일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PLEN-1**
발표분야: 기조강연
발표종류: 특별강연, 발표일시: 목 16:30, 좌장: 장석복

Chiral Diene Ligands for Asymmetric Catalysis

Tamio Hayashi

*Institute of Materials Research and Engineering, A*STAR, Department of Chemistry, National University of Singapore*

As conceptually new chiral ligands, we reported the synthesis of enantiomerically pure chiral dienes, whose basic diene skeleton is bicyclo[2.2.1]hepta-2,5-diene (nbd*) or bicyclo[2.2.2]octa-2,5-diene (bod*). They have two alkyl or aryl substituents on the double bonds, one on each of the two double bonds. The chiral diene ligands were found to be better than the conventional chiral ligands represented by chiral bisphosphines in terms of both catalytic activity and enantioselectivity in some of the catalytic asymmetric reactions. Their high performance was observed in rhodium-catalyzed asymmetric addition of organoboron reagents to α,β-unsaturated ketones, *N*-sulfonylimines, and many other related reactions [1]. In this symposium, I will present some of recent advances on the asymmetric carbon-carbon bond forming reactions catalyzed by chiral diene/rhodium complexes [2].

[1] A review: Shintani, R.; Hayashi, T. Aldrichimica Acta 2009, 42, 31.

[2] (a) T. Nishimura, A. Noishiki, G. C. Tsui, T. Hayashi, J. Am. Chem. Soc. 2012, 134, 5056. (b) T. Nishimura, Y. Takiguchi, T. Hayashi, J. Am. Chem. Soc. 2012, 134, 9086. (c) T. Nishimura, A. Noishiki, T. Hayashi, Angew. Chem. Int. Ed. 2013, 52, 1777. (d) Lim, K. M.-H.; Hayashi, T. J. Am. Chem. Soc. 2015, 137, in press, and references cited therein.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 이동환

AFM in water: Biomarker quantification and single molecule analysis

김영규 이윤희[1] 박준원[1,*]

포항공과대학교(POSTECH) 시스템생명공학부 [1]포항공과대학교(POSTECH) 화학과

본 세미나에서는 수용액에서 원자힘현미경 (Atomic Force Microscope)를 이용하여 분자간 상호작용을 측정하는 방법에 대하여 소개를 하겠습니다. 특히나 나노고깔 모양의 덴드론 분자를 AFM 탐침과 기질에 코팅하여 분석의 정밀도와 재현성을 높일 수 있었는데, 이러한 고유의 접근법을 기반으로 단일 DNA 가닥의 sequence 를 확인하는 방법(J. Am. Chem. Soc., 13754, 2014)과 chaperone 단백질인 AKR2A 가 ribosome 의 RPL23A receptor 와 OEP7 peptide 와 동시에 결합한다는 기작을 밝힌 최근 결과를 발표하고, 아울러 같은 접근법과 기기를 이용하면 DNA, mRNA, microRNA, 그리고 단백질 biomarker 를 아주 낮은 copy 까지 증폭이나 modification 없이 정량 할 수 있다는 진척도 포함하겠습니다.

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장소: 일산 KINTEX
발표코드: **POLY1-1**
발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김동하

Semiconducting Polymers and Small Molecules for Transistors and Solar Cells

Iain McCulloch

Centre for Plastic Electronics and Department of Chemistry, Imperial College, London, UK

The power conversion efficiency (PCE) of single junction organic solar cells has increased significantly during the last decade to 9-10%, now approaching the threshold considered necessary to commercialize the technology. During this period, the structural diversity of semiconducting donor polymers for solar cells has increased dramatically, enabling accelerated development of bulk heterojunction (BHJ) organic solar cells based on polymer donor materials and molecular fullerene derivatives. One aspect of this presentation is to illustrate one molecular design strategy used to optimise a new class of donor polymer. However, the development of electron accepting materials that lead to BHJs with high PCE has been significantly slower. The most commonly used n-type acceptors to date remain [6,6]-phenyl-C61-butyric acid methyl ester (PC61BM) and its slightly larger counterpart PC71BM. These fullerene acceptors have significant limitations including weak absorption and poor tunability of absorption over the range of intense regions of the solar spectrum; morphological instability in thin film blends over time; high synthetic costs and limited scope for synthetic control over electronic and structural properties. For these reasons, we have developed new, synthetically simple electron acceptor materials, based on rhodanine end groups, which have high lying LUMO energy levels and much larger absorption coefficients that fullerenes. In BHJ devices with P3HT donor polymer, the rhodanine molecules were demonstrated to outperform the fullerenes. Our synthetic strategy was to make “dumbbell” shaped dimeric fullerenes where the fullerenes are linked via an alkyl bridge between the ester functional group on PCBM. This was shown to inhibit large scale crystallisation.

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발표코드: **POLY1-2**
발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김동하

Versatile and scalable approaches to chemical processing of nanocarbons

Milo Shaffer

Department of Chemistry, Imperial College, London, UK

Chemical functionalisation is critical to a wide range of nanotube applications, but needs to be versatile and applicable at scale. Existing approaches tend to rely on liquid phase reactions, often requiring damaging sonication or lengthy work up through filtration or centrifugation. The formation of individualized functionalised single wall nanotubes (SWNTs) is a particular challenge. One approach is to shift the modification reaction into the gas phase. We have developed a generic, scalable furnace treatment, based on the thermochemical activation of the CNTs, followed by reaction with functional organic monomers[1]. This approach allows the introduction of a wide variety of functional groups onto the CNT surface whilst maintaining the excellent properties of the untreated materials. The underlying mechanism of the reaction has been established and the distribution of the functionalised sites studied using tagging experiments. The reaction is extremely versatile and can be carried out with a variety of monomers. The reaction and the subsequent product purification can be carried out entirely in the gas-phase, greatly simplifying work-up and improving scalability; the approach is fundamentally compatible with the scale and equipment of many industrial nanotube synthesis processes, and is applicable to multi-walled nanotubes, SWNTs, and other carbon-based materials[6]. The surface properties of these products have been studied by direct wetting experiments on the nanoscale, dispersion studies, and inverse gas chromatography (IGC)[2]. Water dispersible materials with cationic, anionic, and non-ionic surface functionalities provide simple processing routes to a range of applications, and are particularly well suited to studying biological interactions[5,6].A different approach to nanotube processing, relies on reductive charging. Using a liquid ammonia process[3], pure nanotubides can be redissolved, purified, or optionally functionalised without sonication. A key step is to control the ratio of charge to carbons, as it determines both the yield and the nature of the dissolved material. The G/D ratios observed during the dissolution sequence, as a function of metal:carbon ratio, demonstrate a new purification method for removing carbonaceous impurities from pristine SWNTs. The production of individualised SWNT solutions has been confirmed by neutron scattering. A similar approach can be applied to graphene nanoplatelets[4]. The resulting nanocarbon ions can be readily chemically grafted for a variety of applications, depending on the reagent, charge density, and ionic concentration in the reaction medium[9]. The nature of the reactivity of charged graphenides is unusual, due to the continuum density of states of these otherwise molecularly discrete species[10]. Interestingly, the chemical charging agent can be avoided by a pure electrochemical process that yields both nanotube anions[5] and cations[8], suitable for purification, functionalization, or electrodeposition, as desired.

1. R. Menzel et al, Chem. Sci., 2010, 1, 603-8.
2. R. Menzel et al, Langmuir, 2009, 25(14), 8340; R. Menzel et al, Carbon, 2012, 134(20) 8302
3. S Fogden al, ACS Nano, 2012, 6, 54-62
4. E Milner et al, J Am Chem Soc, 2012,8302
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6. Hu et al, Faraday Disc., 2014, 173, 273
7. Hodge et al, ACS Nano, 2013, 1769-1778
8. Hodge et al, Nature Comm, 2013, 1989
9. Morishita et al, J Mat Chem, 2014, 2, 15022
10. Hodge et al, Faraday Disc., 2014, 172, 311

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY1-3**

발표분야: Current Trends in Carbon and Carbon-composite Polymers

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 신관우

Mechanical and Electrical Properties of Carbon Nanotube Fibers

구본철* **이재관**[1]

한국과학기술연구원(KIST) 복합소재기술연구소 [1]*조선대학교 화학교육과/탄소소재학과*

탄소나노튜브(CNT)섬유는 기계적 강도와 전기전도도가 우수하여 차세대 섬유로 알려져 있다. 하지만 전기전도도는 폴리아크릴로니트릴계(PAN) 탄소섬유보다 우수하지만 아직까지 기계적 강도는 이론적인 값에 미치지 못하고 있다. 본 발표에서는 이러한 문제들을 해결하기 위한 방법으로 CNT 섬유를 도핑하거나 기능화하여 개별 CNT 들간의 결합력을 향상시키는 연구결과를 소개하고자 한다. CNT 섬유를 이온성 액체와 아미노산 등으로 도핑을 할 경우 수소결합을 유도하여 강도가 향상 되는 것으로 나타났으며 또한 플라즈마 등으로 처리할 경우에도 같은 메카니즘으로 기계적 강도가 향상되는 것으로 나타났다. 이러한 비공유 결합 뿐만아니라 화학결합에 의해서도 강도가 향상되는 것으로 나타났으며 최대 비강도의 경우 기존의 탄소섬유보다 높은 것으로 나타났다.

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장소: 일산 KINTEX
발표코드: **POLY1-4**
발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 10:25, 좌장: 신관우

Hybrid Nanomaterials Based on Defective Nanocarbons: Promising Energy and Biomedical Applications

김병수

울산과학기술대학교(UNIST) 화학과

Carbon nanomaterials including fullerenes, carbon nanotubes, and graphenes represent the most important class of materials today; their unique physical and chemical attributes advance their roles across most advanced scientific and technology platforms. Defective nanocarbons such as graphene oxide and carbon nanoparticles can offer various opportunities due to their facile synthetic nature, rich surface functional groups as well as interesting photophysical properties. In particular, as a benign alternative to semiconducting quantum dots, carbogenic nanoparticles (also known as carbon dots, CDs) have recently received considerable attention by virtue of their interesting physical, optical, and chemical properties, such as their photoluminescence, photostability, and electron transfer behavior. In the first part of the presentation, the hybrid of carbon-dot-supported silver nanoparticles are exploited to exhibit the versatile surface plasmon resonance of in polymer optoelectronic devices such as PLED and PSC with a record-high efficiency. Moreover, a novel design is described of highly biocompatible, fluorescent, folic acid-functionalized CDs as carriers for the photosensitizer to achieve simultaneous biological imaging and targeted photodynamic therapy. In addition, our early effort in taking advantages of highly biocompatible and photoluminescent CDs in other theranostic applications will be presented.

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장소: 일산 KINTEX

발표코드: **POLY1-5**

발표분야: Current Trends in Carbon and Carbon-composite Polymers

발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 신관우

Preparation of carbon materials using high energy radiation

최재학

충남대학교 고분자공학과

Carbon materials are widely used for a variety of applications such as energy, environment, electronics, and bioelectronics. They have been prepared by various chemical and physical methods. Among them, high energy radiation-based method is an attractive way to prepare and modify carbon materials due to several advantages, such as an eco-friendly process without any harsh chemical agents, a temperature-independent process, fast and easy controllability, and a low processing cost. In this talk, the preparation and modification of carbon materials by high energy radiation, such as electron beams, ion beams, and γ-rays, will be presented.

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발표코드: **POLY1-6**
발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 구본철

친환경 연계형 저비용 탄소섬유 개발 현황 및 발전 방향

신익기

태광산업(주) 탄소섬유공장

최근 자동차 등 수송기기 중심 산업은 "연비 및 환경규제 강화에 따라 철강소재를 뛰어넘는 친환경적인 경량 소재 부품의 연구·개발"에 국가적으로 생태계를 육성해 가고 있는 추세다.이러한 수송기기의 연비·환경규제 강화에 대응 가능한 경량화 신소재로써 탄소섬유 중심의 연구가 활발하게 펼쳐지고 있다.탄소섬유는 전구체 종류에 따라 대표적으로 "PAN 계, Pitch 계, 레이온계 및 기타" 탄소섬유로 구분되며, 이중 높은 기계적 물성 및 우수한 가격 경쟁력으로 인해 PAN 계 탄소섬유가 현재 시장의 90% 이상을 선점하고 있다.탄소섬유의 산업용 시장 확대 및 활성화를 위해서는 높은 제조비용 절감이 중요 Point 로 부각되며, 이러한 높은 제조비용은 전구체 제조비용 및 고에너지 의존도의 문제로 사실상 제조비용 절감에는 한계가 있다.본 강연에서는 기존 고성능 탄소섬유의 물성보다는 상대적으로 낮아지지만 산업용도 중심의 시장접근이 용의한 저비용 탄소섬유에 대한 국내/외 개발 현황 및 발전방향에 대해 소개 하고자 한다.

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장소: 일산 KINTEX
발표코드: **POLY1-7**
발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 구본철

Diverse Carbon-based Nanohybrid Materials for Energy Devices, Photocatalysis, and Sensing

김동하

이화여자대학교 화학나노과학과

Nanostructured carbons have already been recognized as critical element in recent nanotechnological applications with the development of graphene, along with conventional carbon nanotubes or graphites. Coupling carbon moieties with semiconductors play a central role in enhancing the performance of energy conversion and stroge devices, photocatalysis for solar fuel generation and environmental remediation, and electrocatalytic activities. Integrating carbons with noble metal nanostructures have also shown premise for advanced catalytic and sensing properties. A massive amount of efforts have been devoted to the understanding of the interface properties and developing tailored hybrid nanoarchitectures. In this presentation, fabrication of diverse types of hybrid carbon nanostructures utilizing self-assembly, direct carbonization, hybridization of graphene, etc. will be introduced first and their detailed structural assessment is discussed. Application of the resultant nanostructures in electrodes of energy conversion and storage devices, visible light active photocatalysts for solar fuel and degradation of organic pollutants, and surface-plasmon-based enhanced optical biosensing will be the main subject of discussion.Block-copolymer-templated diverse hybrid graphitic carbons have shown promising properties as electrodes in solar cell, fuel cell and metal-air battery. Similar types of carbon nanostructures exhibited viable activity in visible light photocatalysis for water splitting and degradation of toxic chemicals. Finally, charged-, doped-, or neat-graphene oxides and their reduced analogues were assembled in surface plasmon sensing devices and enhanced sensing was demonstrated based on well-defined multilayer thin film geometries.

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발표분야: Current Trends in Carbon and Carbon-composite Polymers
발표종류: 심포지엄, 발표일시: 목 12:05, 좌장: 구본철

PAN 및 pitch기반 탄소섬유의 물성측정

이성호

한국과학기술연구원 탄소융합소재연구센터

최근 탄소섬유는 복합소재의 강화소재로 각광받고 있는데, 이는 탄소섬유의 뛰어난 기계적 물성에 기인한다. 현재 생산되고 있는 탄소섬유는 polyacrylonitrile 과 pitch 를 전구체로 사용하고 있다. 먼저 섬유를 만드는 방사공정, 그리고 크게 두 단계의 열처리 공정(안정화 및 탄화)을 거쳐 탄소섬유가 제조된다. 전구체의 종류에 따라 습식과 용융방사 공정이 필요하고 열처리 공정도 이에 따라 다른 조건이 적용된다. 각 공정의 최적화를 위하여 다양한 물리적, 화학적 물성 측정이 요구된다. 방사를 위하여 습식 및 용융방사에 필요한 전구체의 농도 및 온도에 따른 유변학적 특성이 관찰되어야 하며 전구체 섬유가 만들어진 후 섬유의 배향성, crystallinity 및 기계적 강도 측정이 이루어지게 된다. 또한 안정화 공정에서는 화학적 반응에 따른 functional group 의 변화 및 morphological 변화가 측정이 된다. 탄화공정 후에는 탄소섬유의 구조분석 및 물성을 측정하고 최종적으로 공정-물성-구조의 관계를 분석하여 탄소섬유 제조에 대한 전체적인 이해를 돕게 된다. 본 발표에서는 공정에 따른 물성 측정 방법과 실제 예를 제시하고 탄소섬유의 기초연구에 대하여 논하고자 한다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY2-1**
발표분야: Current Trends in Responsive Polymers
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 유자형

Enhanced Plasmonic Sensing and Catalysis of Hybrid Metal Nanostructures Mediated by Responsive Polymers

김동하

이화여자대학교 화학나노과학과

Stimuli-responsive polymers have been exploited in diverse nanotechnological applications. We introduce our recent efforts to utilize pH- or temperature-sensitive polymers to enhance the function of photocatalysis, electrocatalysis, and optical sensing. Smart bimetallic core@shell nanoparticles were fabricated based on gold nanoparticles (AuNPs) decorated with pH-sensitive polymer shell. The bimetallic nanostructures of AuNP@P4VP nanocomposites containing another type of metal NP at the P4VP periphery exhibit a controlled sensing property in terms of the change in the refractive index of surrounding media and a typical electrocatalytic activity for methanol oxidation reaction. A plasmonic coupling sensing device was also designed, comprising gold nanoparticles (AuNPs) separated from Au substrate through a stimuli-sensitive polymer linker layer. Plasmonic nanostructures coupled with thermo-responsive poly(N-isopropylacrylamide) (PNIPAM) polymers were used to investigate the unique plasmonic-coupling-based SPR sensing properties associated with swelling-shrinking transitions in the polymer linker brush. Noble metal nanostructure coupled with responsive polymer were used to probe unique plasmonic mediated photocatalytic properties associated with swelling-shrinking transitions in polymer chains triggered by specific external stimuli.

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발표코드: **POLY2-2**
발표분야: Current Trends in Responsive Polymers
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 유자형

Volume phase transition of light responsive hydrogels and their application

윤진환

동아대학교 화학과

Hydrogels are three-dimensional network structures of hydrophilic polymers by physical and chemical cross-linking and can be expanded their volumes by absorption water. Some of them change its equilibrium swelling state in responds to external stimuli, such as pH, light, temperature, and electric field. We have found that composite hydrogels consisting of photo-thermal conversion materials embedded within a thermally responsive polymer matrix provide an efficient means to trigger changes in volumetric swelling by visible light irradiation. We maximized degree of volume change triggered by light by adjusting the lower critical solution temperature (LCST) of the hydrogels, providing highly responsive hydrogels that show rapid and significant light-induced volume change. Base on light-responsibility of hydrogels, we have successfully fabricated light-controlled actuators, microfluidic valve, and smart window for energy saving. For more potential applications, light-responsive hydrogels were prepared with controlled size and shape by using microfluidic device and alginate templating method.

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장소: 일산 KINTEX

발표코드: **POLY2-3**

발표분야: Current Trends in Responsive Polymers

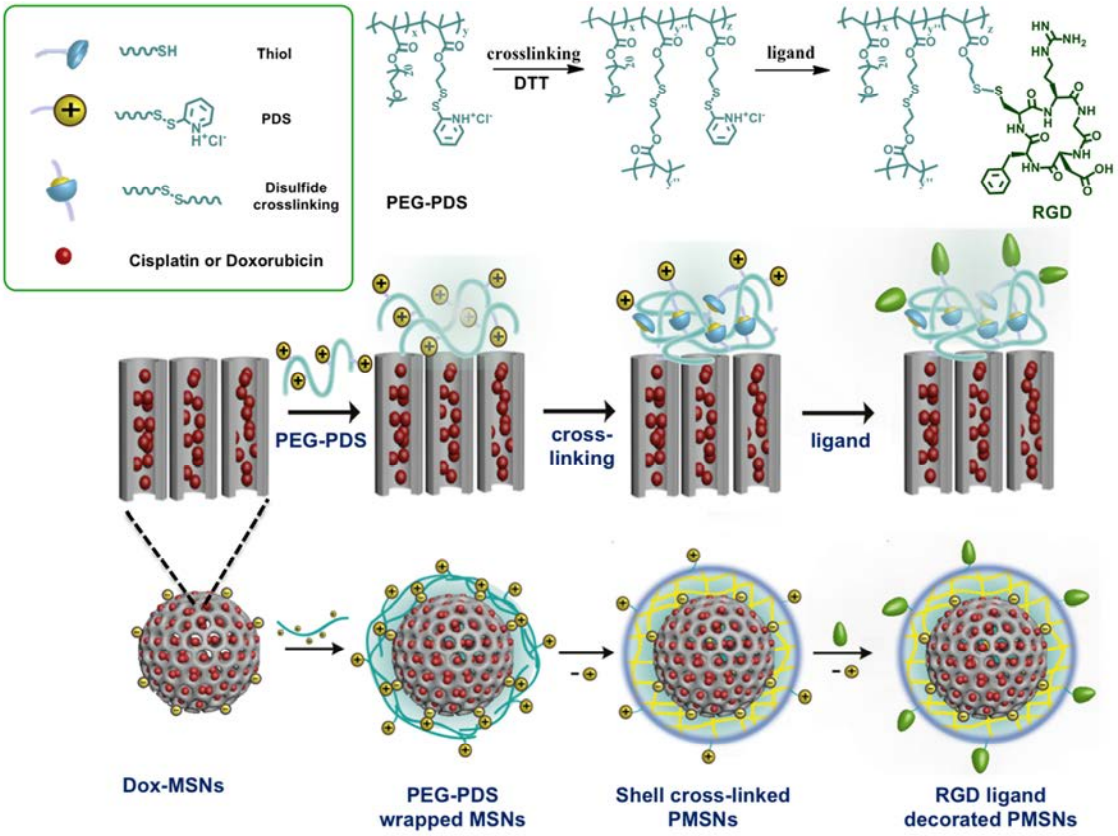
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 윤진환

Noncovalent Polymer-Gatekeeper in Mesoporous Silica Nanoparticles as a Targeted Drug Delivery Platform

유자형

울산과학기술대학교(UNIST) 자연과학부 화학과

Nanoscopic delivery vehicles capable of encapsulating drug molecules and releasing them in response to external stimuli are of great interest due to implications in therapeutic applications. Micellar assemblies are promising scaffolds to overcome many of the problems faced with traditional chemotherapies because of their capacity for non-covalent, hydrophobic guest molecule binding. However, the stability of encapsulation with such self-assembled systems is limited during blood circulation because of a requisite concentration for assembly formation and low encapsulation stability. Thus, deliberate molecular design for stable encapsulation, targeting and triggered release is required. For this purpose, we have developed a facile synthetic method for highly stable, polymer-caged hollow nanoparticles using a simple intra/inter-chain crosslinking reaction. We show a simple method for the preparation of biocompatible nanovehicles that provides the ability to encapsulate hydrophobic or hydrophilic drug molecules. We can control the size of the nano-carriers and release kinetics depending on crosslinking in responsive to stimuli. Nano-carriers showed great stability to encapsulate drug molecules and drugs were only released inside cell. In addition, we can use surface modified nano-carriers for target delivery system. Hence, the stimuli responsive nano-carrier formation using self-crosslinking polymers and the corresponding method of surface modification are a promising platform for creating polymer nanogels for a range of biomedical applications, from drug delivery to biosensing.


SH
Thiol
PDS
Disulfide crosslinking
Cisplatin or Doxorubicin
PEG-PDS
crosslinking
DTT
ligand
RGD
PEG-PDS
cross-linking
ligand
Dox-MSNs
PEG-PDS wrapped MSNs
Shell cross-linked PMSNs
RGD ligand decorated PMSNs

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY2-4**
발표분야: Current Trends in Responsive Polymers
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 윤진환

블록공중합체/이온성 액체 전해질의 Lower Critical Solution Temperature (LCST) 및 이온전달 특성 연구

조병기

단국대학교 화학과

이온성 액체는 비휘발성, 비발화성, 전기화학적 안정성, 높은 전도도 특성으로 인하여, 차세대 전지 전해질 재료로의 응용이 기대되는 물질이다. 한편, 최근 이온성 액체와 블록공중합체의 브렌딩을 통해, 나노 구조화된 전해질제조에 대한 몇몇의 연구들이 보고되고 있다. 이온성 액체와의 혼합을 가능하게 하기 위해, 많은 블록 공중합체들은 poly(ethylene oxide) (PEO)고분자 블록을 사용한다. 그럼에도 불구하고, 블록공중합체 내의 PEO 와 이온성 액체와의 상호작용에 대한 연구가 아직까지도 체계적으로 이루어지지 않은 실정이다. 본 발표에서는 최근 수행된 이온성 액체/블록공중합체 혼합물에서 나타나는 자기조립 나노구조, 온도 증가에 따라 turbidity 가 달라지는 LCST 현상, 이온 전도도 결과에 대해 소개하고자 한다. 특히, 이온성 액체의 분자구조에 따라, 위 특성이 매우 달라지는 현상을 관찰하였으며, 연구 데이타를 기초로 하여, 분자구조-물질특성, 나노구조-물질특성 사이의 상관관계를 정의하고자 한다.

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발표분야: Current Trends in Responsive Polymers
발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 윤진환

Cross-linkable and Degradable Layer-by-Layer Assembly under Cytocompatible Conditions for Cell-Encapsulation

양성호[*] **최인성**[1] **유자형**[2]

한국교원대학교 화학교육과 [1]한국과학기술원(KAIST) 화학과 [2]울산과학기술대학교(UNIST) 나노생명화학공학부

Layer-by-layer (LbL) assembly has recently emerged as a highly versatile and promising method for biochemical and biomedical applications. Accordingly, it is urgently necessary to develop a cytocompatible LbL assembly technique that is stable and offers on-demand degradation and functionalization. In this study, we developed a simple and biocompatible LbL technique that cross-links the layers through covalent bonds under physiological conditions without requirement of any post-treatments or additives. By utilizing the dynamic nature of the disulfide bond, stable LbL films can be spontaneously formed during the process, further functionalized using thiol-maleimide chemistry, and degraded in response to glutathione. In addition, we demonstrated that the method is applicable to plate surfaces, spherical nanoparticles, and even living cells.

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발표코드: **INOR1-1**
발표분야: New Visions in Organometallics and Nanochemistry
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 송현준

Palladium(II) Coordination Cages

정옥상

부산대학교 화학과

Diverse poly-pyridyl *N*-donor ligands that can coordinate two or more remote metal centers were used to construct desirable molecular structures. Unique cage complexes $[(Me_4en)_3Pd_3(L_1)_2](X)_6$ (L_1 = 1,3,5-tris(isonicotinoyloxyethyl)cyanurate; $X^-= BF_4^-$ and ClO_4^-) were constructed. A single water molecule in a skeletal cage was reversibly associated and dissociated via a combination of the adequate space, polar environment, and conformational flexibility of the cage. In Suzuki-Miyaura C-C cross-coupling reactions, the cage complex showed significant catalytic activity along with the effects of the isolated single water molecule. On the other hand, we reported the synthesis and operation of a nano-dimension 24 × 24 × 15 $Å^3$ "ball-joint-type host-guest system" consisting of unprecedented conglomerate of two distinct helical metallacyclophanes, chiral isomer (P)-$[Pd_3X_6(L_2)_2]$@(M)-$[Pd_3X_6(L_2)(L_3)]$ and its enantiomer (M)-$[Pd_3X_6(L_2)_2]$@(P)-$[Pd_3X_6(L_2)(L_3)]$, via the reaction of racemic helical metallacyclophanes, (P,M)-$[Pd_3X_6(L_2)_2]$ with tridentate L_3, or direct reaction of 10 small components (six palladium(II), three L_2, and one L_3, L_2 = *N,N',N"*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide; L_3 = *N,N',N"*-tris(3-pyridinylpropyl)-1,3,5-benzenetricarboxylate; X^- = Cl^- and Br^-). The host-guest aggregation can be ascribed to one π…π interaction and three -NH…O=C- hydrogen-bonds along with the combined helicity. The host-guest system shows a reversible equilibrium between the aggregate and its dissociated species in solution. Such equilibrium control of the host-guest system is reminiscent of "left and right ball-and-socket joint" behavior.

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발표코드: **INOR1-2**
발표분야: New Visions in Organometallics and Nanochemistry
발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 송현준

Nanostructured Bulk Thermoelectric Materials for Energy Harvesting Applications

김성진

이화여자대학교 화학과

Upon confronting present energetic and environmental challenges, the global need for utilizing exhausted waste heat has been accelerated. In effect, thermoelectric materials are gathering a great interest as a potential alternative energy source because of their capability of direct energy conversion between heat and electricity. The increase of thermoelectric efficiencies is one of the main challenges of our scientific community. The performance of a thermoelectric material is assessed with the figure of merit ZT defined as (S2????/k)T; where S is the Seebeck coefficient (or thermopower), ???? electrical conductivity, κ thermal conductivity, and T is the temperature. Recent theoretical and experimental studies show that the use of thermoelectric materials comprising nanostructured components increases ZT relative to that of the bulk counterparts of these materials. Minimizing thermal conductivity while maintaining the electrical conductivity is the key point in formation of nanoscaled or nanocomposite thermoelectric. Controlling the size and content of the nanoscale constituents within the bulk materials is especially important to achieve high ZT. Thus, new routes for the preparation of these components as nanoscale powders are essential for incorporating them as nanoscale constituents of the bulk materials. In this presentation, an overview of recent advances in the development of high performance nanoscaled thermoelectric materials.

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발표코드: **INOR1-3**
발표분야: New Visions in Organometallics and Nanochemistry
발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 송현준

Electrical Activation of Mg-doped GaN Epitaxial Layer by Electrochemical Method

이준기

전남대학교 신소재공학부

GaN 박막을 이용하여 빛을 생성하는 Optoelectric 소자를 제조하기 위하여는 우수한 특성의 n-type GaN 와 p-type GaN 에폐층 필요로 한다. 현재의 제조기술로는 n-GaN 의 성장은 문제가 없지만, p-GaN 의 특성은 n-GaN 의 ~10% 정도밖에 미치지 못하고 있다. 현재의 p-GaN 제조방법은 열처리기법에 의한 것인데, 이 방법은 GaN 를 이용한 기술의 확장에 한계를 보여주고 있으며, 새로운 p-GaN 활성화 방법의 도입이 필요한 시점이다.본 연구는 전기화학적 기법을 이용하여 p-GaN 활성화를 하는 방법을 제안하고 있다. p-GaN 활성화의 걸림돌은 Mg-H complex 로 알려져 있는데, 수소원자가 dangling bond 에 달라붙어서 hole 의 생성을 방해하고 있기 때문으로 알려져 있다. 이러한 수소를 열처리기법을 이용하여 확산공정을 이용하여 제거하는 것에는 한계가 있는 것으로 밝혀져 왔는데, 본 연구는 전기장을 이용하여서는 Mg-H 의 수소원자 제거를 하는 것을 목적으로 하여 실험을 진행하였다. 이러한 전기화학적 공정의 주요변수라고 생각할 수가 있는 용액의 선정, 전압의 세기, 전압을 걸어주는 시간 등을 최적화 하였으며, 각 조건에서의 수소원자가 제거되는 정도를 SIMS 분석을 이용하여 정량분석을 하였다. 여러 분석결과 수소원자를 기존의 열처리 방법에 비하여 거의 1 order 정도 줄일 수가 있다는 것을 확인하였고, hole 농도 또한 확연히 개선되는 것을 확인하였다. 제안된 전기화학적 기법을 활용하여 소자면에서 특성 개선을 확인하였다. 청색 LED 와 Near-UV LED 를 이용하였고, LED 의 광출력 특성이 ~30% 이상 개선되는 특성을 구현하였다. 수소원자의 농도가 줄어들음으로써 Leakage 특성의 mechanism 이 변하는 것을 볼 수가 있었고, LED 소자의 신뢰성이 매우 향상되는 것을 확인할 수가 있었다. 본 연구는 산업적 응용가능성이 높은 것으로 기대되는 기술의 제안으로, 여러 소자에서의 확인과 추가연구가 필요한 분야이다.

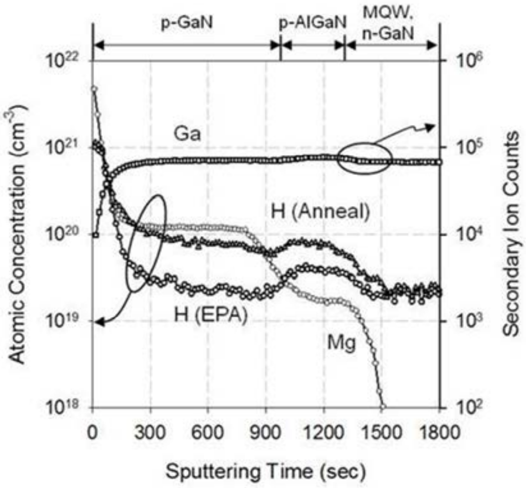

그림 1. SIMS 분석

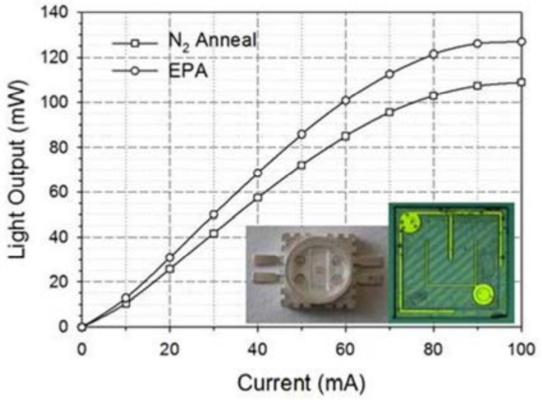

그림2. L-I 특성곡선

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR1-4**

발표분야: New Visions in Organometallics and Nanochemistry

발표종류: 심포지엄, 발표일시: 목 10:15, 좌장: 송현준

Facet-controlled alloy nanoparticles: Design, Synthesis, and Application

이광렬

고려대학교 화학과

Alloying and dealloying behaviors in the nanoscale particles are greatly different from those of bulk materials, because the surface energy of nanoparticles is significant in determining the overall particle energy. We have been particularly interested in the alloy formation in the facet nanoparticles; facet-controlled nanoparticles can now generate geometrically precise energy gradients within the entire nanoparticle and therefore geometrically-predetermined phase segregation is now feasible. Herein I present our recent efforts in the nanoscale alloy formation and nanoparticle-specific reactivities with the ultimate goal of development of atom efficient and highly active nanocatalysts for energy applications.

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발표분야: New Visions in Organometallics and Nanochemistry
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 서원석

Improved Photoelectrochemical Water Splitting Efficiency by the Formation of Metal Oxide Composite

남기민

목포대학교 화학과

Artificial photosynthetic systems are promising approaches to convert sunlight into chemical fuels.The most popular strategy is photoelectrochemical (PEC) water splitting to produce hydrogen sustainably. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary semiconductor that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through the composite. These composite structures are divided into four different configurations depending on the possible electron-hole separation mechanism. These systems elucidate the effect of conduction and valence band positions of the individual components of composite materials.

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발표코드: **INOR1-7**

발표분야: New Visions in Organometallics and Nanochemistry

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 서원석

답사 - 무기화학을 가슴에 간직하고

박준택

(전)한국과학기술원(KAIST) 화학과

답사

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR2-1**
발표분야: Recent Advances in Organometallic Chemistry
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이윤호

N-Heterocyclic Carbenes Mimicking Transition Metal Complexes

이은성

포항공과대학교(POSTECH) 화학과

N-heterocyclic carbenes (NHCs) are well-known to stabilize main group radicals and radical ions. Pioneered by the Bertrand and other groups, phosphoryl, silyl, boryl and other organic radicals stabilized by NHCs have been isolated and characterized. A successful preparation of the radical compounds was explained by NHCs' pi-acceptor character, which imparts remarkable stability because the significant portion of the spin density of the radicals resides on the carbene carbon. We found that NHCs could stabilize nitric oxide (NO) radical in a solution phase to form stable NHC NO radicals. Although nitrous oxide was dominantly formed during the thermolysis of NHC nitric oxide compounds, nitric oxide was also found to be thermally transferred to other N-heterocyclic carbenes. This suggests potential biological applications for NO delivery. Furthermore, this study adds another example of stable singlet carbenes acting as mimics for transition metal centers. Further studies on carbenes' reactivity with other small molecules will deepen our understanding of this interesting resemblance. Full characterization of the compounds including X-ray crystallography, EPR, UV-vis, and cyclic voltammetry will be presented in addition to the mechanistic studies and NO transfer experiments.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR2-2**

발표분야: Recent Advances in Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이윤호

Cycloaddition of Carbon Dioxide to Epoxides Using Catalysts

김영조

충북대학교 화학과

Cyclic carbonates could be easily synthesized via the cycloaddition of CO_2 to epoxides, and they could be widely used as polar aprotic solvents, electrolytes for lithium ion batteries, and precursors for polycarbonates, enantiopure aminoalcohols, thermosetting coatings, and pharmaceutical intermediate. For the synthesis of cyclic carbonates, many examples of homogeneous catalytic systems were reported in the literature. The new advances of catalysts such as metal-based and metal-free compounds for cycloaddition reaction will be presented. Acknowledgment: This work was financially supported by the Korean Ministry of Education (MOE) and the National Research Foundation of Korea (NRF) through the Creative Human Resource Training Project for Regional Innovation (grant number 2014H1C1A1066874).

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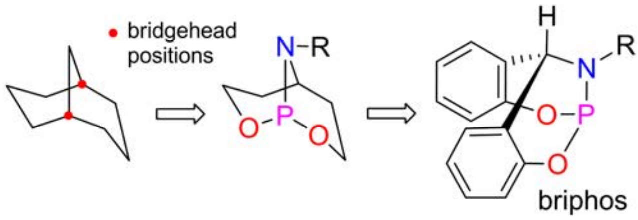
장소: 일산 KINTEX
발표코드: **INOR2-3**
발표분야: Recent Advances in Organometallic Chemistry
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 홍순혁

Briphos: A New Class of π-Acceptor Ligand Induced by Geometrical Constraints

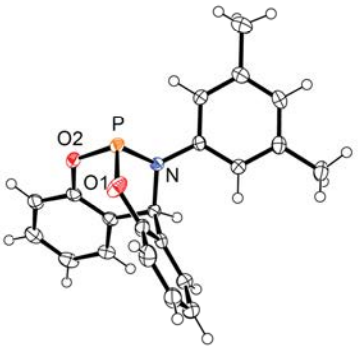
김현우

한국과학기술원(KAIST) 화학과

There has been continuing interest in transition metal catalysis: it is hoped that these reactions will help in the development of unprecedented chemical reactions as well as to providing green chemical processes in the pharmaceutical and find-chemical industries. Indeed, the catalytic performance of the studied transition metals highly depends on the character of the ligands that bind to the central metal atoms. Thus the investigation of ligand effects has been one of the major research topics in the field of transition metal catalysis.We here report a new class of bicyclic bridgehead phosphoramidite (briphos) ligand based on the bicyclo[3,3,1]nonane structure. We show that the geometrical constraints in briphos with respect to its linear analogs enhance π-acceptor ability. Furthermore, facile tuning of briphos leads to highly efficient ligands showing dramatic ligand acceleration effect (LAE), new catalytic reactivity in Rh(I)-catalyzed conjugate additions of aryl boronic acids.The design of briphos ligand is based on our observation that internal hydrogen bonds significantly promote the imine formation of benzophenone and the imine products have been used for stereoselective generation of axial compounds and chiral-at-metal complexes.Reference1. Lee, A.; Ahn, S.; Kang, K.; Seo, M.-S.; Kim, Y.; Kim, W. Y.; Kim, H. Org. Lett. 2014, 16, 54902. Seo, M.-S., Lee, A., Kim, H. Org. Lett. 2014, 16, 2950 3. Seo, M.-S., Kim, K., Kim, H. Chem. Comm. 2013, 49, 11623



bridgehead positions
N-R
O
P
O
H
N-R
O-P
O
briphos



O2
P
O1
N

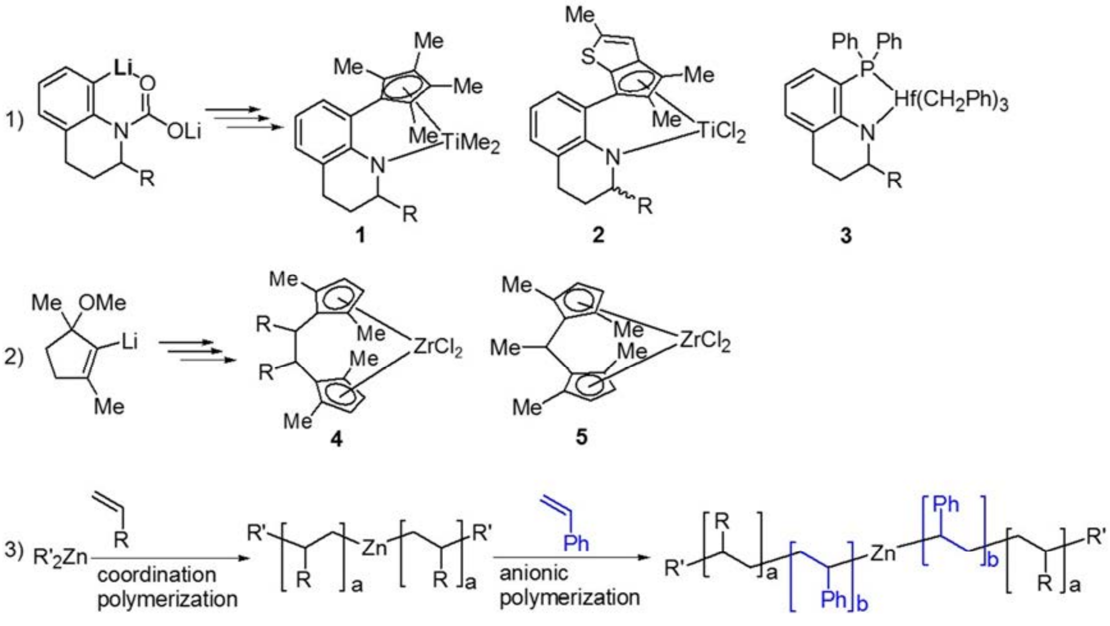
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR2-4**
발표분야: Recent Advances in Organometallic Chemistry
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 홍순혁

Organometallic compounds of transition metals and/or main group metals for precise polymerization of olefin and/or styrene

이분열* 전종엽

아주대학교 분자과학기술학과

Organolithium compounds were efficiently utilized in the construction of various transition metal complexes for olefin polymerizations in our laboratory. Complexes 1-3 exhibited high activity, high 1-octene incorporation, and high molecular weight in ethylene/1-octene copolymerizations. Complexes 4 and 5 showed excellent catalytic performances in 1-decene oligomerizations for lubricant basestock and in ethylene/norbornene copolymerizations, respectively. Recently, we expanded utilization of the main group organometallic compounds, alkyllithium and dialkylzinc, to the area of "catalyzed chain growth" to construct polyolefin-block-polystyrene.



일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS1-1**

발표분야: Biophysical Chemistry: Biological Phenomena Viewed by Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김준수

Computer Simulation Techniques in Biophysical Problems

장락우

광운대학교 화학과

With ever-increasing computational power and developments in user-friendly simulation software, computer simulations have now become indispensible tools in studying biophysical problems including enzyme catalysis, membrane structure and dynamics, and even cell functions. However, since biological systems are still too complex to be studied by first-principle computational techniques, various levels of approximations and techniques are employed depending on the systems of interest. In this talk, I will briefly overview currently available particle-based computer simulation techniques by introducing several biophysical problems I have been investigating in recent years.

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발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김준수

Implications of DNA sequence composition in the chromosome structure and epigenetics

김하진

울산과학기술대학교(UNIST) 생명과학부

The chromosome spends most of its lifetime in the interphase in which it is only loosely condensed and hence viewed as a dynamic polymer. Its structure and dynamics globally affect the gene expression but it is only recent that its average structure was presented through the Hi-C technique by showing the intra- and inter-chromosomal contact map of the whole DNA. We recently discovered that the Hi-C contact map highly and universally correlates with the local AT content. From all-atom molecular dynamics simulations, we hypothesized that the polycation-driven condensation of the DNA explains such global behavior. We proved the hypothesis by designing a simple in vitro system for the single molecule measurement of dsDNA-to-dsDNA interaction.

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Upconverting nanoparticles: a versatile platform for wide-field two-photon microscopy

이강택

광주과학기술원(GIST) 물리화학부 화학과

Lanthanide ion-doped upconversion nanoparticles (UCNPs), which emit in the visible range upon absorption of NIR photons, have attracted great attention in the area of biological imaging owing to their advantageous properties. First, two-photon upconversion of NIR excitation to the emission of a visible photon is so efficient that a tiny CW laser with the output of tens of milliwatts is sufficient as the excitation source even for single-particle detection. Therefore, “inexpensive” “wide-field” two-photon imaging can easily be achieved with UCNPs, which is not possible with organic fluorophores and femtosecond laser systems used in conventional two-photon microscopy. Second, by employing NIR excitation, one can suppress cellular autofluorescence, hardly induce photo-damage to cells, and achieve relatively deep penetration into tissues. In addition, UCNPs are extremely photo-stable without any photoblinking and photobleaching, and finally, their cytotoxicity turns out to be very low. All these aspects strongly suggests that the UCNP-based imaging should provide an excellent platform for “non-scanning” wide-field two-photon microscopy, which is capable of high-speed, high-contrast, biocompatible, uninterrupted, and long-term imaging. Such advanced concepts in microscopy were fully demonstrated in our study on the real-time tracking of single UCNPs in live cells. Furthermore, we employed this technique to investigate the mechanism of gene delivery, addressing the issues such as DNA release, cell division.

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발표분야: Biophysical Chemistry: Biological Phenomena Viewed by Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 김학준

Energetics and Dynamics of Transport of Ions and Biomolecules through Cyclic Peptide Nanotubes

황현석

강원대학교 화학과

Cyclic peptide nanotubes (CPNs) are synthetic proteins which transport ions and biomolecules through lipid bilayer membranes. We used molecular dynamics (MD) simulations to calculate potential of mean force (PMF), position-dependent diffusion coefficients, and force autocorrelation functions (FACs) for ions and glucose through CPNs embedded in a DMPC lipid bilayer membrane.

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Probing protein interactions and dynamics in a single living cell

이남기

포항공과대학교(POSTECH) 시스템생명공학부/물리학

Dynamic interactions between membrane proteins and ligands determine correct cellular responses to diverse environmental changes. Because various protein complexes on a plasma membrane participate in cellular functions, technique identifying complex interactions of membrane proteins with spatio-temporal resolution in a single living cell is highly demanding. Here I present an imaging technique of membrane protein interactions that utilizes the accurate measurement of diffusion coefficient of membrane proteins by tracking individual proteins in a single living cell. We validated this approach that can measure the interactions between ligands and membrane proteins using an epidermal growth factor receptor and show its applicability in measuring dissociation constant of ligands and mutant specific interactions in a single living cell. We extended our technique to G protein-coupled receptors, which confirms the dissociation of Gi-protein at the downstream of ligand interactions. Our results demonstrate that our approach would be a powerful technique for investigating the various interactions of membrane proteins and the processes of signal transduction in a single living cell.

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NMR dynamics study of Z-DNA binding proteins and miRNAs

이준화

경상대학교 화학과

Left-handed Z-DNA is a higher energy conformation than B-DNA and is induced by high salt, negative supercoiling, and complex formation with Z-DNA binding protein (ZBPs). ZBPs have been identified in RNA editing enzyme (ADAR1), DNA-dependent activator of interferon regulatory factor (DAI), viral E3L protein and protein kinase containing Z-DNA binding domains (PKZ). In this study, we determined the solution structure of the free from of $caZ\alpha_{PKZ}$ by multidimensional heteronuclear NMR spectroscopy. We also performed NMR experiments on complexes of $caZ\alpha_{PKZ}$ with DNA duplexes, dT(CG)3 and d(CG)3 under various NaCl concentrations. We investigated changes in the conformation and dynamics of $caZ\alpha_{PKZ}$ induced by increment of NaCl concentration. Comparison of these results to that of $Z\alpha_{ADAR1}$ provides the molecular basis for B?Z transition mechanism of ZBPs, which is modulated by conformational dynamics of a key tyrosine residue in the α3 helix.In plants, the DCL1 enzyme processed primary miR156a into miR156a/miR156a* duplex via a loop-to-base processing mecanism. Some pairing mutants on the B5 bulge (P-B5 mutants) caused earlier flowering than wild-type pri-miR156a. Here, we have investigated the structural and/or dynamics changes of the miR/miR* duplex region induced by P-B5 mutations. This study provides insight into the molecular mechanism on the second cleavage reaction at lower stem structure by DCL1.

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발표분야: Recent Trends in Physical Chemistry

발표종류: 분과기념강연, 발표일시: 목 13:25, 좌장: 장준경

Something happening in a non-adiabatic region: A proton-coupled electron-transfer case

백경구

강릉원주대학교 화학과

A brief description on the backgrounds leading to the interests about non-adiabatic regions of chemical changes will be followed by discussions on detailed dynamics of a proton-coupled electron-transfer (PCET) process as a representative case of the non-adiabatic regions. To capture the 'microscopic yet dynamical view' of the non-adiabatic stage, the time-dependent quantum wave-packet propagation method in conjunction with high-level electron correlation theories, MRCI and IP-EOM-CC methods, was applied to the dynamics of the charge-transfer (CT) excited state of $FHCl$ corresponding to F^+HCl^-. The dynamics of this CT state, generated by the photo-detachment of an electron from the precursor anion $FHCl^-$, corresponds to a bidirectional PCET with two dissociation channels: the electron transfer (ET, generating FH and Cl) and proton transfer (PT, generating F and HCl) paths. Calculated branching ratio of ET/PT disclosed a surprising fact that PT prevail over ET. More importantly, a detailed analysis of the non-adiabatic region suggests that the proton movement starts about 3 femto-seconds earlier than the net adjustment of electron's distribution, and the electron adjustment is triggered by the initial movement of the proton. A few more model systems of X-H-Y will be discussed too, and some comments on recent researches related to this topic will be made as a closing remark.

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Transient Chemical Species : A Study of Reaction Dynamics and Applications

최종호

고려대학교 화학과

Two topics related to transient organic species will be presented.

a) Atom-radical reaction dynamics: Oxidation reaction dynamics of a series of hydrocarbon radicals has been examined as prototypal radical-radical oxidation reactions. High-resolution laser spectroscopy in a crossed-beam configuration was applied to examine the nascent rovibrational state distributions and Doppler profiles of the reactive scattering products. The analyses of the product energy and population distributions demonstrated the existence of unusual dynamic characteristics and competition between the addition and abstraction reaction mechanisms at the molecular level. These features in sharp contrast with those of the oxidation reactions of closed-shell hydrocarbon molecules will be discussed with the aid of the ab initio and quantum statistical calculations.

b) Organic electronic devices Semiconducting π-conjugated organic clusters were utilized to prepare the various organic devices such as OFETs (Organic Field-effect Transistors), OLEFETs (Organic Light-Emitting Field Effect Transistors), inverters, etc. The weakly bound and highly directional neutral cluster beams were quite efficient in producing the high-quality thin films leading to significant improvements in surface morphology, crystallinity and packing density at room temperature. The OFETs and OLEFETs demonstrated good field-effect characteristics, stress-free operational stability, and electroluminescence under ambient conditions. In the cases of organic CMOS inverters ideal performance was realized by integration of unipolar OFETs.

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Femtosecond X-ray liquidography captures the formation of chemical bond in the solution phase

이효철

한국과학기술원(KAIST) 화학과

The pump-probe X-ray diffraction and scattering techniques have now been fully established as a powerful method to investigate molecular structural dynamics [1-5]. We have employed the techniques to study structural dynamics and spatiotemporal kinetics of many molecular systems including diatomic molecules, haloalkanes, organometallic complexes and protein molecules over timescales from ps to milliseconds. X-ray crystallography, the major structural tool to determine 3D structures of proteins, can be extended to time-resolved X-ray crystallography with a laser-excitation and X-ray-probe scheme, but has been limited to a few model systems due to the stringent prerequisites such as highly-ordered and radiation-resistant single crystals. These problems can be overcome by applying time-resolved X-ray diffraction directly to protein solutions rather than protein single crystals. To emphasize that structural information can be obtained from the liquid phase, this time-resolved X-ray solution scattering technique is named time-resolved X-ray liquidography (TRXL) in analogy to time-resolved X-ray crystallography where the structural information of reaction intermediates is obtained from the crystalline phase. We will present our recent results including the achievement of femtosecond TRXL by using an X-ray free electron laser.[1] “Direct observation of bond formation in solution with femtosecond X-ray scattering”, K. H. Kim, J. G. Kim, S. Nozawa, T. Sato, K. Y. Oang, T. W. Kim, H. Ki, J. Jo, S. Park, C. Song, T. Sato, K. Ogawa, T. Togashi, K. Tono, M. Yabashi, T. Ishikawa, J. Kim, R. Ryoo, J. Kim, H. Ihee*, S. Adachi, Nature, 2015, in press.[90] “Volume-conserving trans-cis isomerization pathways in photoactive yellow protein visualized by picosecond X-ray crystallography”, Y. O. Jung, J. H. Lee, J. Kim, M. Schmidt, K. Moffat, V. Srajer, H. Ihee*, Nat. Chem., 2013, 5, 212-220.[3] “Visualizing Solution-Phase Reaction Dynamics with Time-Resolved X-ray Liquidography”, H. Ihee*, Acc. Chem. Res., 2009, 42, 356-366 (Review Article).[4] “Tracking the structural dynamics of proteins in solution using time-resolved wide-angle X-ray scattering", M. Cammarata*, M. Levantino, F. Schotte, P. A. Anfinrud, F. Ewald, J. Choi, A. Cupane, M. Wulff, H. Ihee*, Nature Methods, 2008, 5, 881-887.[22] "Ultrafast X-ray diffraction of transient molecular structures in solution", H. Ihee*, M. Lorenc, T. K. Kim, Q. Y. Kong, M. Cammarata, J. H. Lee, S. Bratos, M. Wulff, Science, 2005, 309, 1223-1227.

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Unprecedented colorimetric responses of polydiacetylene based nanofibers

김명화* 윤주영[1] 이송이[2]

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

Polydiacetylene (PDA) polymers, which were typically prepared by UV irradiation, display unique the blue to red color transition upon environmental stimulation. We report for the first time that polydiacetylenes (PDAs) can be alternatively prepared via plasma induced polymerization process. The degree of polymerization and color transitions could be manipulated by controlling the power of plasma radio frequency, exposure time and by using acrylic mask. In the current study, 10, 12-pentacosadiynoic acid (PCDA) monomers embedded electro-spun fibers, PCDA-HEG embedded fiber bearing hexaethylene glycols (HEG) as head groups and their combinations were explored to study the steric factors of head groups in color transition. We could also demonstrate that patterned colorimetric and fluorometric images could be obtained through a simple acrylic mask with plasma. These results demonstrate not only the first example of PDA polymerization via plasma but also a great potential of plasma process to be used as patterning applications.

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Study on graphene nanoribbon and residual polymer on graphene using Raman spectroscopy

주상용

연세대학교 화학과

라만 분광법은 이차원 나노물질을 연구하는데 있어서 필수적인 요소가 되었다. 본 연구진에서는 라만 분광법을 이용하여 금속성을 가지는 그래핀과는 다르게 반도체성을 갖는 것으로 예상되는 그래핀 나노리본 합성법과 라만 분석법에 대해서 발표하고자 한다. 투과 전자 현미경으로 관찰된 그래핀 나노리본의 다양한 형태에 대해서 논의를 하고 이와 함께 라만에서 관찰된 defect density 와 상관관계에 대해서 연구하였다. 또한 대구경 라만을 이용하여 단일 결정으로 구성된 hexagonal graphene 을 이용하여 잔여 고분자가 그래핀에 끼치는 영향에 대해서 연구하였다. 이상적인 단결정 그래핀을 통해서 기계적으로 박리가 된 그래핀경우와는 다르게 화학기상증착법으로 합성된 그래핀의 경우 고분자가 존재할때 그래핀은 약한 tensile strain 이 존재함을 알 수 있었다. 참고문헌:1. Yoon, W., Lee, Y., Jang, H., Jang, M., Kim, J. S., Lee, H. S., Im, S., Boo, D., Park, J., and Ju, S. -Y., “Graphene Nanoribbons Formed by a Sonochemical Graphene Unzipping using Flavin Mononucleotide as a Template”, Carbon, 81, 629-638 (2014, article).2. Koo, E. -H., and Ju, S. -Y.,“ Role of Residual Polymer on Chemical Vapor Grown Graphene by Raman Spectroscopy”, Carbon, 86, 318-324 (2015, article).

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Electron Transport Characteristics of Molecular & Nano Structures on the Organic Electronic Devices

이상욱

한양대학교 응용화학과

Organic electronic devices based on conjugated small molecules and nano structures have been extensively investigated as promising building blocks for nanoscale optical and electronic devices, such as organic light emitting diode (OLED), organic photovoltaic (OPV) solar cell, thin film field effect transistors (OFET), sensor and molecular electronic devices. However, only the electron transfer can reveal the desired device functions, which strongly depends on the electronic structures of molecular and nano components. Therefore, it is very important to understand how electron flows in a molecular and nano structures and how to manipulate the electron transport behaviors for the development of new functional organic electronic materials. The electron transport behavior can be classified by the phase of organic materials. If the organic electronic devices are composed of bulk solid states, such as crystal and amorphous, the electron transport is governed by inter-molecular hopping mechanism based on the Marcus theory. Whereas, on the single molecule and nanostructure, the electron transport can be explained by the intra-molecular ballistic transfer mechanism based on Non-equilibrium Green’s function (NEGF) theory. Therefore, controlling the bulk and molecular properties, such as morphology, growth direction, and physical and chemical properties, can allow us to design new functional organic electronic devices.In this presentation, I would like to introduce designed molecular and nano structures, and their characteristic electron transport behaviors for on the organic electronic devices.

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Equilibrium Dynamics in Electrolytes of Li-Ion Battery Studied by Ultrafast Pump-probe and Two-Dimensional IR Spectroscopy

곽경원

중앙대학교 화학과

Electrolytes are ubiquitous and indispensable in all electrochemical devices including electrolytic cells, capacitors, fuel cells, or batteries. Moreover, their function is the same in devices for serving as the medium for the ion transport between electrodes. The electrolyte determines how fast the energy could be released by controlling the rate of mass flow within the battery. After making solid electrolyte interphase on the carbonaceous anode, there is no decomposition in electrolyte and Li ion transport occurs through electrolyte. Thus, it has been suggested that the solvation structures and dynamics of Li ions in liquid electrolyte play an essential role to Li-based battery performance. To mimic commercial electrolyte composition composed of carbonates, Li ion were dissolved in diethylcarbonate (DEC) and its solvation behavior was observed with IR spectroscopy as well as time-resolved IR spectroscopies including IR pump-probe and 2D-IR experiments. IR spectroscopic results combined with DFT study reveals the possible solvation structure and major interaction site for Li ion. Subsequent 2D-IR experiments show that there is fast equilibrium solvation dynamics around Li-ion, which might give some clues about the molecular mechanism of Li ion transport through electrolyte.

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발표분야: Recent Trends in Separation Analysis I: Fundamentals
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Analysis of polyethylene terephthalate (PET) by LC-MS and MALDI-TOF

남궁현

(주)코오롱 중앙기술원 분석평가센터

Polyethylene terephthalate (PET) is the most common thermoplastic polymer of the polyester resin family. The PET polymer is used in fiber and stretch blown plastic bottles as well as high end films, especially for the electro-optical application. Depending on the polymerization process and thermal treatment, the PET shows different physical and chemical properties. This semi crystalline polymer contains wide range of oligomers affecting the polymer properties in a different way. Thus it is strongly needed to extract and identify the oligomer from the PET polymer and to investigate the detailed synthesized mechanism. In this work we use the several extraction techniques and LC-MS as well as MALDI-TOF to analyze the oligomers in detail. The cyclic and linear oligomers with molecular weight up to 7,000 are completely identified. Thus using the separation and MASS spectrometry provides the sufficient valuable information to improve the PET quality in a delicate manner.

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Recent trends in Sports Doping Control

이재익

한국과학기술연구원(KIST) 도핑콘트롤센터

In 1999, the International Olympic Committee (IOC) led the way to creating the World Anti-Doping Agency (WADA) through a collective initiative of sport and governments. WADA seeks to foster a doping-free culture in sport. It combines the resources of sport and government to enhance, supplement and coordinate existing efforts to educate athletes about the harmful effects of doping, reinforce the ideal of fair play and detect those who cheat themselves and their sport.The use of performance-enhancing drugs in sport is cheating. They are associated with serious medical complications and, above all, their use is illegal. Procedures to detect prohibited substances in sports have been in operation for many years and the analytical techniques used currently detect minute traces of substances, which may have been taken several weeks ago. In this presentation, the state of the art analytical instruments, technology and various applications will be introduced for anti-doping purpose.This work was supported by Korea Institute of Science and Technology.

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발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 김정권

A Multi-Task, Multi-Dimensional Immunoaffinity Capillary Electrophoresis for the Selective Purification and Characterization of Protein Biomarkers in Biosamples

Norberto A. Guzman

Immuno-Engineering and Bioanalysis, Princeton Biochemicals, Inc., U.S.A.

The long-term survival of patients with chronic diseases, in particular cancer, is influenced significantly by the detection of early-stage disease. Determination of accurate protein biomarkers in biological fluids and cellular structures is of great value in early diagnosis of a disease, surveillance and asymptomatic screening, and the most promising approach to improve prognosis. Biomarker-based companion diagnostics are also becoming of great value in predicting response to treatment. Companion biomarkers are designed to identify responsive patient sub-populations or those likely to experience adverse drug effects. Using companion biomarkers yields safer and more efficacious drug products, reduces clinical trials and development costs, improves post-marketing safety profiles and salvages therapies that otherwise would not be granted approval. The advent of personalized medicine will require change in the traditional paradigms for developing and commercializing new pharmaceutical products. Today, less than 1% of current drugs have a companion diagnostic, and 60% of the drugs in clinical trials have a companion diagnostic in mind. Some drugs which have been withdrawn from market or Phase 3 development due to serious adverse events may have had a different fate if combined with a companion diagnostic to identify responders or to closely monitor toxicity.

The proteome represents all the possible gene products of a cell. Any protein may exist in multiple forms that vary within a particular cell or in different cells, because of modifications derived from co-translational, post-translational, regulatory and degradative processes that affect protein structure, localization, function and turnover. Therefore, a combination of proteomic techniques should be capable to characterize all proteins in a biological system, including complex features, like isoforms, chemical or enzymatic modifications, interactions and functional structures.

Immunoaffinity capillary electrophoresis (IACE), which benefits by using the power of highly selective affinity capture agents with the high-resolving power of capillary electrophoresis (CE), has demonstrated to be a useful tool for the isolation, separation, and quantification of proteins and peptides. When coupled to one or more sensitive detectors, such as a laser-induced fluorescence detector (LIF) and/or a mass spectrometer (MS), IACE is becoming an important tool for the characterization of proteins and peptides present at a wide range of concentrations in simple and complex matrices. Furthermore, when IACE-LIF and/or IACE-MS are coupled with artificial intelligence based pattern recognition systems, it could result in a powerful tool to study early changes in the underlying pathophysiology of many diseases and toxic conditions.

In this seminar I will discuss the use of a multi-dimensional, multi-task immuno-separation instrument adapted to be coupled to one or more detectors, including a mass spectrometer, for the capture, separation, quantification, and characterization of protein and peptides biomarkers in biological fluids, cell extracts and exhaled breath. Furthermore, I will address the use of IACE for the analysis of isoforms, modified proteins and peptides, degradants, and protein-drug conjugates. The IACE instrument can be manufactured as a portable miniaturized point-of-care instrument to be used in doctor’s office, ambulances, and remote locations.

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발표코드: **ANAL1-4**
발표분야: Recent Trends in Separation Analysis I: Fundamentals
발표종류: 심포지엄, 발표일시: 목 10:35, 좌장: 한상윤

Sequential injection - capillary electrophoresis: Fundamental design and applications

Michael Charles Breadmore Daniel Gstoettenmayer Adam J Gaudry Ala Alhusban Joan Marc Cabot Leile Ranjbar Hong Heng See Petr Smjekal[*]

School of Chemistry, University of Tasmania, Australia

Traditional capillary electrophoresis instrumentals operate in the batch mode: the capillary is transferred from one vial to another for flushing, injection and separation. This is advantageous because of the flexibility and level of automated throughput that can be achieved, particularly for method development and optimisation. However, it is also limited in the ability to couple with other processes streams. Flow-based systems offer an alternative instrument design that makes it easier to achieve regular and routine monitoring of a particular sample as a function of time. Here, the construction and capabilities of a number of flow-based capillary electrophoresis systems based on sequential injection will be discussed. Unique to this design is the ability to efficiently inject all ions from a specific sample volume under stacking conditions to provide superior detection limits. Applications of these systems for water monitoring, cell cultures and for homemade explosives will be discussed.

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발표코드: **ANAL1-5**

발표분야: Recent Trends in Separation Analysis I: Fundamentals

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 한상윤

Development of a Multiuple Channel Capillary Electrophoresis System

박상열

한국표준과학연구원(KRISS) 바이오임상표준센터

Capillary electrophoresis (CE) features unique advantages of high separation efficiency and small sample volume-requirement. In addition, instrumentation for electrophoretic separation is simple, which facilitates implementation of multiple channel separation for high throughput analysis. We have devised a sample introduction method that allows simultaneous introduction of multiple samples without the help of individualized sample wells. In a hydrophobic environment created with a non-polar solvent, aqueous samples attached at the tips of sample loaders autonomously form hydrophilic sample bridges with the entrances of CE channels. The hydrophilic bridges not only prevent samples from dispersing toward others but also maintain themselves against possible agitations. Therefore, samples are to be intendedly introduced into the separation channels without interfering others, which renders highly simple apparatus design acceptable. Our plan is to develop an automated multiple channel CE analysis system for high throughput analysis of routine samples based on the unique sample introduction method. The goal of development is to realize a highly competitive commercial instrument.

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발표분야: Recent Trends in Separation Analysis I: Fundamentals
발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 한상윤

The chemical structures of newely identified analogures of drugs in adulterated foods

조수열

식품의약품안전평가원 첨단분석팀

The various forms of dietary supplements have been developed, because consumer demand for dietary supplements that support their new or continuing healthy lifestyle has increased steadily in recent years. The various forms of analogues of erectile dysfunction and anti-obesity drugs in the dietary supplements which produced to avoid skillfully the regulation of the Ministry of Food and Drug Safety have been increased. Recently, the most widely prescribed drug, sibutramine, was withdrawn from the market. However, phosphodiesterase-5 (PDE-5) inhibitors have been developed to treat erectile dysfunction (ED) and various ED drugs such as sildenafil, tadalafil, vardenafil, and mirodenafil have come onto the market. Some manufacturers dope synthetic drugs into these products to increase treatment efficacy. To date, the 57 analogues of drugs such as PDE-5 inhibitors and sibutramine in adulterated health food products have been identified and our laboratory has been continuously identifying these kind of drugs. The 8 illegal analogues of drugs identified in adulterated foods in 2013 to 2014 were registered in the Criteria and Standards for Food by MFDS and the analogues are continuously being discovered. The 6 out of 8 newely identified analogues of drugs have been first reported in Korea. The structures of 8 analogues of erectile dysfunction(ED) were consistent with a proproxyphenyl-linked sildenafil, an acetylated product of aminotadalafil or methylated tadalafil, and the new analogues were also found as impurities in illegal analogues of drugs. Many analogues of ED may exist because of their chemical structures and the analogues are becoming increasingly diversified and sophisticated in terms of their products and processes. Therefore, it is essential to continuously monitor existing and newly identified analogues of ED, along with elucidating its structural characteristics.

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발표코드: **ANAL2-6**

발표분야: Recent Trends in Separation Analysis II: Applications

발표종류: 분과기념강연, 발표일시: 목 15:45, 좌장: 김성환

Online MW sorting-based enzyme reactor for jumping over the limitation of conventional shotgun proteomics

강덕진

한국표준과학연구원(KRISS) 삶의질측정표준본부

In general proteomics, advanced mass spectrometry coupled with diverse liquid chromatography techniques (LC-MS) has been considered as a fundamental way to both identify and quantify protein(s) of interest in biological sample, as well as to study protein post-translational modifications (PTMs). To this end, proteolytic preparation for protein sample, which is an essential step for bottom-up proteomic analysis, is carried out by in-gel or in-solution digestion with various proteases. However, it is well known that this step is generally labor-intensive and time-consuming (over 12 hours). In this presentation, we introduce a microbore hollow fiber enzyme reactor (mHFER)-LC-MS platform developed recently for online digestion with complementing the issues in general proteolytic preparation. Furthermore, we also present a simple, ease-to-use, and online antibody-specific shotgun proteomics for understanding the biological functions of protein PTMs study

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발표코드: **ANAL2-1**

발표분야: Recent Trends in Separation Analysis II: Applications

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 오진우

Chemical profiling of various alkaloids in herbal medicines using pH control liquid-liquid extraction and LC-ESI-tandem mass spectrometry

홍종기

경희대학교 약학과

Alkaloids with significant biological effects are frequently found to be the main constituents of various herbal medicines. Several types of alkaloids extracted from Fangchi (F.) and Corydalisis (C.) species were characterized using liquid chromatography-electrospray ionization tandem mass spectrometry (LC-ESI-MS/MS). These interesting compounds were extracted from F. and C. species by sonication with 70% CH3OH, and the extract was partitioned at pH values of 2 and 12. LC chromatographic separation of alkaloids were investigated on reversed-phase C18 column with pH variation and composition of mobile phase. Separation of these alkaloids in herbal extracts was found to be significantly affected on mobile phase composition using gradient elution. Chemical profiling of alkaloids in F. and C. species was successfully obtained for the classification of geographic origins and quality evaluation of herbal medicines. Eight-types of alkaloids (aporpine, protoberberine, tetrahydroprotoberberine, benzylisoquinoline, protopine, phthalide, morpine, and bisbenzylisoquinoline) observed in herbal medicines were analyzed by electrospray ionization tandem mass spectrometry in positive ion mode. Several types of fragmentations such as inductive and α-cleavage, retro-Diels-Alder cleavage, imminolization process or simple bond cleavage were observed according to their structural characteristics. These fragmentation patterns could enable to instantly classify the specific alkaloid type in MS/MS spectra of various alkaloids. Based on the MS/MS fragmentations, some of new alkaloids were observed in herbal medicines.

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발표분야: Recent Trends in Separation Analysis II: Applications
발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 오진우

Direct Characterization of Glycosylated Proteins by Ultrahigh-Performance Nano LC-MS/MS

임재민* Lance Wells[1]

창원대학교 화학과 [1]The Complex Carbohydrate Research Center, The University of Georgia

Protein post-translational modification (PTM) increases the functional diversity of the proteome by the covalent addition of proteins. Therefore, identifying and understanding PTMs is critical in the study of protein bioscience. Protein glycosylation is acknowledged as one of the major post-translational modifications, with significant effects on protein folding, conformation, stability and activity. The need to characterize glycoproteins continues to increase as more irrefutable examples of the essential role that covalent carbohydrates in the proteins play in biological processes and functions. The extant challenge of glycobiology and glycotechnology is to approach the extremely low level of sensitivity, used for PTM analysis over the protein identification.In this study, several biologically important proteomic samples was analyzed by shotgun proteomics method, the resulting modified peptides are separated and detected by ultrahigh-performance nano liquid chromatography-tandem mass spectrometry (nano LC-MS/MS). We, for the first time, identified specific O-GlcNAc modification sites of Oct1 and O-linked glycosylation site of Tango1 with the state-of-the-art nano LC-Orbitrap Fusion Tribrid mass spectrometer. Additionally, we focused on the analysis of native glycopeptide of endopolygalacturonases (EPGs) from Botryotinia fuckeliana and polygalacturonase inhibiting proteins (PGIPs) from Phaseolus vulgaris to define their structural interaction. The reports offer comprehensive information for the glycosylation characterization of the EPGs and PGIPs including site identification of glycan attachment, microheterogeneity determination of glycosylation, and N- and O-linked glycan profiles.This work presents an overview of the methods, which have been successfully applied to the detection of level-limited glycopeptides in the glycoproteins.Key Words: Oct1, Tango1, PGIPs, EPGs, Glycosylation, Site mapping, and Nano LC-MS/MS

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A novel derivatization method of free cyanide including cyanogen chloride for the sensitive and rapid analysis of cyanide in chlorinated drinking water by liquid chromatography-tandem mass spectrometry

신호상

공주대학교 환경교육과

A novel derivatization method of free cyanide (HCN + CN-) including cyanogen chloride in chlorinated drinking water was developed with D-cysteine and hypochlorite. The optimum conditions (0.5 mM D-cysteine, 0.5 mM hypochlorite, pH 4.5, and a reaction time of 10 min at room temperature) were established by the variation of parameters. Cyanide (C13N15) was chosen as an internal standard. The formed β-thiocyanoalanine was directly injected into a liquid chromatography-tandem mass spectrometer without any additional extraction or purification procedures. Under the established conditions, the limits of detection and the limits of quantification were 0.07 ?g/L and 0.2 ?g/L, respectively, and the inter-day relative standard deviation was less than 4% at concentrations of 4.0, 20.0, and 100.0 ?g/L. The method was successfully applied to determine CN- in chlorinated water samples. The detected concentration range and detection frequency of CN- were 0.20-8.42 ?g/L (14/24) in source drinking water and 0.21-1.03 ?g/L (18/24) in chlorinated drinking water.

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발표분야: Recent Trends in Separation Analysis II: Applications

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 김성환

Determination of vaccenic and elaidic acid in commonly consumed foods using a silver ion cartridge solid phase extraction method coupled with GC × GC-TOFMS

하재호

한국식품연구원 식품분석센터

This study aimed to develop an analytical method for accurately estimating the ratio of vaccenic to elaidic acid (V/E value). To estimate an accurate V/E value, a silver ion cartridge (SIC) solid phase extraction (SPE) method was performed for removing cis-fatty acids. The removal efficiency of cis-fatty acids was greater than 97.8%. However, the analytical values of total trans-fatty acids (TFAs) were not significantly different between with SIC SPE method and without SIC SPE method. Comparison tests of the V/E values produced by two different methods (without SIC SPE method and with SIC SPE method) using comprehensive two-dimensional gas chromatography combined with time-of-flight mass spectrometry (GC × GC-TOFMS) were also carried out. Those two methods exhibited significant differences in the estimated V/E values because removing cis-fatty acids affected the V/E value but did not affect the total TFAs. The SIC SPE method coupled with GC × GC-TOFMS suggested in this research is available to estimate accurate V/E values in commonly consumed foods, such as margarines, milk products and beef tallow.

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발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김성환

Digital Microfluidics as a Versatile Bioanalysis Tool

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. In this talk, I will present two recent projects using solid samples on a DMF device. First, I will describe the work integrating solid-phase microextraction (SPME) in DMF. In the new system, a SPME fiber is used to extract analytes from a complex sample, and is then inserted into a DMF device. Solvent droplets are then used to extract analytes from the fiber with continuous actuation, followed by analysis with liquid chromatography and mass spectrometry. Compared to conventional methods, the new technique allows for fast, efficient desorption of analytes from the SPME fiber using a small volume of solvent. The miniaturized system allows for preconcentration of analytes and was applied the analysis of steroid hormones in human urine. Second, I will describe our 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. Using this automation system allowed for parallel sample processing and full factorial design of experiments (DOE) optimization. Relative to macroscale methods, this DMF approach reduced reagent volumes and analysis time, and moreover, this represents the first DOE optimization for immunoassays implemented in a microfluidic system. I propose that these techniques have great potential for numerous applications in bioanalysis and beyond.

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Foot-and-mouth disease virus: a major global agricultural problem in need of antiviral therapy

고윤영

한국화학연구원 바이러스시험연구센터

Foot-and-mouth disease (FMD) is a highly contagious disease of the cloven-hoofed animals caused by the foot-and-mouth disease virus (FMDV; family Picornaviridae; genus Aphthovirus). FMD is the most economically important veterinary pathogen due to its highly infectious nature, ability to cause persistent infection and long-term effects on the condition and productivity of the many animal species it affects. Due to the enormous socioeconomic consequences related to an FMD incursion, the main concern of FMD-free major livestock producing countries is to prevent the introduction of the virus and/or to rapidly eradicate it in case of an outbreak. Although vaccines have been crucial in controlling and eradicating FMD from some parts of the world, the disease still affects millions of animals around the globe and remains as the most important veterinary disease limiting trade of animals and animal products. The use of current FMD vaccines to induce early protection is limited; thus, alternative/supplementary methods to rapidly reduce the spread of FMDV in outbreak situations are urgently needed. One possible alternative would be the use of antiviral drugs in a vaccinated zone to control viral dissemination and fill the “immunity-gap” between time of vaccination and development of protective immunity. Unfortunately, there are not yet commercially available antiviral therapies for prevention or treatment of FMDV infection. In this presentation, the current efforts to discover FMD-antiviral drugs will be reviewed to help and provide insights to investigators for identification of potential therapeutics to fight against this devastating animal disease.

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Regulating the regulators: Basic concept and clinical application for PD-1/PD-L1 interaction

하상준

연세대학교 생화학과

For more than 100 years, immunotherapy for infectious disease and cancer has played an ever-increasing role as a therapeutic regimen even though there are not many approved drugs and regimens. Activating the immune system for therapeutic benefit in infectious disease and cancer has long been a goal in immunology and oncology. After repetitive failures, the tide has finally changed due to the success of recent proof-of-concept clinical trials using antibodies to blockade immune inhibitory molecules such as CTLA-4 and PD-1. These successes suggest that tolerance raised by immune suppressive microenvironment is a major obstacle for immunotherapy and therefore, blocking the tolerance is the first step to rejuvenate antigen-specific T cell immune responses. In this seminar, the basic concept of T cell exhaustion and the role of inhibitory molecules expressed by the exhausted T cells and regulatory T cells. In addition, a representative inhibitory molecule, PD-1, and its current clinical use to treat infectious disease and cancer will be introduced. Finally, future strategy to enhance the efficacy of the regulator blockade therapy will be discussed.

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Characterization and Lead optimization of a novel hepatitis C virus inhibitor acting on early and late steps of the viral life cycle

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Approx. 200 million patients Hepatitis are chronically infected with hepatitis C virus (HCV) and are at risk of developing life threatening liver diseases. Until to date, there are obvious unmet medical needs which encouraged us to identify, characterize and develop novel HCV interventions.

We devised strategies using the infectious HCV cell culture system and carried out a phenotypic, target-free screening campaign. By excluding compounds active in the replicon system and including those active on HCV E1/E2 mediated entry, we identified inhibitors interfering with early and late steps of the HCV life cycle. A promising hit was selected and further characterized in order to determine the mechanism of action, antiviral potency and to evaluate properties crucial for drug development.

By conducting time-of-addition experiments with this favorable hit compound, inhibition of attachment and internalization of HCV particles was observed. In addition, cell-to-cell spread and the secretion of infectious virions was inhibited, whereas HCV RNA secretion and density of viral particle was unaffected. Furthermore, this potent (EC50 0.0005uM, CC50 >5uM) inhibitor is synergistic in combination with selected direct acting antivirals and IFN-alpha, and viral drug resistance profiling revealed the HCV glycoprotein E1 as putative molecular target. Concerning DMPK, amongst other properties, metabolic stability, solubility, CYP inhibition and other PK properties are being evaluated and improved.

In summary, we identified and characterized a very potent novel inhibitor acting on early and late steps of the HCV life cycle. A Lead optimization campaign has been initiated to further improve drug-like properties and to evaluate in vivo efficacy in order to move towards preclinical studies.

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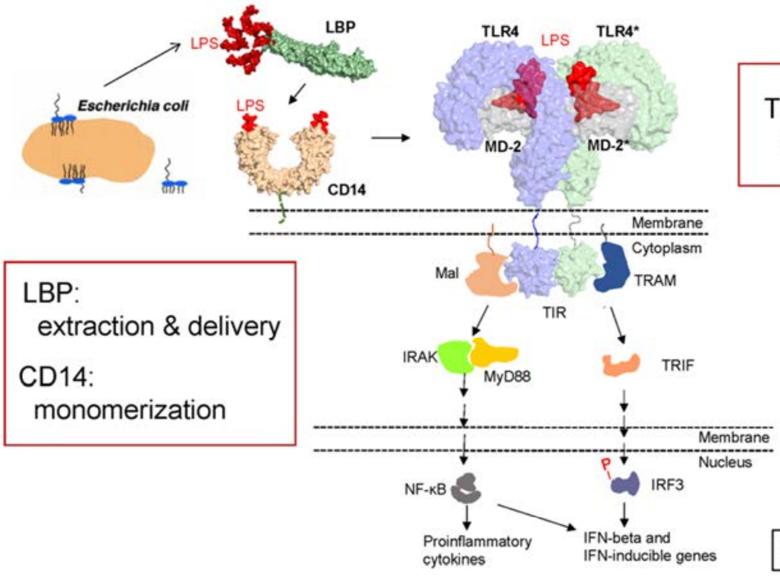
Recognition of Lipopolysaccharides by TLR4 and its Accessory Proteins

이지오

한국과학기술원(KAIST) 화학과

Lipopolysaccharide (LPS) is a bacterial glycolipid that is the major component of the outer membrane of gram-negative bacteria. It serves as an early warning signal of infection by initiating a potent immune response. Lipid A, the lipid part of the LPS, is responsible for the majority of the immunological activity of LPS and binds to the cell surface receptor, TLR4-MD-2 heterodimer. LPS binds to the hydrophobic pocket in MD-2 and induces the dimerization of TLR4. Efficient activation the TLR4 signal in vivo requires accessory proteins, LBP and CD14. LBP is a serum glycoprotein that can extract LPS from bacterial membranes or vesicles released from it. CD14 accepts a monomeric form of LPS from LBP and delivers it to the TLR4-MD-2 complex. The structures of these LPS recognition proteins in a complex with LPS and related molecules provide us insight into how our immune system recognizes bacterial infections and initiates efficient defense mechanisms. I will summarize recent structural studies of these LPS receptors and accessory proteins.



TLR4-MD-2:
signaling

LBP:
extraction & delivery

CD14:
monomerization

sepsis

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발표분야: Infectious Disease Research in Biochemistry and Structural Biology
발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 이형호

Structure-guided discovery of a novel inhibitor against class C beta-lactamases with extended substrate spectrum

차선신

한국해양과학기술원 생물연구본부

The emergence and dissemination of drug-resistant pathogens are great threat to public health in the world. The expression of beta-lactamases, which inactivate antibiotics, is a prevalent resistance mechanism of bacteria to beta-lactam antibiotics. Therefore, the development of inhibitors against beta-lactamases is a challenge to treat drug-resistant pathogens. Recently, a non-beta-lactam inhibitor against class C beta-lactamases has been discovered in my lab. The chemical structure of this novel inhibitor is different from those of existing inhibitors. In addition, this inhibitor exhibited an in vivo efficacy without side-effects in mouse models. In this talk, I present the molecular features of this inhibitor.

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Structural biology of cell-shape determining proteins from *Helicobacter pylori*

서세원

서울대학교 화학부

Helicobacter pylori is the major human pathogen associated with various gastrointestinal diseases such as gastritis, ulcer, and gastric cancer. Its colonization of the human gastric mucosa requires high motility, which depends on the helical cell shape. At least seven cell shape-determining genes (csd1, csd2, csd3/hdpA, ccmA, csd4, csd5, and csd6) have been identified in *H. pylori*. These proteins play key roles in determining the cell shape through modifications of the cell-wall peptidoglycan by alteration of crosslinking or by trimming of peptidoglycan muropeptides. To provide a framework for a better understanding of their molecular functions and for the discovery of novel inhibitors that would prove helpful in fighting infections by *H. pylori*, we are carrying out determination of their crystal structures by X-ray crystallography. Csd4 is a Zn-dependent D,L-carboxypeptidase that cleaves the bond between the γ-D-Glu and mDAP of the uncrosslinked muramyl tripeptide (L-Ala-γ-D-Glu-mDAP) of the peptidoglycan to produce the muramyl dipeptide (L-Ala-γ-D-Glu) and mDAP. We have determined its crystal structure in three different states, i.e., the ligand-unbound form, the substrate-bound form, and the product-bound form. H. pylori Csd4 consists of three domains: (i) the N-terminal D,L-carboxypeptidase domain of the typical carboxypeptidase fold, (ii) the central β-barrel domain of a novel fold, and (iii) the C-terminal immunoglobulin-like domain. The D,L-carboxypeptidase domain recognizes the substrate by interacting primarily with the terminal mDAP moiety of the muramyl tripeptide. It undergoes a significant structural change upon binding either mDAP or the mDAP-containing muramyl tripeptide. We also show that Csd5, another cell-shape determinant, is capable of interacting not only with H. pylori Csd4 but also with the dipeptide product of the reaction catalyzed by Csd4.

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발표분야: Recent Advances in Bioconjugation and Related Applications
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김양미

A tumor suppressor of ubiquitin ligase substrate receptor

강창원

한국과학기술원(KAIST) 생명과학과

Cancers are promoted by oncogene upregulation or tumor suppressor gene downregulation. This study of genetic epidemiology, cell biology and proteomics proposed a novel tumor suppressor, for which no biological function had been known. Firstly, this gene was discovered to be statistically associated with susceptibility to gastric cancer in this Korean case-control study using 1271 gastric cancer patients and 1303 healthy controls. Secondly, this gene expression was downregulated in gastric and several other cancers. Its knockdown using siRNA or shRNA increased cell proliferation, piling up and anchorage-independent growth, which are characteristics of tumor progression. Thirdly, proteomic and western blot analyses identified this protein as a substrate receptor component of E3 ubiquitin ligase complex, as binding to other components of E3 complex, TCEB1 (elongin C) and TCEB2 (elongin B). This substrate receptor additionally bound to IMP dehydrogenases, IMPDH1 and IMPDH2, which appeared to be E3 ubiquitination substrates and had been associated with tumor transformation and progression. Accordingly, this substrate receptor-containing E3 complex appears to exert a tumor suppressive role via ubiquitination-dependent degradation of cancer-associated IMP dehydrogenases among other oncoproteins.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-2**
발표분야: Recent Advances in Bioconjugation and Related Applications
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 최수혁

Bioconjugation of polymers for gene and drug delivery

김원종

포항공과대학교(POSTECH) 화학과

In this research, siRNAs were utilized for two functions: therapeutic agent and cross-linking building block for nanoconstruct. We developed a novel nanoconstruct (NC) which was composed of siRNA-conjugated natural polymers through spontaneous hybridization of sense- and antisense strand siRNAs conjugated to dextran polymer. This siRNA mediated cross-linked NC is a condensed nano-sized particle through gathering each polymer chains by siRNA double helix formation. Increasing the concentration of NC inhibited gene expression more efficiently up to about 40 %. Herein, we also designed self-assembled nanoparticles for Paclitaxel (PTX) delivery toward tumor cell. Self-assembled nanoparticles were constructed through host-guest chemistry between PTX and β-cyclodextrin (β-CD). CD and PTX are covalently conjugated with poly maleic anhydrides via ester linkage that provide higher solubility of nanoparticles. This inclusion complex forms a stable nano-sized particles, in which hydrophilic polymers cover outside nanoparticle and the inclusion complex of CD/PTX is located inside nanoparticle. It was revealed that this nanoparticle effectively inhibited the tumor growth in vivo by delivering PTX into tumor site.

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장소: 일산 KINTEX
발표코드: **BIO2-3**
발표분야: Recent Advances in Bioconjugation and Related Applications
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 최수혁

Applications of sticky moieties directly to living organisms

이해신

한국과학기술원(KAIST) 화학과

The unique water-resistant adhesive property represented by poly(dopamine) has been widely implemented to a variety of fields such as material, energy storage, bioconjugation, biomaterials, drug delivery, and others. In chemical structure, poly(dopamine) and its derivative polymers such as poly(DOPA) and poly(norepinephrine) are similar to natural or synthetic melanin, the bio-pigment found in human skin, eye, and brain. Unlike conventional approaches utilizing poly(dopamine) and its related sticky compounds, this presentation will introduce a new approach in which the sticky moiety can also be applied directly to living cells such as bacteria or virus. Furthermore, property conversion when displaying the mussel-inspired sticky moieties will be discussed, and useful applications will be proposed based on recent results.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-4**
발표분야: Recent Advances in Bioconjugation and Related Applications
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 최수혁

Supramolecular nanoprobes based on rationally designed block molecules

이은지

충남대학교 분석과학기술학과

Self-assembly of organic block molecules can give rise to the various nanostructures such as spheres, cylinders and vesicles. Incorporation of a specific block with desired functions into molecular architecture leads to a variety of functional nanomaterials. Recently, we have developed the supramolecular nanoprobes based on the self-assembly of amphiphilic block molecules in response to the metal ions and inorganic nanoparticles which results in the drug- and imaging agent-loaded nanohybrids. Interestingly, the metal-binding process of amphiphiles induced nanoassemblies even below the CMCs, and the binding stoichiometry affected the morphologies of the resultant nanostructures. In addition, the bioconjuagated block molecules with assembly-monitoring fluorophore pendant showed the solution-state molecular organization within the nanoaggregates and specific fluorescence turn-on or turn-off response as a function of metal ion. In this talk, the fabrication of supramolecular nanoprobe for metal ion sensing in aqueous solution and its applications toward live cell imaging and antimicrobial agent will be discussed.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-5**
발표분야: Recent Advances in Bioconjugation and Related Applications
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 최수혁

Aptide-based bioconjugates for biomedical applications

전상용

한국과학기술원(KAIST) 생명과학과

Aptides, a novel class of high-affinity peptides, are designed to possess a “tweezers-like” structure comprising a unique structure-stabilizing scaffolding region and two high-affinity target-binding components. We have produced aptides with nanomolar-range binding affinities for several targets using phage display selection, demonstrating the utility of this technology. Indeed, peptides with high target affinity isolated from aptide libraries have offered the potential for use as diagnostic or drug candidates. We have utilized several aptides specific to target proteins for various biomedical applications, including targeted drug delivery, cancer imaging by MRI, and targeted protein therapeutics. In this lecture, a couple of biomedical applications using aptide-based bioconjugates will be presented.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN1-1**
발표분야: Current Trends in Organic Chemistry I: Catalytic Organic Reactions
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 윤재숙

Part 1. A Catalytic Enantioselective Glycolate Aldol Reaction via Lewis Base Activation of Lewis Acids
Part 2. A General Enantioselective Approach to the Chemical Synthesis of the Chlorosulfolipids

정원진

GIST 화학과

Part 1. A general, efficient, Lewis-base catalyzed enantioselective addition of glycolate-derived silyl ketene acetals to a wide range of aldehydes will be presented. Both *syn*- and *anti*-diastereomers are accessible without changing the catalyst or controlling the geometry of the silyl ketene acetal. Simple modification of the size of alkyl groups on the silyl ketene acetal is sufficient to reverse the stereochemical course of the addition. The observed diastereoselectivity and reactivity could be rationalized by the analysis of six open transition state structures with the aid of computational analysis.

Part 2. A concise and general approach has been developed for the enantioselective synthesis of three structurally related chlorosulfolipids. Key advances include highly stereocontrolled additions to a,b-dichloroaldehydes, kinetic resolution of complex chlorinated vinyl epoxide intermediates, and *Z*-selective alkene cross metathesis of *cis*-vinyl epoxides. This strategy facilitated the synthesis of enantioenriched danicalipin A, mytilipin A, and malhamensilipin A in nine, eight, and eleven steps, respectively.

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일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN1-2**
발표분야: Current Trends in Organic Chemistry I: Catalytic Organic Reactions
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 윤재숙

Development of DNA Hybrid Catalyst Using a Rational Design Approach and Application in the Asymmetric Synthesis

박소영

교토대학교 화학과

The application of DNA-based hybrid catalysts for asymmetric synthesis emerged very recently. These catalysts consisting of DNA and a metal complex with a specific ligand through supramolecular or covalent anchoring strategies, have demonstrated high enantioselectivity in a variety of carbon?carbon or carbon?heteroatom bond-forming reactions and have expanded their role in asymmetric catalysis. We have developed a DNA-based hybrid catalyst containing an intrastrand bipyridine ligand through direct ligand incorporation and successfully performed asymmetric intramolecular Frieldel-Crafts alkylations. This is the first report on the DNA hybrid catalyst system that intrastrand ligand is covalently introduced into the phosphate backbone. We have generated a series of active site to investigate the structural details of DNA hybrid catalysts and demonstrated that catalytic properties of DNA hybrid catalysts are governed by the disposition of the metal-binding site in the DNA duplex, the size of catalytic cavity and the composition of nucleobases in the catalytic pocket.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN1-3**

발표분야: Current Trends in Organic Chemistry I: Catalytic Organic Reactions

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 윤재숙

Pd-catalyzed asymmetric hydroamination and hydroalkoxylation of allene: Development and application

이영호

포항공과대학교(POSTECH) 화학과

In this presentation, our recent discovery will be discussed which describes the Pd-catalyzed asymmetric intermolecular hydroamination and hydroalkoxylation of alkoxyallene. Combined with the ring-closing-metathesis, these reactions offer a new pathway toward stereodefined cyclic allylic O,O- and N,O-acetals. Application of this method will be revealed, which focuses on the stereochemically flexible syntheis of highly functionalized azacycles and various mono- and disaccharides.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN1-4**

발표분야: Current Trends in Organic Chemistry I: Catalytic Organic Reactions

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 민선준

Efficient Synthesis of Organic Molecules using Transition Metal Catalyst

전철호

연세대학교 화학과

There are some efficient ways to prepare functional organic molecules by transition metal catalysis. Some of typical examples are 6-membered heterocycles such as pyridine and isoquinoline. Pyridine and isoquinoline derivatives are prepared by the reaction of alpha,beta-unsaturated ketone and acetophenone with internal alkynes under Rh(III) and Cu(OAc)2 through C-H bond activation of sp2-C-H bond. Another interesting substrate is ester, which can be prepared in one pot from alkene, sodium formate, and alcohol under cooperative catalyst of 2-pyridine methanol and Ru3(CO)12 complex. In this protocol, various esters can be prepared from above three components using chelation-assistant strategy. With this protocol modification of polybutadiene can be achieved to afford functionalized polymer. The reaction of aryl chloride with primary alcohol is carried out in the presence of Pd/C catalyst and NaF to form ester, arene, and alkane. In this reaction, aryl chloride acts as both oxidant and coupling partner, while alcohol serves as both carbonyl source and alkoxy component of the final ester product.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN1-5**

발표분야: Current Trends in Organic Chemistry I: Catalytic Organic Reactions

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 민선준

Drug Discovery in Academia: A Successful Case Study

Michael E. Jung

Department of Chemistry and Biochemistry, UCLA

The process of drug discovery in academia will be discussed with examples of prior and ongoing collaborations, including at least one success story. The areas of research include antitumor agents, osteogenic materials for spinal fusion and osteoporosis, and anti-leukemic agents. In particular, the biology and chemistry leading to the approved drug, enzalutamide (Xtandi) will be described.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry II: Organic Supramolecular Chemistry

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 이희승

From the Reversible Sensor to the Irreversible Biological Probe

김해조

한국외국어대학교 자연과학대학 화학과

Keywords: Fluorescence, Imaging, Optical, Probe, Sensor

Although a lot of reversible optical sensors for metal cations and anions have been developed utilizing H-bonds of crown ethers and self-assembled supramolecules over the several decades, few molecules are capable of assessing biologically meaningful analytes due to the weak intermolecular forces between a host molecule and guest molecules in the aqueous environment. To reinforce the host-guest interaction, recently are designed reaction-based chemical probes,[1] which play a good role of biological probe in water. In this lecture, we will review the reversible sensors and present our approach to the irreversible chemical probes, especially focusing on the biological probes for mitochondrial GSH with high selectivity and with NIR fluorescence capable of noninvasive imaging in biological samples.[2] In order to monitor mitochondrial GSH with low background autofluorescence, we designed a heptamethine-nitroaryl conjugate as an NIR fluorescent probe by introducing a tunable lipophilic cation unit as the biomarker for mitochondria or tumor and a nitroaryl group as the GSH-selective reaction site as well as the fluorescence quencher. The probes exhibited dramatic Off-On NIR fluorescence responses in the presence of GSH with high selectivity toward GSH over other amino acids including Cys and Hcy. Further application to cellular imaging and tumor diagnostics indicated that the probes were highly responsive to GSH in cancer cells.

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일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN2-2**

발표분야: Current Trends in Organic Chemistry II: Organic Supramolecular Chemistry

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이희승

Development of Thermoresponsive Amphiphilic Molecules Utilizing Monodisperse Oligoethylene Glycols

Kazushi Kinbara

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

Polyethylene glycol (PEG) is one of the most popular water-soluble organic compounds, which has been used in wide fields of chemistry. One of the important properties of PEG its thermal response: PEG undergoes a conformational change from the gauche-rich to anti-rich form upon temperature elevation. Thus, we have interests in development of thermoresponsive functional amphiphilic molecules including monodisperse oligoethylene glycol units in a macrocyclic skeleton.

Recently, we have synthesized macrocyclic structured PEG consisting of three tetraethylene glycol (TEG) and pentaerythritol units, respectively. This triangle molecule undergoes hydrophilicity/hydrophobicity switching accompanied by the conformational change at lower temperature than conventional linear PEGs, and effectively suppressed thermal aggregation of proteins. In addition, we have also developed cyclic amphiphilic multiblock molecules, consisting of linearly connected oligoethylene glycol units and hydrophobic 1,4-bis(4-phenylethynyl)benzene units. Interestingly, these molecules show unique phase-transition behaviors upon temperature change. Unique features of such thermoresponsive molecules will be presented.

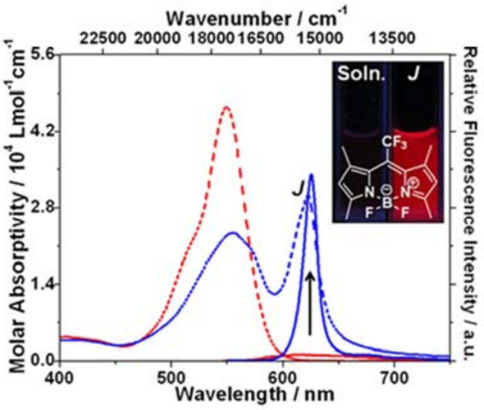
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN2-3**
발표분야: Current Trends in Organic Chemistry II: Organic Supramolecular Chemistry
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이희승

Aggregation Induced Emission of Organic Dyes and Thier Applications

김영미

단국대학교 화학과

Due to their excellent spectroscopic properties, high photochemical and chemical stabilities, and the facile alteration of their photophysical properties by molecular design, 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) dyes are among the most popular organic fluorophores and have been widely employed as labeling reagents in molecular biology, lasing medium in liquid solution dye lasers, and chemosensors or molecular probes. However, while many BODIPY dyes exhibit high fluorescence quantum yields in dilute solutions, they scarcely emit in the solid state as a result of emission quenching upon aggregation, which remains a major challenge in the application of BODIPY dyes. In this talk, we present the first unequivocal example of structurally characterized emissive BODIPY J-aggregate, formed by the simple meso-trifluoromethyl-substituted dye 1 (CF_3-BODIPY), which contrasts with the quenched condensed-phase photophysics that are typical for BODIPY dyes such as CH_3-BODIPY 2 (Figure 1). Figure 1. Absorption (dotted lines) and emission (solid lines) spectra of 1 (left) and 2 (right) at concentrations of 2×10^{-5}mol/L in CH_3CN (red) and CH_3CN/H_2O solution (blue, $CH_3CN/H_2O = 1:99$ (v/v)). Excitation at 530 nm for 1 and 460 nm for 2, respectively. Inset shows photographs of each solution (left: CH_3CN, right: $CH_3CN/H_2O = 1:99$ (v/v)) under irradiation at 365 nm.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20000
18000
16500
15000
13500
Molar Absorptivity / 10^4 Lmol^{-1}cm^{-1}
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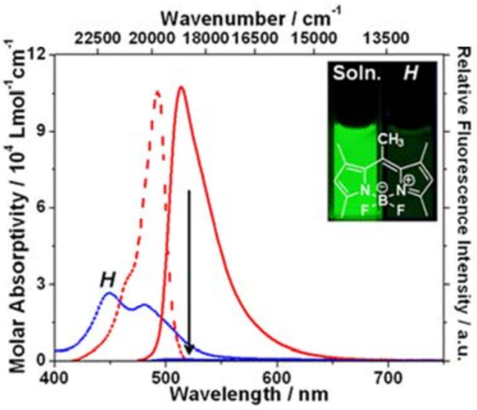
4.2
2.8
1.4
0.0
400
500
600
700
Wavelength / nm
Relative Fluorescence Intensity / a.u.
J
Soln.
J
CF$_3$
N
B
N
F
F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22500
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15000
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Molar Absorptivity / 10^4 Lmol^{-1}cm^{-1}
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9
6
3
0
400
500
600
700
Wavelength / nm
Relative Fluorescence Intensity / a.u.
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Soln.
H
CH$_3$
N
B
N
F
F

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN2-4**

발표분야: Current Trends in Organic Chemistry II: Organic Supramolecular Chemistry

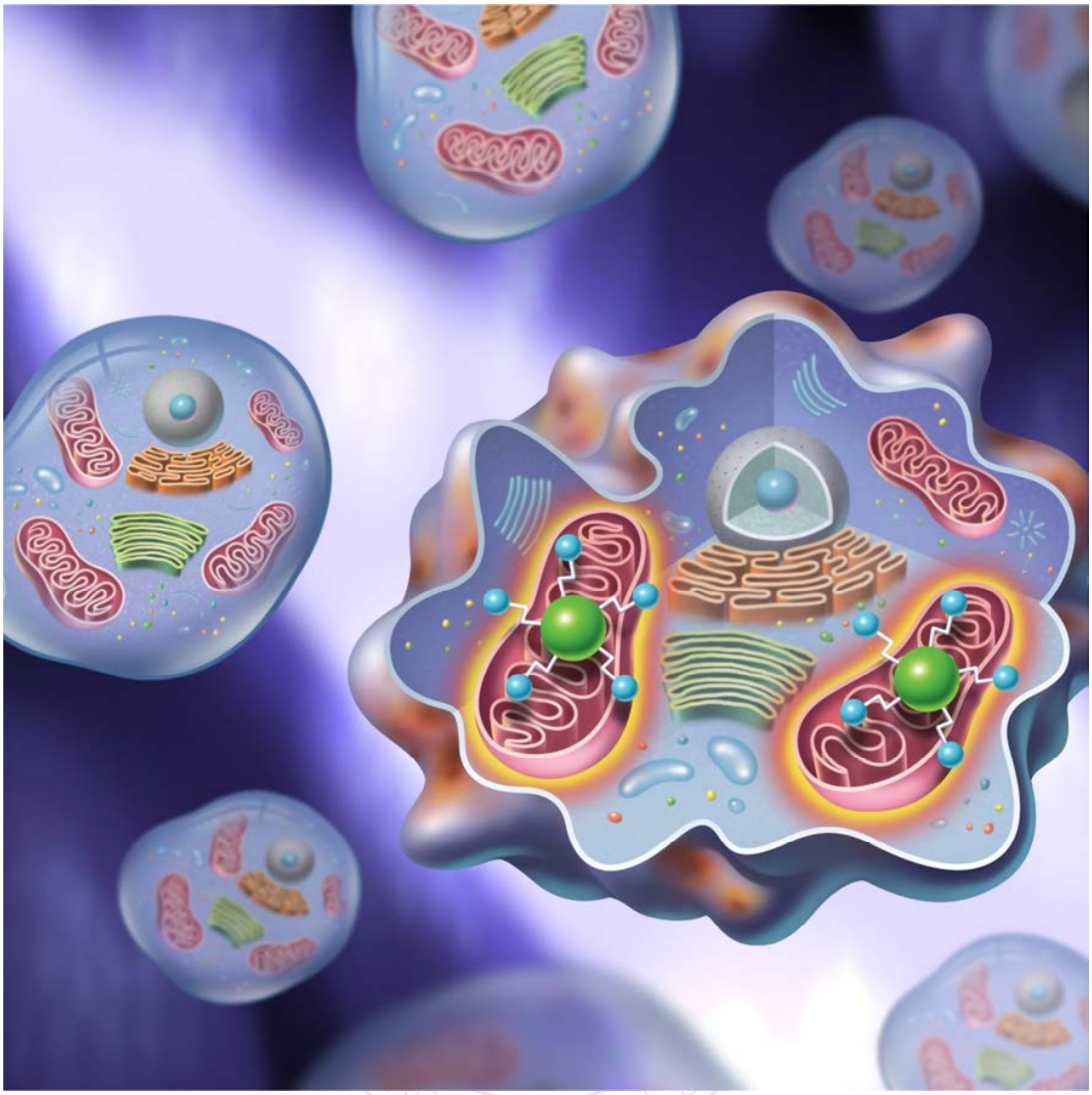
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김영미

Small molecule based drug delivery with fluorescence imagings

정효성 이재홍 이윤학 장주희 신원섭 엄수진 구세영 김원영 선우경 강철훈[1] 김종승*

고려대학교 화학과 [1]경희대학교 동서의학대학원

Mitochondria are organelles that are readily susceptible to temperature elevation. We prepared a new mitochondria-targeting iron oxide NP fabricated with two functional groups: TPP as the mitochondrial targeting unit and coumarin as a fluorescent signalling unit. Upon irradiation with a 740 nm NIR laser at 2.0 W/cm2, the solution temperature of Mito-CIO was increased by 13 °C, whereas no such changes occurred in an NP-free solution. Laser irradiation of HeLa cells incorporating Mito-CIO increased the cellular temperature by 2.1 °C within 5 min. In HeLa cells, Mito-CIO and CIO were localized to the mitochondria and the ER, respectively. Mito-CIO induced significantly more cell death after 20 min NIR irradiation than did CIO, and the differential cytotoxicity can be attributed to the mitochondrial localization of NPs. Furthermore, in vivo therapy using mitochondria-directed hyperthermia clearly displayed tumour suppression, which is in agreement with the in vitro cytotoxicity results. Together, these results strongly support our hypothesis that mitochondria are more susceptible to hyperthermia than the ER. From this study of both the in vitro and in vivo effects of mitochondria-targeted MPs, we conclude that this heat generating system can enhance the therapeutic efficacy of hyperthermia in cancer treatment and may allow the development of new photothermal therapeutics.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN2-5**
발표분야: Current Trends in Organic Chemistry II: Organic Supramolecular Chemistry
발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 김영미

Click Chemistry + Supramolecular Chemistry = Functional Materials

조병기

단국대학교 화학과

많은 유기합성법 중에, 최근에 가장 각광받고 있는 합성법인 클릭 화학 (click chemistry)은; 1) 물에서 반응이 가능, 2) 생성물이 regio-specific, 3) protecting group 이 별도로 필요하지 않고, 4) 반응성이 매우 높아 실온에서도 반응이 가능하다는 합성적인 장점을 갖고 있다. 이러한 클릭 반응은 최근 기능성 유기소재개발의 중요한 구성요소로서의 응용이 시도되고 있음에도 불구하고, 대부분의 경우, 서로 다른 블록을 연결하는 linking method 로 사용되고 있는 실정이다. 본 연구실에서는 최근 수년간 액정 및 기능성소재 디자인에 본 클릭화학을 이용하여, 자기조립 초분자 유기소재개발연구를 수행하고 있다. 특히, 2 차원 원판형, 3 차원 프로펠러형, 수소결합 액정 초분자시스템, 브렌치형 블록공중합체등을 클릭화학을 통해 디자인하여, 형광변색소재, 이온전달체, 나노다공성과 같은 기능성 유기소재특성을 조사하였다. 본 발표에서 관련 연구결과를 소개하고자 한다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI-1**
발표분야: Recent Trends of Targeted Therapy for Cancers and Drug Discovery
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 남기엽

Development of BCR-ABL1 tyrosine kinase inhibitors in chronic myeloid leukemia

김동욱

가톨릭대학교 혈액내과

Imatinib which was first successful tyrosine kinase inhibitor (TKI) has revolutionized the treatment of chronic myeloid leukemia (CML) with markedly improved survival. However about 30-40% of patients who initially respond to imatinib subsequently develop resistance or intolerance. Recently, second generation BCR-ABL1 tyrosine kinase inhibitors (2G TKIs) such as dasatinib, nilotinib, radotinib, bosutinib and ponatinib have been developed.Radotinib (IY5511HCL), a novel and selective BCR-ABL1 TKI developed by ILYANG co., has shown pre-clinical and clinical activity in CML. The phase 2 clinical study was conducted in 77 chronic phase CML patients with resistance and/or intolerance to other TKIs. For 12 months of treatment with radotinib 400 mg twice daily, major cytogenetic response (MCyR) was achieved in 50 (65%) patients, including 36 (47%) patients with complete cytogenetic response (CCyR). Overall survival rate at 12 months was 96.1%. All newly-occurring or worsening grade 3/4 hematologic abnormalities included thrombocytopenia (24.7%) and anemia (5.2%); grade 3/4 drug-related non-hematologic adverse events included fatigue (3.9%), asthenia (3.9%), and nausea (2.6%). The most common biochemistry abnormality was hyperbilirubinemia (grade 3/4 23.4%), and 12 of 18 patients were managed with dose modification. Study findings suggest radotinib is effective and well tolerated. As already stressed by a CML expert panel, globally, treatment penetration and compliance rates of TKIs are low due to high prices. However, Korean prices for 2G TKIs are approximately 20%-30% that of Western countries because of the approval of radotinib based on our study. Finally, cost-effectiveness of radotinib could improve drug accessibility and may be necessary in emerging regions.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI-2**
발표분야: Recent Trends of Targeted Therapy for Cancers and Drug Discovery
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 남기엽

E3 ubiquitin ligase-dependent pathway as a novel therapeutic strategy

진동훈

서울아산병원 아산생명과학연구원 암연구단

PTEN is one of the most frequently mutated or deleted tumor suppressors in human cancers. NEDD4-1 was recently identified as the E3 ubiquitin ligase for PTEN, but a number of important questions remain regarding the role of ubiquitination in regulating PTEN function and the mechanisms by which PTEN ubiquitination is regulated. In the present study, we demonstrated that p34, which was identified as a binding partner of NEDD4-1, controls PTEN ubiquitination by regulating NEDD4-1 protein stability. p34 interacts with the WW1 domain of NEDD4-1, an interaction that enhances NEDD4-1 stability. Expression of p34 promotes PTEN poly-ubiquitination, leading to PTEN protein degradation, whereas p34 knockdown results in PTEN mono-ubiquitination. Notably, an inverse correlation between PTEN and p34/NEDD4-1 levels was confirmed in tumor samples from colon cancer patients. Thus, p34 acts as a key regulator of the oncogenic behavior of NEDD4-1 and PTEN.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI-3**
발표분야: Recent Trends of Targeted Therapy for Cancers and Drug Discovery
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 함정엽

Anticancer activities of novel pyrazolo[3,4-d]pyrimidine derivatives on thyroid cancer

심태보

한국과학기술연구원(KIST) 화학키노믹스연구센터

RET (REarranged during Transfection) is a receptor tyrosine kinase (RTK) and RET mutations are implicated with thyroid cancers. Chromosomal rearrangements of RET are associated with papillary thyroid carcinoma (PTC) and point mutations of RET are responsible for medullary thyroid cancer (MTC). Based on structure-based drug design, we have identified a series of novel pyrazolo[3,4-d]pyrimidine derivatives as potent and selective RET inhibitors. Our lead compounds possess excellent potency against various point-mutants of RET including gatekeeper mutations (V804M, V804L). These novel RET inhibitors will be presented in this talk.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI-4**
발표분야: Recent Trends of Targeted Therapy for Cancers and Drug Discovery
발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 함정엽

EGFR Inhibitors for Lung Cancer Treatment

이광호

한국화학연구원 신물질본부/난치성

Erlotinib (Tarceva) & Gefitinib (Iressa) are currently in clinic use as epidermal growth factor receptor (EGFR) kinase inhibitors for non-small-cell lung cancer (NSCLC). However, their clinical efficacy is limited by both their mechanism-based toxicity and the development of drug-resistance mutations, including the gatekeeper T790M mutation. Unlike their quinazoline-based core scaffold, a new pyrimidine-based irreversible inhibitor has been identified for the EGFR gatekeeper T790M mutant specific activities. These pyrimidine-based EGFR inhibitors may provide improved therapeutic window and more effective clinical treatment for NSCLC patients.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT1-1**

발표분야: Recent Trends in Soft Nano/Micro Materials

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 유효종

Surface-engineered Nanomaterials as X-ray Absorbing Adjuvant Agents for Auger-mediated Chemo-radiation

이상민

가톨릭대학교 화학과

We demonstrate a prototype approach to formulating gold nanoparticle (AuNP)-based X-ray absorbingadjuvant agents through surface-engineering of cisplatin pharmacophore (Pt) with lipoic acid-modifiedpolyacrylate (Pt-AuNPs). Design of Pt-AuNPs was examined and further validated using a combinationof physicochemical characterization methods. Our results show Pt-AuNPs exhibits very high capacity forPt-loading via the mechanism of multidentate coordination between Pt(II) ions and surface-boundpolyacrylate. The Pt-AuNP vector demonstrated excellent colloidal stability in an acid-sensitive mannerthat enables Pt drug-release, and exhibited high in vitro cytotoxicity to the cancer cell lines MCF-7 andSK-OV-3. Secondary electron emissions from both Pt(II) and AuNPs are triggered by an external ionizingradiation source via the Auger cascade. As a result, Pt-AuNPs exhibit therapeutic potential as an adjuvantagent for concurrent chemo-radiation cancer therapy

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT1-2**

발표분야: Recent Trends in Soft Nano/Micro Materials

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 유효종

Designer Functional Colloids Using Drop-based Microfluidics

김진웅

한양대학교 응용화학과

This talk introduces a flexible and straightforward method for fabrication of monodisperse complex colloidal materials by using a microcapillary-based microfluidic technique. The use of this approach enables tight control over the size and monodispersity of droplets as well as their surface functionality, which is essential for not only determining the loading level of solutes, but also regulating their transport kinetics. We show that fine-tuning of fluids that flow through a geometrically controlled tiny channel enables fabrication of a wide variety of novel structures: elastomeric colloidal sensors, polymer shells, and hollow microcapsules. The robustness and versatility of our microfluidic approach can make the complex colloidal systems more controllable, thus opening up new possibilities to engineer key functions that are most suitable for many practical applications, including electronic skins, drug delivery, biomineralization, and so on.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT1-3**
발표분야: Recent Trends in Soft Nano/Micro Materials
발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 유효종

Utilizing advanced stop flow lithography techniques for the synthesis of complex anisotropic multifunctional particles in microfluidic devices

봉기완

고려대학교 화공생명공학과

Stop Flow lithography (SFL) has been emerging as a powerful synthesis technique for creating anisotropic multifunctional particles with applications that range from MEMs to biomedical engineering. Combining photolithography with microfluidic methods, the technique has been used to mass-produce hydrogel microparticles with geometrical and chemical patterns. However, in the early version of SFL, the geometrical and chemical patterns in particles have been limited to 2D and 1D, respectively. Moreover, the technique has required gas permeable polydimethylsiloxane flow channels which are incompatible with many organic solvent flows. In this presentation, we introduce advanced stop flow lithography techniques that can address the aforementioned problems, and achieve much higher degree of geometrical and chemical complexity in particles than before.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT1-4**
발표분야: Recent Trends in Soft Nano/Micro Materials
발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 이상민

Protein-based Hybrid Colloidal Nanostructures for Theranostic Applications

남윤성

한국과학기술원(KAIST) 신소재공학과

In this talk I will introduce serum-stable hybrid nanocapsules of human serum albumin (HSA) cross-linked with six-arm-branched polyethylene glycol (PEG). The HSA/PEG hybrid nanocapsules are prepared by emulsifying an organic solution of amine-reactive six-arm-branched PEG into an aqueous solution of HSA. The successful formation of nanocapsules are kinetically determined by several processes: diffusion of PEG molecules out of the organic phase, adsorption of HSA onto the emulsion surfaces, and cross-linking reactions between PEG and HSA at the organic/aqueous interface. The nanocapsules are employed as in vivo delivery carriers for paclitaxel and inorganic nanocrystals. In several types of cells, the surface modification of nanocapsules with a cell-penetrating peptide or cancer-targeting molecule greatly facilitates cellular uptake and apoptosis-inducing effects of paclitaxel. Furthermore, the targeted anti-tumor activities of the paclitaxel-loaded nanocapsules in a mouse tumor model suggest that the shell cross-linked nanocapsules are very promising oil-free nanoscale delivery vehicles for water-insoluble anti-cancer agents. In addition, cadmium-free CuInS/ZnS quantum dots, and monodisperse iron oxide nanocrystals are encapsulated within the shell as an imaging probe. I will discuss physicochemical properties of the prepared hybrid nanocapsules in relation with their cytotoxicities and in vivo destinations. This study demonstrates that the HSA/PEG hybrid nanocapsules can be utilized as a biocompatible, cell-targeting platform for in vivo systemic delivery of various therapeutic and imaging agents.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT1-5**
발표분야: Recent Trends in Soft Nano/Micro Materials
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 이상민

Biogenic nanoparticles and their biomedical applications

박태정

중앙대학교 화학과

Some of the strategies found in natural science, especially in the normal metabolisms of microorganisms, are common and well-known examples of creating various types of inorganic materials that have great potential to further nanotechnologies. Many researches have been recently performed to provide fundamental understandings for synthetic formation processes of inorganic metal nanomaterials showing fluorescence and specific optic properties and magnetic affinities. In this symposium, we discuss the use of microorganisms for the synthesis of inorganic metal particles as a novel platform technology and describe different types of microorganisms for biosynthetic processes. The great advantages of this approach are non- and less-toxic to the cells, which are those by properly adopting the detoxification mechanisms of organisms. It can be synthesized the metal nanoparticles and rare nanoparticles at room temperature or simple condition, it is eco-friendly, it has low energy intensiveness, and it has high economic feasibility. This study crosses research boundaries between biology, chemistry, material science and nanotechnology, with the aim of accelerating the merging of different techniques to develop biosynthetic methods for the production of inorganic metal nanoparticles and to support their biomedical applications.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT2-1**

발표분야: Synthesis and Application of Exotic Nanoparticles

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 박성호

Toward molecular designing on nano-materials for catalytic applications

박성진

인하대학교 화학과

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

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-2**
발표분야: Synthesis and Application of Exotic Nanoparticles
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 박성호

Synthetic Approach to Controlled Assembly of Nanoparticles: Raspberry-like Metamolecules

박소정* **Zhaoxia QIan[1] Zahra Fahkraai[1] Chen Li[1] Nader Engheta[1]** 서명주

이화여자대학교 화학나노과학과 [1]University of Pennsylvania, USA

Here, we present a new synthetic approach to produce raspberry-like plasmonic nanostructures with unusually strong magnetic resonances. The synthesis is based on the surfactant-assisted templated seed-growth method, which allows for the simultaneous one-step synthesis and assembly of well-insulated gold nanoparticles. The aromatic surfactant used for the syntheses protected nanoparticles from touching each other and made it possible to place discrete nanoparticles at close distances, which are key requirements for the fabrication of metamolecules supporting magnetic resonances at optical frequencies. The resulting isotropic gold nanoparticle clusters, which are termed raspberry-like metamolecules (raspberry-MMs), exhibited unusually broadband surface plasmon resonance in the visible and near-IR region. A series of syntheses with varying structure parameters, along with finite-difference time-domain modeling and mode analyses of corresponding model structures showed that the close-packing of a large number of metal nanoparticles in raspberry-MMs is responsible for the unusually strong magnetic resonances and broad extinction spectra observed here.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-3**
발표분야: Synthesis and Application of Exotic Nanoparticles
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 박성호

Tailored Synthesis and Application of Anisotropic Nanomaterials

유효종

한림대학교 화학과

By using unique and efficient soft-templates, and changing reaction conditions controllably, we could synthesize interesting anisotropic nanomaterials. Solubilization of specific anions into an aqueous CTAB (cetyltrimethylammonium bromide) or CTAC (cetyltrimethylammonium chloride) solution led to the formation of rod-shaped micelles and became a key shape directing factor to generate one-dimensional Au structures. Through this strategy and seed-mediated methods, nanoscaled Au rods and Au bipyramids were synthesized. The structural factors of these metallic systems were effectively controlled by varying the amount of spherical gold nanoparticle seed or salicylate ion. We could also fabricate a variety of Au nanofibers in solution by adjusting CTAB or mixed surfactants of CTAB and Brij35. We show the syntheses of unique “Au Raspberry-Like Nanoparticles (Au RLNPs)” by use of nonionic Brij surfactants and “Star-shaped gold nanoparticles (Au SSNPs)” through a facile seed-mediated method using cetyltrimethylammonium bromide (CTAB), Brij35, Au seed nanoparticles, Ag^+ ions, ascorbic acid, and salicylic acid. In particular, it is noteworthy that the lengths of each branch of Au SSNPs were finely tuned by the change of molar ratio of surfactants, and salicylate ion. These are novel and simple synthetic approaches for generating anisotropic nanomaterials, which can be applied to a variety of areas such as catalysis.We also describe a facile method for the fabrication of Ni-based coordination polymer nanoparticles using modulators (e.g. acetic acid, benzoic acid, or pyridine) to control their size. The resultant coordination polymer nanoparticles were then calcinated at controlled temperature to produce porous nickel oxide (NiO) nanomaterial with high surface area. We successfully deposited NiO nanostructures onto an indium tin oxide (ITO) serving as an efficient matrix for the immobilization of urease (Ur) for urea detection. The prepared bioelectrode (Ur/NiO/ITO/glass) is successfully employed for urea sensing using amperometric techniques.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT2-4**

발표분야: Synthesis and Application of Exotic Nanoparticles

발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 박성호

Development of Effective Heterogeneous Sensors Based Upon FluorescentCoordination Polymer Particles

오문현

연세대학교 화학과

Heterogeneous sensors are considered as promising next-generation sensors due to their good chemical stability, low contamination, and recyclability, in spite of their low sensitivity and weak signal. Not only the excellent dispersity of solid sensors but also the signals from the outside of solid sensors are important features for the excellent sensing sensitivity and selectivity. Herein, we report the development of ideal solid sensors based upon fluorescent coordination polymer particles. Ideal heterogeneous solid sensors are achieved by constructing them in small, uniform, or thin core-shell particles. They displayed high sensitivity and outstanding recyclability for sensing events.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-5**
발표분야: Synthesis and Application of Exotic Nanoparticles
발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 박성호

Noble Metal Nanocrystals with Unprecedented Morphologies

한상우

한국과학기술원(KAIST) 화학과

The morphology of metal nanocrystals explicitly determines their plasmonic, electrical, and catalytic characteristics. In particular, the catalytic activity and selectivity of nanocrystals can be tuned by controlling their shape, because the exposed surfaces of nanocrystals have distinct crystallographic planes that can determine their overall catalytic properties. However, the control of the size, shape, and composition of NCs has been limited due to the complex kinetics in the reduction of cationic metal precursors and to the difficulty in finding suitable stabilizing agents. Therefore, the development of an efficient synthesis route for the preparation of nanocrystals with a specific morphology is still a radical issue to study their properties and applications. Here, facile wet-chemical synthetic processes of noble metal nanocrystals with unprecedented morphologies and their applications in catalysis are reported.

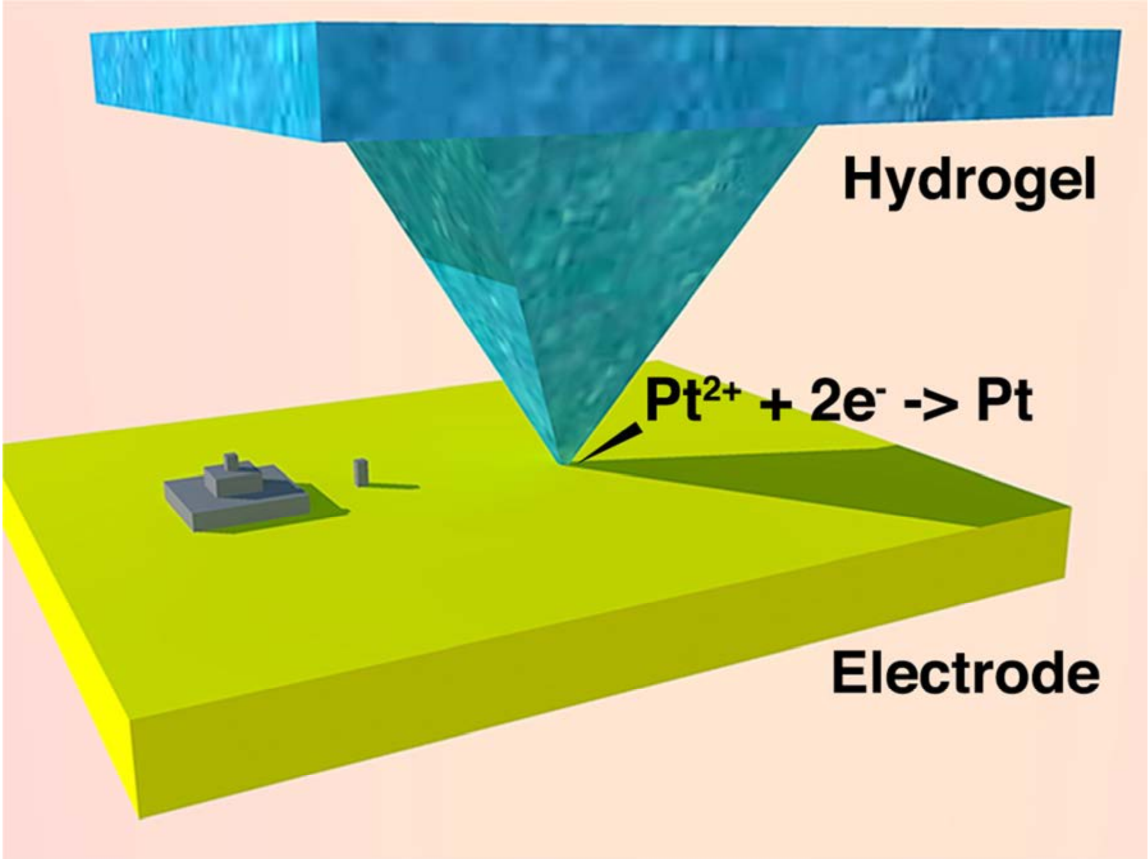
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC1-1**
발표분야: Recent Developments of Electrochemical Microdevices
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 장병용

Hydrogel Pen for Electrochemical Metal 3D Printing in Nanoscale

강호석 황성필[*] 곽주현[1,*]

고려대학교 신소재화학과 [1]한국과학기술원(KAIST) 화학과

Incorporation of chemical process to fabricate small devices is highly effective way due to its intrinsic properties to modify surface in molecular level. Among many chemical processes for surface modification in a small scale, electrochemical processes provides very accurate and effective way in small scale surface modification, which is crucial for fabrication of microdevice by both of additive and subtractive surface modification at an interface between electrolyte and conductive surface. In this presentation, extremely localized electrochemistry within nanometer area using a hydrogel pen for electrochemical reaction (HYPER) made of a microscopic pyramid containing electrolyte will be present. The hydrogel pen merges the fine control of atomic force microscopy and makes nanoscale contact area with macroscale working electrode, producing faradaic current that depends on the electroactive area. The theoretical and experimental investigations of the mass transport behavior within the hydrogel to establish a criteria for quantitative electrochemical reaction. The steady- state current from the faradaic reaction is linearly proportional to the deformed length of the hydrogel pen by contact, i.e. signal transduction of deformation to an electrochemical signal, which enables the fine control of the electroactive area in the nanometer-scale regime. Combined with electrodeposition, localized electrochemistry of the hydrogel pen results in the ability to fabricate small sizes (110 nm in diameter), tall heights (up to 30 μm), and arbitrary structures, thereby indicating an additive process in 3 dimensions by localized electrodeposition.


Hydrogel
$Pt^{2+} + 2e^{-} \rightarrow Pt$
Electrode

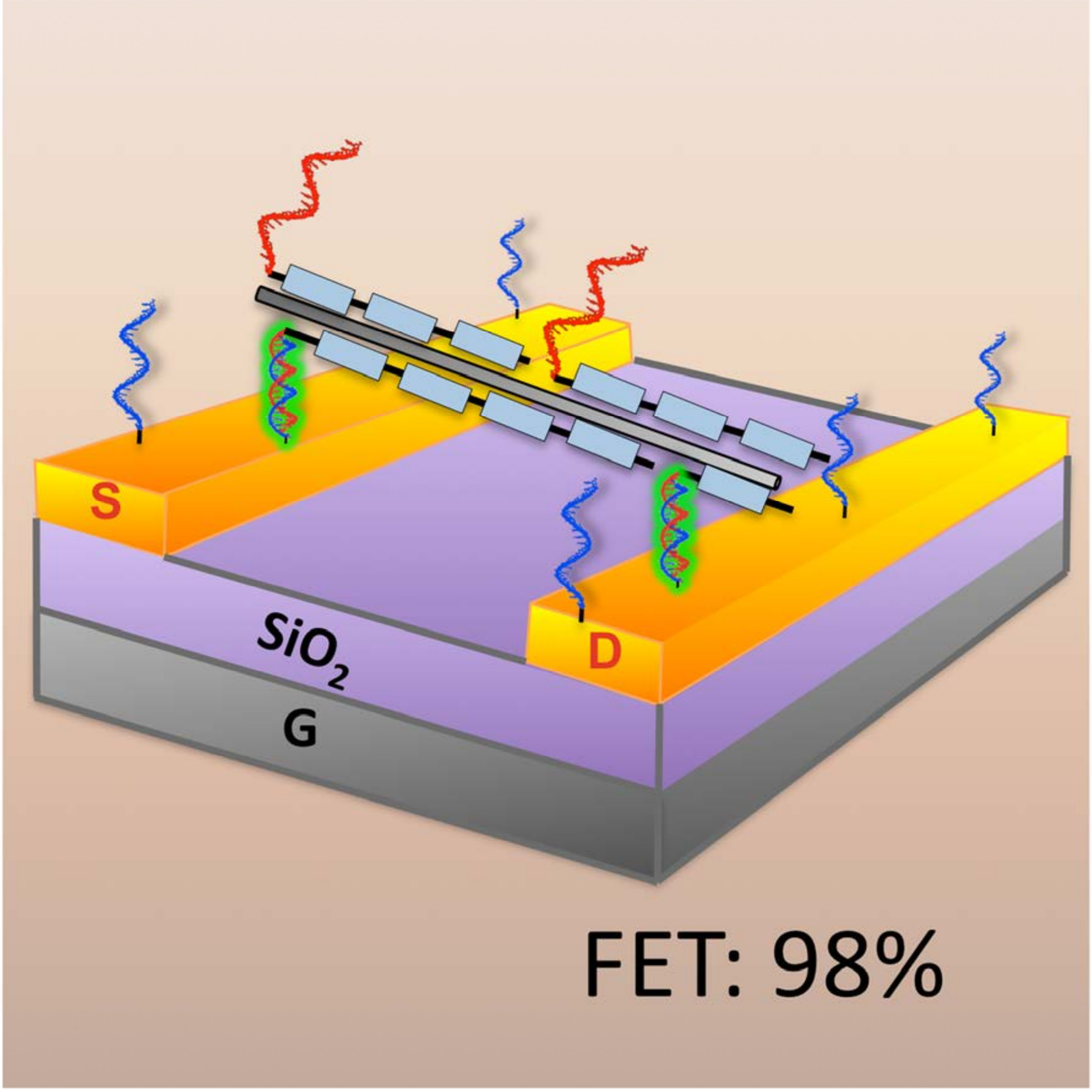
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC1-2**
발표분야: Recent Developments of Electrochemical Microdevices
발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 장병용

DNA-CNT Transistor: from Selection of Semiconducting Species to Self-Assembly onto Substrate Entirely through Solution Process

곽민석

부경대학교 화학과

This talk deals with utilization of DNA block copolymers (DBCs) with one of the most promising nanomaterials, single-walled carbon nanotube (SWNT), for eventual incorporation into practical technologies. So far the use of SWNTs is limited by difficulties in solubilizing and isolating individual species and precisely manipulating the structures while preserving their superb properties. Dispersing SWNT with DBC is a potentially scalable solution to these obstacles using DBCs consisting of a single-stranded DNA block covalently connected to a hydrophobic polymer segment. This combination of materials enables each to contribute its full potential ? self recognition and sorting semiconducting SWNTs, respectively ? to the utilization of SWNTs. It is demonstrated that one such hybrid is capable of the whole gamut of solution-based SWNT technologies, from selective dispersion to non-destructive functionalization to high-yield device fabrication such as field-effect transistors. These powerful applications are mediated by simple programmed DNA self assembly, opening the door to broader multidisciplinary materials research in the field of carbon nanotubes.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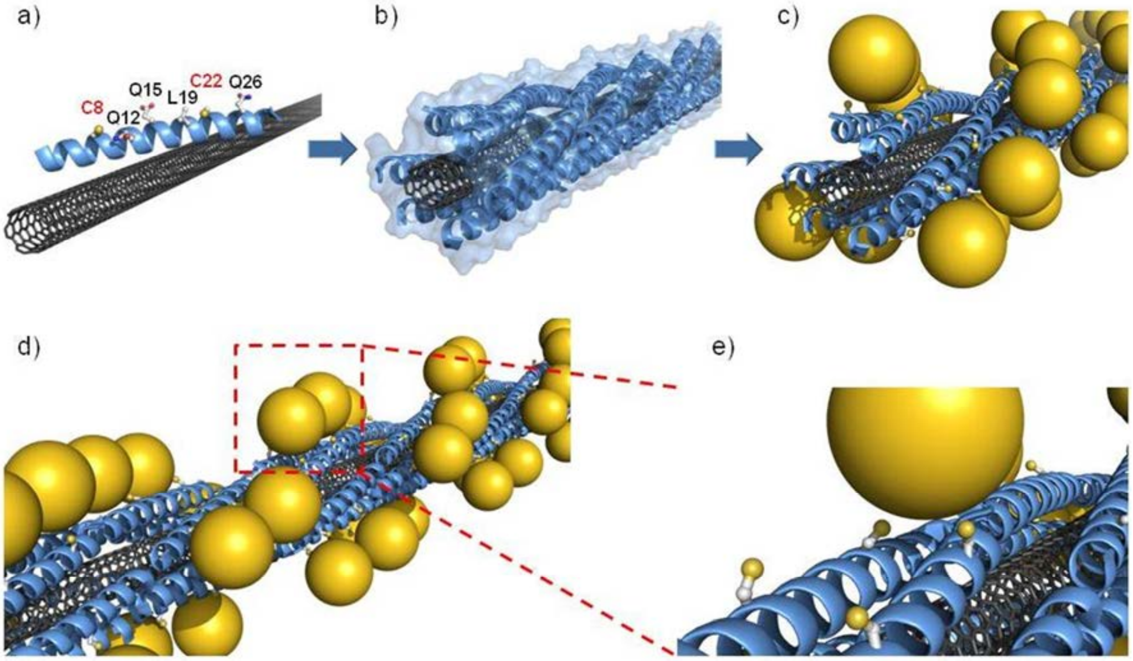
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC1-3**
발표분야: Recent Developments of Electrochemical Microdevices
발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 장병용

Design of peptide-based biomaterials for energy and biomedical devices

김용호

성균관대학교 자연과학대학/화학과, 성균나노과학기술

Protein-based biomaterial driven from biological principles of supramolecular protein assembly for energy application is a weighty mean of nanotechnological fabrication, achieving next generation energy devices. Here we demonstrate new design approach to engineer the protein-nanomaterial complexes using unique nanostructure of self-assembled peptides that would allow for the wrapping of single walled carbon nanotubes (SWNTs) with containing catalytic metal nanoparticles. For the purpose of enhancing catalytic activity of oxygen reduction reaction (ORR), we introduced the selection rule whereby precisely controlling the geometry and position of functionality within such superstructures constrains a variety of arrangement of bimetallic AuPt nanoclusters. The elected positions of functionality from the selection rule precisely alter their arrangement and density of catalytic nanoparticles and result in significantly improved ORR activity and durability. The remarkable electrochemical property of nanoparticle-protein-SWNT superstructures corresponding to controlling of interparticle distance, particle size and alloy composition of single-phase nanoparticles suggests a route to the construction of new functional protein materials tailored to unique energy applications.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일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC1-4**
발표분야: Recent Developments of Electrochemical Microdevices
발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 방진호

Electrochemical Sensors Integrated with Microfluidic Systems

조윤경

울산과학기술대학교(UNIST) 생명공학과

We present an electrochemical-sensor system integrated in microfluidic platform that monitors the liquid flow by recording an amperometric signal created by the solution movement. This approach allows the in-situ monitoring of flow rates. In the first example, the proposed method of electrochemical velocimetry is employed to accurately monitor flow on rotating microfluidic platform. On-disc flow rates, determined by electrochemical velocimetry, agreed well with theoretically expected values and with optical measurements. In addition, the electrochemical detection set-up integrated on the centrifugal microfluidic platforms were further employed to achieve flow-enhanced immunoassay detection sensitivity. Furthermore, the similar electrochemical velocimetry was used to monitor the flow in porous materials, which is critical for the engineering of paper-based microfluidic bioassays. This approach allows the in situ monitoring of the different hydrodynamic conditions depending upon specific paper composition or geometry. As a proof of concept demonstration, the electrochemical velocimetry was used to characterize the flow behavior of different nitrocellulose paper strips depending upon different surface treatment of the paper materials. In conclusion, we believe the proposed electrochemical method offers a valuable alternative to existing optical-based detection method for flow measurements either in centrifugal or paper-based microfluidic systems.

References
[1] K. Abi-Samra et al. Lab. Chip.,13, 3253-3260, 2013
[2] T. Kim et al, Lab Chip, 13, 3747-3754, 2013

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC1-5**
발표분야: Recent Developments of Electrochemical Microdevices
발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 방진호

Micro/Nanoscale Electrodes for Photoelectrochemical Water Splitting

이민형

경희대학교 응용화학과

Due to the increasing concerns about environmental issues associated with fossil fuel consumption increase, hydrogen has drawn great interest as an alternative energy source because it is a sustainable and green fuel without producing harmful byproducts after combustion. Photoelectrochemical (PEC) water splitting have been considered as most clean and simple way to produce hydrogen compared to other methods. However, the solar-to-hydrogen (STH) conversion efficiency is still very far from industrial demand, because it is very difficult to fulfill the all requirements for highly efficient PEC cells (i.e. high VIS absorption, long-term stability, and fast kinetics). In this talk, we will report our recent efforts to enhance STH conversion efficiency by designing micro/nanoscale electrodes with synergistic effect of combining optimized design, oxide passivation, and cocatalyst.

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발표분야: Recent Developments of Electrochemical Microdevices
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의료용 펌프로 적용 가능한 전기삼투펌프의 개발

신운섭

서강대학교 화학과

전기삼투펌프는 다공성막과 양단의 다공성전극으로 구성된 가장 간단한 펌프로서 전기화학자에게는 친숙한 MEA 시스템인데, 그 동안 기계공학자, 유체역학자들에 의해 주로 연구되어 왔고 전기화학적 관점에서의 접근은 거의 이루어진 바 없다. 전극은 전압을 거는 도구로만 고려되었지 이에 따른 전기화학반응은 크게 고려된 바 없었다. 본 연구진은 전기삼투펌프의 전극반응을 바꿈으로 그 동안 백금전극 사용으로 인한 물분해 반응 등 제기되었던 문제를 일시에 해결하였고 효율적인 시스템 구성을 가능케 하여 실제적인 소형펌프로서 응용 가능함을 보여준 바 있다. 이러한 신개념전기삼투펌프를 활용한 인슐린펌프, 체내이식형 펌프로의 적용 및 개발 현황을 본 발표를 통해 보여주고자 한다.

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장소: 일산 KINTEX

발표코드: **ELEC2-1**

발표분야: Electrochemical Research Using Functionalized Electrodes

발표종류: 심포지엄, 발표일시: 목 13:35, 좌장: 신재호

Improving Amperometric Biosensing Platforms with Nanoparticles and Liquid/liquid Interfaces

이혜진

경북대학교 화학과

In this talk we will highlight our latest efforts to develop highly sensitive and selective amperometric biosensors for protein biomarkers and environmentally toxic reagents. Two different types of biosensing platforms will be presented: (i) a platform utilizing surface enzyme reactions and various biofunctionalized nanoparticles in conjunction with the formation of surface sandwich complexes. (ii) A sensor based on ion transfer reactions across a polarized water/organic gel layer interface. For example, a novel surface sandwich bioaffinity assay in conjunction with aptamer functionalized Au nanoparticles deposited onto carbon electrodes and an antibody-alkaline phosphatase conjugate was developed for the detection of protein biomarkers. This approach was successfully applied to detect 100 fM concentrations of proteins in serum as well as in buffer samples. Another example is to utilize the layer by layer assembly of Au nanoparticles onto carbon electrodes followed by the attachment of tyrosinase for the sensitive detection of catechol and phenol. Finally, a single micro-hole on a thin polymer substrate interfacing a water and gelified polymeric organic phase was fabricated for sensing applications. Voltammetric responses for the transfer of Cu(II) ions and anticancer drug molecules across the polarized microhole supported interface was characterized and the currents associated with the ion transfer reaction was used to develop highly sensitive and selective amperometric sensors.

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발표코드: **ELEC2-2**
발표분야: Electrochemical Research Using Functionalized Electrodes
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 신재호

Application of Conducting Polymer Modified Electrodes for Electrochemical Detection of Dopamine

이재준

건국대학교 응용화학과

Interference-free detection of dopamine (DA) was studied by using conducting poly(thionine) (PTH) films which could be prepared in two different ways onto the glassy carbon electrode (GCE). The sensitivity of the DA detection is significantly dependent on the polymerization condition on a substrate and it was analyzed to interpret the cause of the sensitivity variation. A simple variation of electropolymerization conditions dramatically changed the PTH formation mechanism and the catalytic activity of the PTH films towards the oxidation of DA in the presence of ascorbic acid (AA) and uric acid (UA). The variation of the accumulated surface charge of the PTH films possibly corroborated the signal suppression and/or the separation of electrochemical response of AA and UA with respect to that of DA. The interaction mechanism of DA, AA, and UA at PTH films was also investigated in terms of the variations of the pH of phosphate buffer solutions (PBS). Similar effect was also expected for the functionalized low-dimensional carbon based electrode surface.

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발표분야: Electrochemical Research Using Functionalized Electrodes
발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 신재호

Electrochemical control of organic ion transport through a conducting polymer modified membrane and its selectivity for the ions

PIAOHUSHAN 손용근*

성균관대학교 화학과

Studies for separating a mixture of inorganic ions including heavy metals into components by using a conducting polymer membrane (CPM) system have been published well. However, studies about organic ion separations with the CPM system were hardly found even though organic ions are used in so many fields. Because comparing with the inorganic ions, organic ions have more complex characters which affect their transport property. Thus, transport of organic ions under a certain condition should be studied on a case by case basis. In this study, we investigated the transport phenomenon of two organic ions which are different in specific adsorption property with the CPM under different applied potentials and demonstrated their transport mechanism in detail. Benzylamine (BA) and Methylene blue (MB) were chosen as the transporting ions and the experimental results showed that their transport tendency were different from each other under same potential condition. Thus, the transport mechanism of each ion was demonstrated in detail. In addition, we compared the transport property of BA to that of MB under a negative applied potential and suggested a possibility that organic ions could be separated based on the membrane selectivity. This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy(No. 2010501010002B)

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발표분야: Electrochemical Research Using Functionalized Electrodes
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 권성중

Preparation of functionalized electrode materials through novel thermal treatment process

박원철

서울대학교 융합과학기술대학원 나노융합학과

In this presentation, the preparation of various functionalized electrode materials through novel thermal treatment processes is introduced. (I) Through a simple heating procedure using a single precursor for both carbon and metal oxide, self-assembled and uniform-sized metal oxide nanocrystals embedded carbon nanosheets were synthesized simultaneously. The shape and size of the nanoparticles decorated on carbon could be easily controlled by changing the experimental conditions. As a demonstration of the nanocomposite as anode material for Lithium-ion battery, electrochemical experiments were carried out in a coin type cell assembly. The nanocomposite electrodes exhibited large power capability with good cycling stability. The superior performance of the nanomaterial is due to its short diffusion path and large accessible surface area for the effective insertion of lithium ions. (II) Our recent advances in the preparation of graphene based nanocomposite materials as well as their applications as electrode materials for electrochemical energy storage devices are also introduced.

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발표분야: Electrochemical Research Using Functionalized Electrodes
발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 권성중

Improving the microstructure and electrochemical performance ofcarbon nanofibers containing graphene-wrapped silicon nanoparticlesas a Li-ion battery anode

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대구대학교 과학교육학부 [1]전남대학교 고분자 섬유 시스템공학과

A novel anode material for lithium-ion batteries, graphene-wrapped Si nanoparticles (NPs) embedded incarbon composite nanofibers (CCNFs) with G/Si, is fabricated by electrospinning and subsequent thermaltreatment. In CCNFs with G/Si, Si NPs are distributed and preserved inside the CNF surface because thegraphene wrapping the Si NPs help prevent agglomeration and ensure a good dispersion of Si NPs insidethe CNF matrix. 20-GSP prepared from a weight ratio of 20 wt% of G/Si to polyacrylonitrile exhibits stablecapacity retention and a reversible capacity of above 600 mAh g————————————1 up to 100 cycles. The high cyclingperformance and superior reversible capacity of the 20-GSP anode can be attributed to the onedimensionalnanofibrous structure with non-agglomerated Si NPs in the CNF matrix, which promotescharge transfer, maintains a stable electrical contact, and buffers the Si volume expansion.

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발표분야: Electrochemical Research Using Functionalized Electrodes

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 권성중

Direct electro-deposition of metal catalysts on functionalized insulators

이진영 이재경 신재호 정택동*

서울대학교 화학부

Electrochemistry on a dielectric-layer-modified electrode has a potential to provide new insight and application. Highly n-doped silicon electrode (n^+-Si) was modified with 6-nm-thick thermal silicon oxide (SiO_2), which is one of the dielectric materials used as gate insulators. Si electrode modified with thermal SiO_2 has been known to bring hydrogen-atom-mediated electrochemistry . Several kinds of catalysts are electrodeposited on thermal SiO_2, inert supports, by constant potential method. In order to improve affinity between metal catalysts and supports, amine-terminated thermal SiO_2 was introduced by silanization. Electrodeposited Palladium (Pd) nanoparticles are more disperse on amine-terminated thermal SiO_2 compared to the bare thermal SiO_2, looking like grains consisting of numerous small particles. Herein, it is also demonstrated that other bimetallic catalysts can be directly deposited on amine-terminated SiO_2/n+-Si electrode by a simple electrochemical method. Direct electro-deposition of metal catalysts on inert supports such as SiO_2 can be expected to simplify the manufacture of chemical and biological sensors as well as that of oxide-supported metal catalysts.

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발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 강석진

2015 개정 과학/화학 교육과정의 지향 및 개발

박현주[*] 김명화[1,*] 최중철[2,*] 김현정[3,*] 김현경[4,*] 현종오[5,*] 방담이[6,*] 전화영[7,*] 박상희[8,*]

조선대학교 과학교육학부 [1]이화여자대학교 화학 나노과학과 [2]동국대학교 화학과 [3]한국교육과정평가원 대학수학능력시험본부 [4]한국교육과정평가원 교육평가본부 [5]월계고등학교 [6]가톨릭대학교 ELP학부대학 [7]경복고등학교 자연과학부 [8]인천청량초등학교 교무부

2015 개정 교육과정은 학교교육을 통해 모든 학생들이 인문·사회·과학기술에 대한 기초 소양을 함양하여 인문학적 상상력과 과학기술 창조력을 갖춘 창의융합형 인재로 성장할 수 있도록 우리 교육을 근본적으로 개혁하고자 하는 것이다. 많이 가르치는 교육에서 배움을 즐기는 '행복 교육'으로 교육 패러다임의 전환을 기본으로 한다. 2015 개정 교육과정의 기본 원칙은 인문·사회·과학기술적 기초 소양 함양을 위한 교육 강화, 학생의 꿈과 끼를 키우는 교육, 미래 사회가 요구하는 역량 함양이 가능한 교과 교육, 교육과정과 연계하여 교육정책 전반을 종합적으로 개선이다. 이에 따른 총론 개정의 주요 방향은 미래 사회를 대비하는 교육 방향 제시하고, 현행 교육과정의 연속성 유지하고 개선점을 모색하며, 학생의 꿈과 끼를 키우는 교육과정을 개발하는 것이다. 과학기술 소양의 함양 교육을 강화하는 방안으로, 자연현상에 대한 통합적인 접근과 융·복합적 사고가 가능하도록 대주제(Big Idea) 중심의 고교 '통합과학' 과목을 신설하였다. 초·중등학교의 물질 및 고등학교의 화학과 교육과정의 개발 방향은 2009 과학/화학과 교육과정의 내용을 기본으로, 기존 교육과정에 대한 현장 교사의 의견을 수렴하여 반영하고, 화학의 핵심 개념과 필수 개념을 검토하고, 학습자의 수준 및 과학의 다른 분야와의 통합의 가능성을 고려하여 개발하였다.

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2015 개정 과학과 교육과정: 초등학교 과학 물질 영역

장신호

서울교육대학교 과학교육과

본 연구는 의 시안을 개발하여, 초등학생들이 과학의 개념을 통합적으로 이해하고 과학 탐구 실행 능력과 태도를 함양하여 일상생활의 문제를 과학적이고 창의적으로 해결하는 데 필요한 과학적 소양을 기르기 위한 성취기준과 내용목표를 구성하는 것을 목적으로 한다. 2009 과학과 교육과정을 기준으로, 새로 개정해야 할 내용들은 최근 수행되었던 교육과정 분석연구, 교과서 비교연구, 문이과 통합형 교육과정 연구 결과 및 현장교사들의 의견 등을 참고하여 개정하고자 하였다. 이 세션에서는 2009 교육과정과 비교하여 새롭게 변화되거나 개정되는 내용을 중심으로 발표하고자 하며, 본 연구를 통한 초등학교 과학 물질 영역 교육과정의 전체적인 개정의 방향은 다음과 같다. 초등학교 ‘물질’ 영역은 초등학교 1, 2 학년의 슬기로운 생활, 중학교 ‘물질’과 긴밀한 연계를 가지도록 구성하며, 물질의 기본개념을 통합적으로 구성하고 기본 개념과 과학 탐구 실행이 학년 및 영역 간에 연계되도록 한다. 분과적이고 단편적인 지식의 획득보다는 기본 개념의 통합적인 이해를 토대로 일상생활의 문제를 과학적으로 해결하는 능력을 함양하도록 한다. 개념의 통합적 이해, 과학탐구실행을 통하여 정보활용능력, 비판적 사고력, 의사소통능력, 문제해결력, 개인적·사회적 책무성, 진로개발 능력 등의 핵심역량을 함양하도록 한다. 초등학교 ‘물질’의 주요 개념을 학습자의 경험과 밀접한 관련이 있는 상황에서 지도하고, 학습한 지식과 탐구 방법을 일상생활이나 사회 문제 해결에 적용할 수 있는 기회를 제공함으로써 과학의 가치뿐만 아니라 과학, 기술, 사회의 상호 관계를 인식할 수 있도록 한다. 이러한 개정의 방향을 바탕으로 물질 영역의 세부 개정 내용을 발표하고, 이를 통해 미래 과학교육의 방향과 교육적 시사점을 논의하고자 한다.

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2015 개정 과학과 교육과정: 중학교 과학 물질 영역

김현정

한국교육과정평가원 대학수학능력시험본부

미래사회가 필요로 하는 창의 융합형 인재의 육성을 위하여 문 이과 통합형 교육과정과 창조경제 사회에 적합한 핵심역량 중심의 과학과 교육과정으로의 개정이 필요하다. 이에 개정되는 과학과 교육과정의 방향은 문과와 이과 분야의 균형 잡힌 소양과 역량을 갖춘 미래시민을 양성하는 기초가 되는 교육과정으로 물리 화학 생명 과학 지구 과학의 분과적인 구분을 넘어서 통합원리를 중심으로 재구조화하려 한다. 구체적으로 중학교 과학 교육과정의 경우 교육 내용 적정화를 위해 중학교 과학 교과의 핵심 개념과 중학교 학습자에의 적절성 등을 준거로 질적인 접근을 통해 실질적인 내용을 감축하고, 학년별로 통합 단원을 구성하여 통합원리를 중심으로 연관된 개념을 통합하여 내용의 중복을 방지하고 연계성을 강화하도록 하고 있다. 또한 중학교 과학 교육과정의 성취기준은 교과의 핵심개념과 기능을 반영하여 구체화하며, 학생 수행을 중심으로 진술하는 방향으로 개발되고 있다. 현재 구성되어있는 중학교 과학 교육과정 안은 2009 개정 과학과 교육과정의 내용 요소를 바탕으로 과학 교과 핵심 개념과 학습자에의 적절성을 중심으로 내용을 감축하는 방향으로 개발되었으며, 학년마다 과학 전 교과가 통합 원리를 바탕으로 통합 단원을 구성하였다. 2009 개정 과학과 교육과정과 비교하여 변화되는 내용은 구체적인 성취기준을 통해 파악할 수 있으며, 2009 개정 과학과 교육과정의 현장 의견과 검토를 통해 변화 내용이 결정되었다. 변화되는 내용은 2009 개정 교육과정부터 고등학교에서 중학교 3 학년으로 내려온 여러 가지 화학 반응 단원의 고등학교 통합과학으로 이동하고, 중학교 2 학년의 혼합물의 분리 단원의 혼합물의 분리의 예를 성취기준으로 구체적으로 분리하여 학습량을 감축하도록 하였으며, 중학교 2 학년에서 구체적으로 배우는 앙금생성반응을 중학교 3 학년의 화학반응의 규칙성의 반응의 예로 포함하고, 학년별로 통합 단원이 구성되는 등의 변화가 나타날 예정이다. 이에 개발중인 중학교 과학 물질 영역의 구체적인

내용을 발표하고, 이를 통해 중학교 1, 2, 3 학년의 내용 적정화, 단원 위계, 단원 제목들의 적절성, 핵심개념 등에 대한 다양한 의견을 수렴하고자 한다.

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2015 개정 과학과 교육과정 '통합과학' 성격 및 내용

<u>전화영</u>

경복고등학교 자연과학부

2015 개정 과학과 교육과정의 ‘통합과학’은 고등학생의 미래 진로 및 진학 경로와 무관하게 모든 학생들이 반드시 이수해야 하는 필수과목으로서, 과학탐구 시험의 대상 과목이다. 통합과학은 자연 현상을 통합적으로 이해하고, 이를 기반으로 자연 현상과 인간의 관계, 과학기술의 발달과 미래 생활 예측과 적응, 사회문제에 대한 합리적 판단 능력 등 미래 사회에 필요한 과학적 소양 함양을 위한 과목이다. 따라서 교과목의 초점은 학생들에게 과학에 대한 통합적 이해를 바탕으로 우리주변의 자연 현상과 현대사회의 문제에 대한 스스로의 이해를 추구하고 합리적 판단을 할 수 있는 민주시민으로서의 기초 소양을 기르는 데에 주어진다. 최근 미국의 NGSS 및 기타 선진국들의 과학 교육과정에서 강조되고 있는 과학의 통합적 이해를 위한 통합개념을 새로운 과학과 교육과정의 내용 영역을 구성하는 핵심 축의 하나로 도입한다. 이러한 통합개념은 물/화/생/지의 학문분야에 따라 파편화된 지식과 이해를 넘어서는 과학에 대한 통합적이고 유기적인 이해를 돕기 위한 것으로 ‘물질과 규칙성’, ‘시스템과 상호작용’, ‘다양성과 변화’, ‘에너지와 환경’으로 구성되었다. 이 중 화학은 ‘물질과 규칙성’ 단원에 주기율과 화학 결합, ‘다양성과 변화’ 단원에 산화와 환원, 중화 반응을 포함한다. 또한 ‘에너지와 환경’ 단원에서는 화석연료의 연소 및 연료 전지 관련 내용을 포함하여 구성한다.

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2015 개정 과학과 교육과정: 고등학교 화학I

현종오

중경고등학교 수학과학부

2015 개정 과학과 교육과정의 ‘화학Ⅰ’은 통합과학을 이수한 학생들을 대상으로, 우리 생활과 밀접하게 관련된 물질 및 현상들의 탐구를 통해 화학 기본의 개념을 이해하고, 과학 탐구 실행 능력과 태도를 함양하여 일상생활의 문제를 과학적이고 창의적으로 해결하는 데 필요한 과학적 소양을 기르기 위한 교과이다. ‘화학Ⅰ’은 통합과학에 포함된 화학의 기초 개념의 확장을 위해 다양한 물질 및 현상에 대해 관찰, 실험, 조사, 토의 등 다양한 탐구 실행 중심의 학습으로 제공된다. 화학의 기본 개념을 학습자의 경험과 밀접한 관련이 있는 상황에서 학습하고, 학습한 지식과 탐구 방법을 일상생활이나 사회 문제 해결에 적용할 수 있는 기회를 제공함으로써 과학의 가치뿐만 아니라 과학, 기술, 사회의 상호 관계를 인식할 수 있도록 한다. ‘화학Ⅰ’의 내용은 통합과학에 포함된 화학 개념과 긴밀한 연계를 가지고, 원소와 주기율, 화합물과 화학 결합, 산화와 환원, 산과 염기, 발열반응과 흡열반응 등을 보다 심층적으로 이해하는데 유용한 화학적 개념을 포함한다. ‘화학Ⅰ’의 내용은 화학의 유용성, 화학 반응의 양적 관계, 물질의 구성 입자, 화학 결합, 화학 반응 등의 화학의 기초 개념을 이해할 수 있도록 구성한다. 또한 화학적 현상과 물질의 성질에 대한 관찰과 실험 연구, 모형과 구조를 활용하여 현상을 해석·설명하며, 화학 기호와 모형 등으로 현상을 이해하는 과정으로 구성한다. ‘화학Ⅰ’을 통하여 화학 기본 개념의 이해, 과학 탐구 실행을 통하여 정보 활용 능력, 비판적 사고력, 의사소통 능력, 문제해결력, 개인적·사회적 책무성, 진로개발 능력 등의 핵심역량을 함양하도록 한다.

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2015 개정 과학과 교육과정: 고등학교 화학Ⅱ

김현경

한국교육과정평가원 교육평가본부

본 연구는 ‘2015 과학과 교육과정 개정을 위한 시안 개발 연구’의 일환으로, 고등학교 화학Ⅱ 교육과정의 성격 및 목표 진술과 내용 요소 및 성취기준 등을 개발하는 것을 목적으로 한다. 2015 교육과정 총론 주요사항 발표에서 고등학교 과학 교과의 경우 모든 고등학생이 필수 공통으로 이수할 통합과학을 개설하기로 하였고 선택과목 군으로 일반선택과 진로선택 과목 군을 구분하여 개설하는 것으로 발표가 되었다. 일반 선택 과목 군에는 물리학Ⅰ, 화학Ⅰ, 생명과학Ⅰ, 지구과학Ⅰ으로 구성되어 있으며 각 교과별 학문의 기본적인 이해를 바탕으로 한 과목으로 수능 대상 과목으로 권장이 되는 교과 군이다. 진로선택 과목 군에는 교과 융합 학습, 진로 안내 학습, 교과별 심화 학습, 실생활 체험 학습 등이 가능한 과목으로 정의가 되어 있어 물리학Ⅱ, 화학Ⅱ, 생명과학Ⅱ, 지구과학Ⅱ, 과학사, 생활과 과학, 융합과학이 포함되어 있으며, 여기에 생태와 환경 교과를 추가하여 개발할 예정이다. 이들 교과의 기본 이수 단위는 과목별 특성을 고려하여 다양하게 설정할 것으로 제안되었다. 특히 2015 개정 교육과정은 학교교육을 통해 모든 학생들이 인문-사회-과학기술에 대한 기초 소양을 함양하여 인문학적 상상력과 과학기술 창조력을 갖춘 창의융합형 인재로 성장할 수 있도록 하기 위해 진로선택 교과 군에 포함된 각 Ⅱ과목은 이공계 진학을 목적으로 하는 학생 대상 교과목으로, 기타 교과목은 인문계 학생들이 선택할 수 있는 교과목의 성격을 갖도록 총론에서 제시하고 있다. 현재까지의 화학Ⅱ 과목은 화학Ⅰ 과목에서 학습한 개념을 바탕으로 이공계 진학을 할 학생을 대상으로 하는 교과로서 학업의 부담이 과중하지 않는 한도에서 심도 있는 개념을 다루고자 한다. 이러한 개정의 방향을 바탕으로 화학Ⅱ 교육과정의 내용 요소를 추출하고, 성취기준은 핵심개념과 기능을 반영하고 구체화시켜 학생 수행을 중심으로 진술하는 방향으로 개발되고 있다. 이에 개발된 화학Ⅱ 교육과정의 내용 요소 및 성취 기준 등과 같은 세부 개정 내용을 발표하고,

이를 통해 구체적인 개선 방안에 대한 의견을 수렴하고 미래 화학 교육의 방향과 교육적 시사점을 논의하고자 한다.

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발표분야: Environmental Implication of Nanomaterials
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이승학

Development of a new detection method for carbon nanotube contamination in water

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Carbon nanotubes possess unique properties that have led to an increase in research in a wide variety of fields. This growing demand and use of carbon nanotubes poses a potential health risk and may have detrimental effects in the environment. There is a significant gap of information of the actual quantity of carbon nanotubes in the environment. However the detection methods that are specific to carbon nanotubes are very limited mainly due to the ubiquitous carbon chemistry of carbon nanotubes. In response to these deficiencies, a novel method that utilizes a structural differentiation of carbon nanotubes was developed for carbon nanotube detection in water. The specific affinity between single walled nanotubes (SWNT) and G/T alternating ssDNA was employed to capture SWNT in water. A rapid, SWNT-specific separation was obtained by the use of magnetic field. Dual fluorescent labels that are attached to sandwich ssDNA probes were used for the precise quantification. A calibration curve (r2 = 0.90) was successfully made using a range of SWNT concentration against the planar graphene that was used as a negative control. The findings of this research suggest that this method is of great sensitivity and specificity for carbon nanotube detection in aqueous environment.

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Analysis of nanoparticles in environmental samples

이병태

광주과학기술원(GIST) 환경공학부

The measurement and characterization of nanoparticles in the environmental and biological samples are essential to understand the fate, behavior, and potential toxicity of nanoparticles. Single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) is a promising technique that has the potential to determined particle size, number concentration, and aggregataion state in environmental samples at environmentally relevant low concentrations (ng/L) . The samples containing particles in a short period of time (dwell time) can be analyzed by SP-ICP-MS and converted to the particle number-based size and concentrations . It was applied to predict the aggregation structure of nanoparticles in water samples. The mass of an aggregates measured by SP-ICP-MS calculated the number of the primary(single) nanoparticle in an aggregates. The dispersed nanoparticles in the environmental waters (e.g., tap water, river water, and municipal waste waters) and biological tissues (e.g., chicken breast and Daphnia) were also determined by measuring mass concentrations and nano range sizes.

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환경 중 제조나노물질의 거동 연구 (Environmental fate and transport of engineered nanomaterials)

황유식

안전성 평가연구소 미래환경연구센터

최근 급속한 나노기술 발전과 더불어 나노물질이 가지는 인체 및 환경위해성에 관한 관심과 우려가 증대되고 있는 실정이다. 이에 EU 및 미국 등의 주요 선진국을 중심으로 나노물질 및 제품에 대한 본격적인 규제화의 움직임이 있으며, 최근의 연구동향을 살펴보면 초기 단편적인 나노물질의 물성 및 독성 평가 중심에서 점차 인체 및 생태계를 고려한 위해성 평가 및 관리 중심으로 전환되고 있는 상황이다. 이에 본 발표에서는 나노물질 노출 및 위해성 평가에서 매우 중요한 역할을 하는 환경 중 나노물질의 주요 거동 현상들을 소개하고자 한다. 특히 나노물질의 경우 환경으로 노출 후 다양한 환경인자들에 의해 물리화학적 특성이 완전히 다른 물질로 쉽게 변화 될 수 있다. 이에 실제 환경조건에서 일어날 수 있는 나노물질의 응집(home- and hetero-aggregation), 용해(dissolution), 표면변환(surface transformation) 등 주요 변환반응에 대한 최신 연구결과들을 발표하고 이러한 변환과정들이 궁극적으로 그들의 위해성에 어떤 영향을 미칠 것인지를 발표하고자 한다. 본 연구결과들은 환경 중 나노물질의 존재형태를 규명하는데 큰 도움을 줄 뿐만 아니라 환경 중 나노물질의 분석기술 개발 및 노출평가에 중요한 정보를 제공할 것이다.

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장소: 일산 KINTEX

발표코드: **ENVR1-4**

발표분야: Environmental Implication of Nanomaterials

발표종류: 심포지엄, 발표일시: 목 10:35, 좌장: 이승학

Nanoinformatics for the study of environmental implications of nanomaterials

윤태현

한양대학교 화학과

Nanomaterials are known to have very unique physicochemical properties, biological toxicities, and environmental implications.. However, due to the ever-increasing numbers of novel nanoparticles (NPs) and related consumer products, toxicity assessment and environmental implication studies of all these novel NPs are still limited. Therefore, systematic categorization (or grouping) of NPs as well as computational nanoinformatics approaches are considered as promising alternatives for the efficient assessment of NPs' environmental implications and screening those NPs with higher potential hazards for further toxicity tests. In this presentation, current status of nanoinformatics studies in EU, USA, as well as Korea will be introduced. Particularly, I will present current progress and future direction of nanoinformatics project in Korea (a.k.a. S2NANO:QNTR, funded by Korean MOTIE).

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발표코드: **ENVR1-5**
발표분야: Environmental Implication of Nanomaterials
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 이승학

Transport and Retention Behaviors of Zinc Oxide Nanoparticles in Saturated Porous Media: Role of Biofilm, Ionic Strength and pH

한요셉 황국화 김동현 최시영[1] 이병천[2] 김현중[*]

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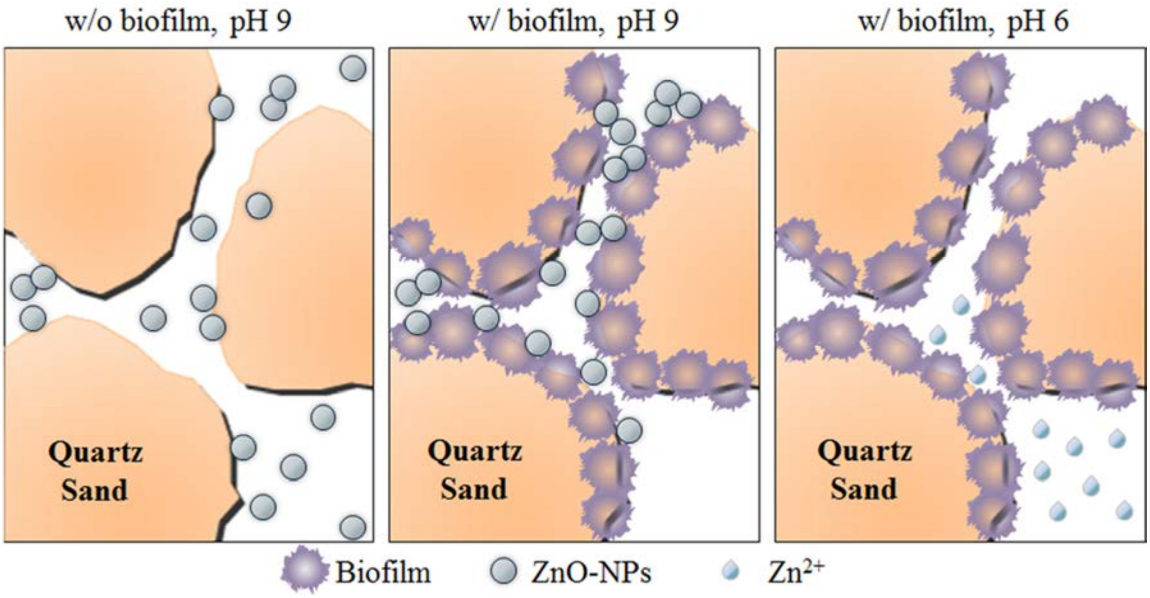
We investigated the initial-post transport and retention behavior of zinc oxide nanoparticles (ZnO-NPs) in saturated quartz sand porous media coated with biofilm. The initial transport of the ZnO-NPs in a solution of pH 9 showed significant retention at the inlet of the column with hyper-exponential retention profiles regardless of the solution ionic strength investigated and biofilm coating. However, increasing the solution ionic strength and biofilm coating led to the enhanced retention of ZnO-NPs in a column, resulting from more favorable NPs-NPs interaction and greater surface roughness, respectively. This was supported by DLVO interaction energy profiles and Electron Microscopic observations. Meanwhile, breakthrough curves and time-lapse retention profiles were obtained from a series of post-transport tests. After continuous long-term injection of pH 6 solution without added ZnO-NPs through the NPs retained in the column after the initial transport, the reducing solution pH largely released the initially retained NPs more rapidly on the bare silica. This eventually led to nearly complete transport regardless of the presence of the biofilms. We attribute this post-transport to the dissolution of Zn due to the change of pH, because ZnO is well-known to be soluble in this pH. We verified this hypothesis by conducting additional column tests of post-transport behaviors with different pHs, which showed significantly reduced post-transport, and even nearly no post-transport at pH 10. Our study suggests that since the pH of various soil environments typically ranges from 5 to 9, long-term transport of ZnO-NPs would eventually lead to the complete transport of toxic Zn ions into groundwater, even without sign of ZnO-NPs dissolution or Zn transport during the initial stage.


w/o biofilm, pH 9
w/ biofilm, pH 9
w/ biofilm, pH 6
Quartz Sand
Quartz Sand
Quartz Sand
Biofilm
ZnO-NPs
Zn^{2+}

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발표코드: **ENVR1-6**

발표분야: Environmental Implication of Nanomaterials

발표종류: 심포지엄, 발표일시: 목 11:25, 좌장: 이승학

Visual evidence of trophic transfer of nanopaticles using bio-imaging

안윤주

건국대학교 보건환경과학과

Nanoparticles have a range of applications. They can be accumulated in ecological biota and delivered to other organisms via food chain. This study investigated trophic transfer of fluorescent nanoparticles, quantum dots (QDs). With bio-imaging technique, we visually and quantitatively proved that quantum dots (QDs) from low-level to high-level organisms in the food chain using intravital multi-photon laser scanning microscope. Bioaccumulation was also observed in the higher trophic levels. This study has implications for safe use of nanoparticles. Acknowledgement-This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and future Planning (NRF-2014R1A2A1A11050513)

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발표코드: **ENVR2-1**

발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 한영수

Reductive transformation of tetrachloroethene by substitution of H_2O in aqua-cobalamin by sulfide in nano-mackinawite suspensions

최경훈

충남대학교 환경공학과

Persistent chlorinated organic compounds are ubiquitous in the environment due to their intensive use, release during industrial activities, and leakage from non-point sources. Tetrachloroethene (PCE), one of the most frequently found chlorinated organics in contaminated soil and groundwater systems and widely known to be carcinogenic, can be degraded by iron-bearing soil minerals (IBSMs) (e.g., magnetite, green rust, and mackinawite (FeS)), anaerobic microorganisms (e.g., dechlorination bacteria), and interactions between them, in natural and engineered environments. Interactions between extracellular substances (e.g., cobalamin) produced by dechlorination bacteria and IBSMs may occur in complex soil and groundwater systems, and have the potential to significantly influence degradation kinetics and reaction pathways in the reductive degradation of PCE. In this presentation, we introduce (1) the reductive substitution of H_2O in aqua-cobalamin(III) (Cbl(III)-H_2O), (2) the reduction of Cbl(III)-H_2O at different concentrations of S^{2-} in nano-mackinawite (nFeS) suspension, (3) reductive degradation kinetics of PCE by Cbl(III)-S^{2-} in nFeS suspension, and finally (4) transformation products and reaction pathways for the reductive dechlorination of PCE by Cbl(III)-S^{2-} in nFeS suspension.

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발표코드: **ENVR2-2**

발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics

발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 한영수

Characterization of Metal Sorption Behavior on Phosphate and Carbonate Minerals

이영재

고려대학교 지구환경과학과

Metal partitioning to minerals has been shown to be a key factor in controlling the fate and transport of metals as well as their bioavalibility. Phosphate and carbonate minerals have been the subject of interest in geochemical and biological processes because of its high reactivity but also because of being ubiqotous in various environments. Metals such as Hg, As, Se, and Zn are notorious in ecosystems due to its toxicity. In this study, systematic batch experiments were conducted to investigate Hg sorption on hydroxylapatite (HAP, [$Ca_5(PO_4)_3OH$]) over a wide range of physicochemical conditions, and EXAFS spectroscopy was used to examine the modes of incorporation of As, Se, and Zn with HAP.Hg sorption increases with increasing pH up to pH 6.0 whereas the sorption decreases with pH at pH ≥ 7.0. It is found that Hg sorption on HAP increases with increasing Hg concentration. At pH 5.0 and 7.0, Hg uptake by HAP steeply increases up to $[Hg]_{ini.} \leq 10$ μM, and then gently increases at higher concentration. At pH 9.0, however, the Hg sorption on HAP shows linear slope with increasing Hg concentration. Upon Hg sorption edges and isotherms, it is shown that the sorption is little influenced by variation of ionic strengths, providing that Hg would form inner-sphere surface complexes at the HAP. In kinetics, Hg sorption on HAP reaches ~70 % of total sorbed Hg within the first 3 hr, indicating that adsorption plays a major role in cotrolloing the initial uptake of Hg by HAP.As(V)-, Se(VI)- and Zn-doped HAP samples were synthesized at 75 oC to provide dopant concentrations up to 900 ppm for study by EXAFS. Fitting results for As-doped HAP show that the local coordination of As is similar to that found in johnbaumite ([$Ca_5(AsO_4)_3(OH)$]), with ~9 Ca atoms at distances of 3.25-3.68 Â. Se local coordination in Se-doped HAP samples yielded similar fitting results with ~8-9 Ca atoms at 3.17-3.65 Â. These results confirm that As(V) and Se(VI) substituting for P in HAP. Zn K-edge XANES spectra of Zn-doped HAP are found to differ from model compounds suggesting that precipitation of a Zn phase is unlikely. Best fit EXAFS

results indicate that Zn occurs in tetrahedral coodination with O at ~1.96 Â. More distant shells were fitted with ~1 P at ~3.16 Â, ~1 P at ~3.58 Â and 1~2 Ca at ~4.05 Â, suggesting Zn incorporation into Ca sites in HAP with highly distorted local environments expected. Results of this study also provide coprecipitation systematics, as well as insight to metal incorporation mechanisms in human bone and teeth.

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발표코드: **ENVR2-3**
발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 한영수

The Effects of Microorganisms on the Behavior of Heavy Metals and Application to Environmental Remediation

이종윤

전남대학교 에너지자원공학과

Bacteria have exerted significant influence on geochemical behavior of elements. Numerous evidence of their control on geochemistry through geologic history has been observed in a variety of natural settings. They have mediated weathering rate, formation of secondary minerals, redox transformation of metals and metalloids, and thus global cycling of elements. Therefore, effective applications of the bacterial activity to the environmental bioremediation of toxic metals and radionuclides are possible through various remediative techniques including natural attenuation. Some recent subjects of geomicrobiology which are studied extensively are as follows: 1) Dissimilatory metal reducing bacteria conserve energy to support growth by oxidation of organic matter coupled to reduction of some oxidized metals and/or metalloids. They can be effectively used in remediation of the environments contaminated with U, As, Se, and Cr. 2) Functional groups distributed on bacterial cell walls adsorb dissolved cations onto cell surfaces by electrostatic surface complexation, which is followed by hydrous mineral formation in some cases. 3) Bacteria increase the rate of mineral dissolution by excreting proton and ligands such as organic acids into aqueous system. Acidophiles can be used in extraction of metals from contaminated soil and sediments. 4) Thorough investigation on the effects of biofilm on geochemical processes is needed, since most bacteria are adsorbed on solid substrates and form biofilms in natural environments.

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발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 한영수

Reductive Dechlorination of Chloroethenes on Zerovalent Iorn (ZVI) From First-Principles

임동희

충북대학교 환경공학과

본 연구는 염소화합물의 영가철(Fe^0) 표면에서의 상대적 반응성을 양자화학계산 모델링을 통하여 규명하였다. 대표적 염소화합물인 perchloroethene (PCE, C_2Cl_4), trichloroethene (TCE, C_2HCl_3), 그리고 *cis*-dichloroethene (*cis*-DCE, $C_2H_2Cl_2$) 물질들의 영가철 표면에서의 흡착 및 분해 특성을 고찰하였다. 영가철에 의해 염소화합물의 탄소-염소 결합이 끊어지는 메카니즘에 대한 이해가 아직 많이 부족한 현실을 감안할 때, 염소화합물들의 상대적 반응성을 이해하는 일은 환경오염정화 측면에서 매우 중요한 일이다. 이는 영가철을 이용하여 염소화합물로 오염된 식수원을 정화 시키는 시스템을 최적화하기 위한 모델을 개발할 때 핵심적인 요소이기 때문이다. Fe(110)표면이 본 연구를 위해 선택되었는데, 이는 실제 자연계에서 흔히 발견되는 영가철 표면중의 하나이며, 열역학적으로 가장 안정된 표면을 대표할 수 있기 때문이다. 앞서 언급한 세가지 염소화합물들의 영가철 표면에서 가장 안정된 흡착 구조를 알아 내기 위해서 periodic density functional theory (DFT)와 generalized gradient approximation (GGA) 방법을 사용하였다. Climbing image nudged elastic band (CI-NEB) 방법을 사용하여 환원적 탈염소 메카니즘에서 염소 원자가 염소 화합물로부터 분해되는 과정에서의 활성화 에너지 (activation energy)를 계산하였고, 염소화합물의 vibrational frequencies 를 계산함으로써 Arrhenius equation 을 바탕으로 탈염소 분해율 상수를 계산하였다. 염소화합물의 가장 안정적인 흡착 구조는 염소화합물이 철 원자 바로 위에 위치할 때 이며, 흡착된 염소화합물의 전기적 특성을 분석한 결과 염소화합물의 두개의 탄소원자들과 철 원자 사이에 강한 파이 결합이 형성되어 있음을 알 수 있었다. 영가철에 의한 실제 염소화합물의 분해 반응이 수중에서 발생함으로 인해, 이들 반응의 용매 효과 (solvation effect)를 고려하여 DFT 계산값을 보정하였다. 염소화합물의 영가철 표면에서의 흡착 강도는 PCE 가 가장 컸으며, 다음으로 TCE 와 *cis*-DCE 순이었으며, 이는 다른 문헌의

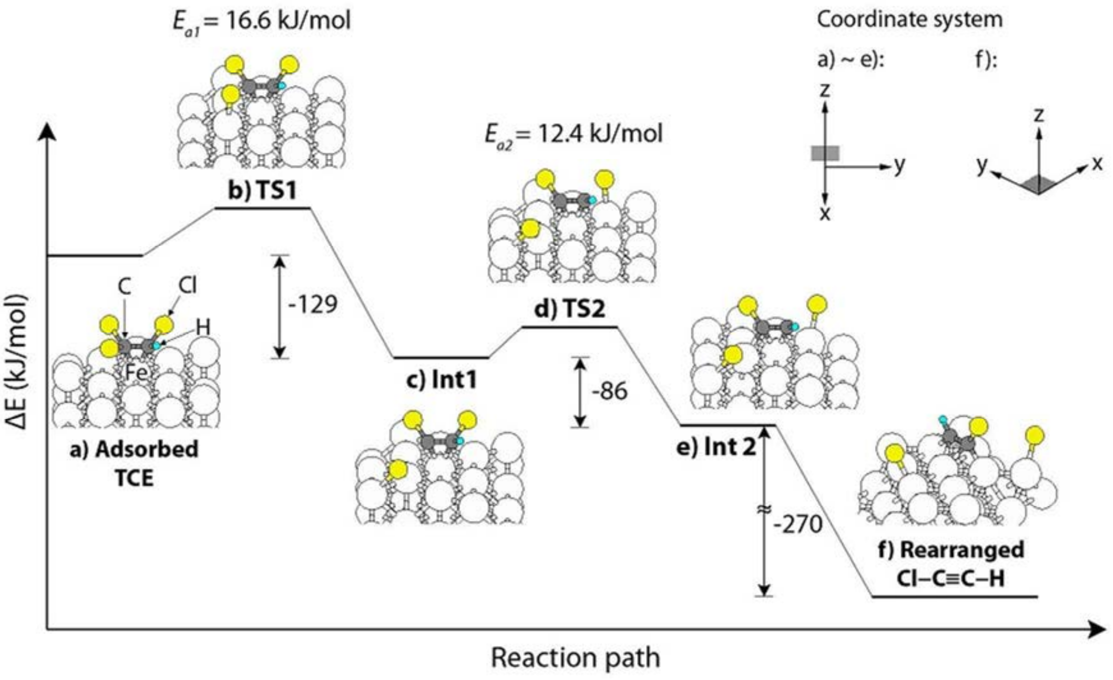
실험결과와도 일치함을 보여 주었다. 염소의 분해 활성화 에너지는 PCE 가 9.9 kJ/mol, TCE 가 16.6 kJ/mol, 그리고 *cis*-DCE 가 23.8 kJ/mol 로서, 염소 원자의 갯수가 많아 질 수록 활성화 에너지가 낮아 지는 특성을 보였다(그림 1 참조). 열역학 계산을 활용하여 상온 300 K 에서의 PCE 염소 분해율이 TCE 와 *cis*-DCE 보다 각각 14 배와 338 배 더 빠르게 나타난다는 것을 보였다. 이는 실험결과 문헌과도 일치하는 염소화합물 분해 경향이다. 이로써, 본 연구는 염소화합물의 자세한 흡착 모형과 분해 메카니즘의 중간 생성물 모형에 대한 전자기적 및 물리적 특성을 분석하여 염소화합물의 분해 메카니즘 이해를 돕는데 기여하였다.

References

(1)Lim, D.-H.; Lastoskie, C. M.; Soon, A.; Becker, U., Density functional theory studies of chloroethene adsorption on zerovalent Iron. Environmental Science & Technology (2009), 43 (4), 1192-1198.

(2)Lim, D.-H.; Lastoskie, C. M., Density functional theory studies on the relative reactivity of chloroethenes on zerovalent Iron. Environmental Science & Technology (2009), 43 (14), 5443-5448.

그림 1. Fe(110) 표면에서 TCE 가 분해되는 반응 경로. Ea1 과 Ea2 는 각각 첫 번째, 두 번째 염소원자가 분해될 때 요구되는 활성화 에너지를 나타낸다. 염소화합물 원소표시: Cl-가장 큰 원형 (노란색), C-중간 크기 원형 (회색), H-가장 작은 원형 (하늘색).



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발표코드: **ENVR2-5**

발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 박진희

Applications of Biogeochemical Redox Reactions in Environmental Biotechnology Field

정석희

전남대학교 환경에너지공학과

Electron transfer reactions (redox reaction) dictates element cycling on the earth, where microbial reaction is crucial. Using the knowledge on biogeochemical redox reactions, novel engineered systems have been invented and performance of existing engineering systems have been enhanced. In this talk, two representative applications of redox reactions in environmental biotechnology field will be introduced. A passive treatment of acid mine drainage (AMD) is a well-known traditional application of biogeochemical reactions. This process utilizes microbial sulfate-reducing reaction and ferrous-oxidizing reactions to precipitate acidity and metal levels in AMD. Microbial fuel cell (MFC) technology is an innovative environmental technology that utilize the redox reaction of metal-reducing microorganisms. The pollution treatment together with energy recovery from wastewater streams or contaminated soils can be fulfilled by using MFC technology, and MFC technology has other fascinating potential applications. Regarding these traditional and emerging technology, current status, perspective and my research will be presented.

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Correlation between micro speciation and reactivity in iron Redox chemistry

김동욱

육군사관학교 화학과

난분해성 환경오염물질의 제거를 위해 수많은 산화 환원 공정이 적용되어 왔다. 이러한 공정에는폐수 내의 유기물질을 처리하기 위한 AOP, 지하수 내의 유기염소화합물, 중금속 등을 제거하기 위한 다양한 환원공정 등이 포함된다. 산화반응, 환원반응 모두 다양한 환경변수(예; pH, 반응물질의 농도, 온도 등)에 따라 대상 오염물질과의 반응성이 크게 달라지곤 한다. 이중에서도 pH 는 반응성에 매우 중요한 역할을 하는 것으로 알려져 왔다. pH 가 변함에 따라 수용액 내의 많은 화학종의 농도가 변하게 되며, 이 화학종의 농도에 따라 반응성이 달라지게 된다. 때로는 다른 화학종에 비해 농도가 수백 수천 배 이하의 적은 농도를 가진 화학종이 반응성의 대부분을 설명하는 경우도 있다. 본 발표에서는 pH 와 수용성 유기물질의 양에 의해 변화되는 반응물질의 micro speciation 과 반응성의 상관관계에 대해 알아보고자 한다. 이를 위해 폭약에 사용되는 고에너지 유기화합물인 TNT, RDX 등과 같은 나이트로계열 폭발물질과 수용성 철이온(Fe ions)과 유기계리간드 물질의 결합체와의 반응을 살펴본다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR2-7**
발표분야: Biogeochemical Redox Processes and Their Impact on Contaminant Dynamics
발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 박진희

Desorption of heavy metals by using iron-chelated persulfate reaction in soil and adsorption of As(III) and As(V) using waste reclaimed alginated bead in aqueous phase

이홍균

한국과학기술연구원(KIST) 환경연구그룹

오염된 토양 및 지하수 오염 정화에 있어 각 물질별 또는 오염 대상에 따른 다양한 처리기법이 적용되어 지고 있다. 따라서, 본 연구에서는 토양에서의 중금속 탈착과 수용액상에서의 비소 (As) 흡착의 효율과 기작에 대하여 규명한다. 토양에 오염된 중금속 처리의 경우, 산/염기 또는 저분자 유기산 등을 이용한 토양세척 (soil washing)이 보편적으로 적용되고 있으며, 많은 연구결과들이 있다. 하지만, 산화제인 과산화수소 (hydrogen peroxide) 또는 과황산 (persulfate) 반응에서 발생되는 다양한 산화 또는 환원 radical 들에 의한 중금속 탈착현상이 보고되고 있으며, 본 연구에서는 토양에 흡착된 중금속 탈착에 기인하는 radical 을 규명한다. 더하여, 비소로 오염된 지하수 또는 폐수처리를 위한 흡착공정에서 폐기물 재활용 흡착제 (waste reclaimed adsorbent)인 acid mine drainage sludge bead (AMDS bead)를 이용한 흡착효율과 기작을 규명하고, 더하여 흡착제에 함유된 manganese oxide 에 부수적인 As(III)의 As(V)로의 산화에 대하여 확인한다.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS1-1**

발표분야: 국가와 기업이 원하는 과학기술 인재상

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 석차옥

국가 R&D 혁신: 출연(연) 시각에서 KIST사례를 중심으로

이병권

한국과학기술연구원(KIST)

오늘날 우리 사회가 직면하고 있는 위기를 극복하기 위해서는 결국 과학기술의 혁신을 통해 근원적 돌파구를 찾아야한다. 하지만 현재 우리나라의 연구개발은 그 수행방식에 있어 여러 문제점을 내포하고 있다. 특히, 우리나라 연구개발에 있어 중요한 부분을 차지하는 출연(연)의 연구개발 방식에 전반적인 변화와 혁신이 필요한 실정이다.

KIST 는 우리나라의 대표적 출연연구기관으로, 국가 발전의 성장동력을 되살리고, 국가와 국민이 체감하는 연구성과 창출을 위해, 최근 몇 년 간 수많은 변화의 노력을 기울여왔다. 특히, 연구조직, 기획, 평가, 성과확산에 이르는 전 과정에서 변화와 혁신에 매진해왔고, 이러한 노력을 인정받아 출연(연)의 혁신 사례로 회자되고 있는 상황이다. 본 강연에서는 KIST 의 R&D 혁신 사례를 통해 우리나라 과학기술의 혁신 방향을 공유하고자 한다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS1-2**
발표분야: 국가와 기업이 원하는 과학기술 인재상
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 석차옥

Creative leadership of King Sejong & Happiness Sharing 125

손욱

차세대융합기술연구원

Introduction to the organizational culture building measures appropriate to the nature of Korean, Sharing Movement for happiness. King Sejong the Great King Sejong era of science and technology and report back to the lessons of this practice, and technology management, creating a fusion of Korean leadership circle and creating culture, introduction to the debate, just like King Sejong.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS2-1**

발표분야: Photochemistry Tutorial for Material Scientists; Fundamental and Applications

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 한민수

Photochemistry Tutorial for Material Scientists; Fundamental and Applications

윤웅찬

부산대학교 화학과

The field of photochemistry covers all processes which involve chemical changes brought about by absorption of visible or ultraviolet radiation. These photochemical processes and photophysical processes involve the direct participation of an electronically excited state of a molecule and compete with each other. Further quenching processes other than the photochemical change and photophysical processes like energy transfer- or electron transfer processes accelerate decay of the electronically excited state of a molecule in a competitive manner. In this tutorial factors and issues involved in production, time-independent properties, time-dependent phenomena, and quenching of electronically excited states will be presented; (1) absorption and emission of light, (2) intensity of electronic transitions and its related selection rules, (3) singlet-triplet excited states, (4) dissipative pathways including radiative transitions (fluorescence/phosphorescence) and nonradiative transitions (internal conversion/intersystem crossing), (5) excimer and exciplex formation, (6) electron transfer quenching (Rehm and Weller equation/Marcus theory), (7) heavy atom quenching, (8) electronic energy transfer processes. Further photochemical changes (reactions) occurring in electronically excited states of common organic chromophores will be briefly introduced.

As well as background knowledge on (organic)photochemistry is highly essential for photochemists who are interested in designing and developing new photochemical reactions, the knowledge can provide a solid basis not only in understanding and explaining the phenomena observed in the area of material science involving electronically excited states but also in designing and developing new functional molecules, like optoelectronic, light emitting diode (LED), and light emitting sensor materials whose key functions are largely related to the properties of their electronically excited states.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS3-1**

발표분야: Research Funding Sponsor Promotion Forum

발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 윤성호

LG화학의 산학 협력 프로그램 소개 (Introduction of LG Chem's University Collaboration Programs)

이성만

LG화학

LG 화학의 현사업과 관련된 연구분야와 간략한 연구개발 현황을 소개하고 미래 중점적으로 연구하고자 하는 연구분야를 소개하고자 한다. 효과적인 연구개발을 위해 Open Innovation 차원에서 주로 대학과 진행하고 있는 다양한 협력 프로그램에 대한 소개를 통해 대학과의 보다 진전된 협력 기회를 모색하고자 한다.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS3-2**

발표분야: Research Funding Sponsor Promotion Forum

발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 윤성호

Opportunities through Open Innovation - How solution providers are participating NineSigma Open Innovation Programs sponsored by Global Fortune 500 companies

이준혁

Ninesigma

(미정)

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS3-3**

발표분야: Research Funding Sponsor Promotion Forum

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 윤성호

삼성미래기술육성사업 소개 (Introduction of Samsung Research Funding Program for Future Technologies)

김현주

삼성전자 미래기술육성센터

(미정)

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS4-1**

발표분야: IoT 미래소재 심포지엄 - 세상과 만물 그리고 사람, 마음으로 通하라

발표종류: 심포지엄, 발표일시: 목 13:45, 좌장: 최우

스마트한 세상을 위한 사물인터넷(Internet of Things)기술과 미래기술

김동현

부산대학교 IT기반 융합산업 창의인력양성 사업단

사물인터넷기술은 우리 주변의 다양한 사물에 네트워크 기능을 탑재하여 사물 본래의 기능을 향상시킬 뿐만 아니라 다양한 네트워크 기술을 이용하여 연결함으로써 언제 어디서나 제어, 모니터링 할 수 있는 연결 기술을 의미한다. 사물인터넷은 교통, 물류, 헬스케어, 에너지, 엔터테인먼트, 디스플레이 등 다양한 분야에 영향을 미칠 것으로 예상된다. 본 심포지엄에서는 사물인터넷에 대한 정의와 사물에 인터넷을 지원하기 위한 시스템 프레임워크 등을 통해 사물인터넷 기술 설계 및 구현을 위한 프레임 워크를 설명한다. 실제 응용사례를 통해 어떠한 분야에서 사물인터넷에 대한 연구 및 상용화가 진행 중인지 확인하고, 특히 소재 부문에서 사물 인터넷을 지원하기 위한 미래 기술 트랜드에 대하여 알아보겠다. 그리고, 향후 사물인터넷의 발전방향을 통해 다양한 산업을 견인할 길잡이 역할을 할 사물인터넷기술에 대하여 폭 넓게 알아볼 것이다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS4-2**
발표분야: IoT 미래소재 심포지엄 - 세상과 만물 그리고 사람, 마음으로 通하라
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 최우

Wearable 전자 소자 응용을 위한 기능성 박막 소재와 공정 연구

박진성

한양대학교 신소재공학부

세계 소비자 가전 박람회 2014 년도의 가장 주목 받은 주제는 사물인터넷 (ITOs, Internet of Things)의 등장을 이야기하는 것 이였다. 또한, 이와 함께 미적 기능이 첨가된 휘어지는 디스플레이들과 입고 다닐 수 있는 소형 전자제품들은 매년 500%이상의 예상 성장치를 가지고 급변화하고 있다. 이를 수용하고 응용할 수 있는 새로운 전자 소재와 공정에 대한 연구와 관심도 급성장하고 있다. 특히, 유연한 기판/섬유의 기능성 부여와 3D 구조체에 기능성 박막 소재/공정은 매우 중요한 연구주제로 주목되고 있다. 본 발표에서는 원자층 증착법 (Atomic Layer Deposition, ALD)을 활용한 유연한 소재에 적용이 가능한 기능성 박막 소재와 공정 기법들을 설명하고자 한다. 투명산화전도막과 반도체등은 향후 섬유소재나 3D 구조체등의 복잡한 표면을 가지고 있는 곳에 높은 밀착력과 도포성으로 코팅되어지며, 얇으면서도 우수한 전기적, 광학적 물성등을 보여줬다. 그리고 저온 원자층 증착기법을 통한 산화막과 금속박막등의 응용 공정을 발표할 예정이다. 그리고 진공기반의 공정에서 벗어나 저원가 기반의 상압 증착 기법에 대한 요구가 늘어나고있고, 이를 활용한 유연 기반의 전자 소재/공정등에 대해서도 소개할 예정이다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS4-3**
발표분야: IoT 미래소재 심포지엄 - 세상과 만물 그리고 사람, 마음으로 通하라
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 양민수

Required materials, processes and devices in printed electronics for realizing printed IoT

조규진

순천대학교

For the realization of ubiquitous society, providing thin film transistors (TFTs) based inexpensive IoT-network and signage will be a key step since all of goods need to have wireless sensor tag or label with signage to communicate with human via wireless means.1-4 As a consequence of developing the IoT and signage, I would like to show the way of developing materials, process and device design to fully print the inexpensive IoT and signage based on a continuous roll-to-roll (R2R) gravure printing process. As a reference example, fully gravure printed wireless-sensor tags with the signage, humidity sensor and electrochemical sensor on PET foils are R2R printed and can display the logo whenever the tags sense the analytes. Since we are using R2R gravure to print wireless tag, signage and sensor, we can integrate this R2R printing system with the R2R package printing to remove the extra cost in tagging and labeling for the fabrication of IoT wherein wireless tag, signage and sensors are integrated. In this presentation, I would like to show the details of R2R gravure system to print prototype of all printed wireless devices and sensors for realizing IoT.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS4-4**

발표분야: IoT 미래소재 심포지엄 - 세상과 만물 그리고 사람, 마음으로 通하라

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 양민수

Wearable, Portable 중심의 Flexible OLED 기술

권장혁

경희대학교 정보디스플레이학과

Mobile 용 AMOLED 기술은 최근 빠르게 Flexible 기술로 바뀌고 있으며 향후 Wearable 기술로 전개되리라 예측이 되고 있다. Flexible AMOLED 로는 LG 의 G Flex 제품과 삼성 갤럭시 S6 양면 edge 제품이 출시되었고 우수한 디자인성을 기반으로 새로운 시장을 창출해 나갈 것으로 예측되고 있다. 본 발표에서는 이러한 Flexible AMOLED 가 기존 유리기판 제품과 비교해서 어떤 기술적인 차이점을 가지고 있는지 소개하고 우리가 향후에 추가 연구가 필요한 기술은 어떤 것이 있는지 소개하고자 한다. 또 향후 Wearable AMOLED 로 가기 위한 신기술개발 현황도 같이 토의하고자 한다.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.O-1**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 박문정

Reversible Morphological Transformation between Polymer Nanocapsules and Thin Films through Dynamic Covalent Self-Assembly

백강균 김지홍[1] 김기문[1,*]

기초과학연구원 복잡계자기조립연구단 [1]포항공과대학교(POSTECH) 화학과

In biological systems, morphological transformations of nano/microstructures in response to environmental stimuli are integral to many of the processes necessary for life. Synthetic nanostructures that can similarly undergo morphological transitions in response to physical and chemical stimuli have attracted a great deal of attention, particularly for the development of smart functional materials. Herein, we developed a facile method for synthesizing polymer nanocapsules and thin films by multiple in-plane stitching of monomers through the formation of reversible disulfide linkages. Owing to the reversibility of the disulfide linkages, the nanostructured materials readily transform their structures in response to environmental changes at room temperature. For example, in reducing environments, the polymer nanocapsules release loaded cargo molecules. Moreover, reversible morphological transformations between these structures can be achieved by simple solvent exchanges. This work is a novel approach for the formation of robust nano/microstructured materials that dynamically respond to environmental stimuli.

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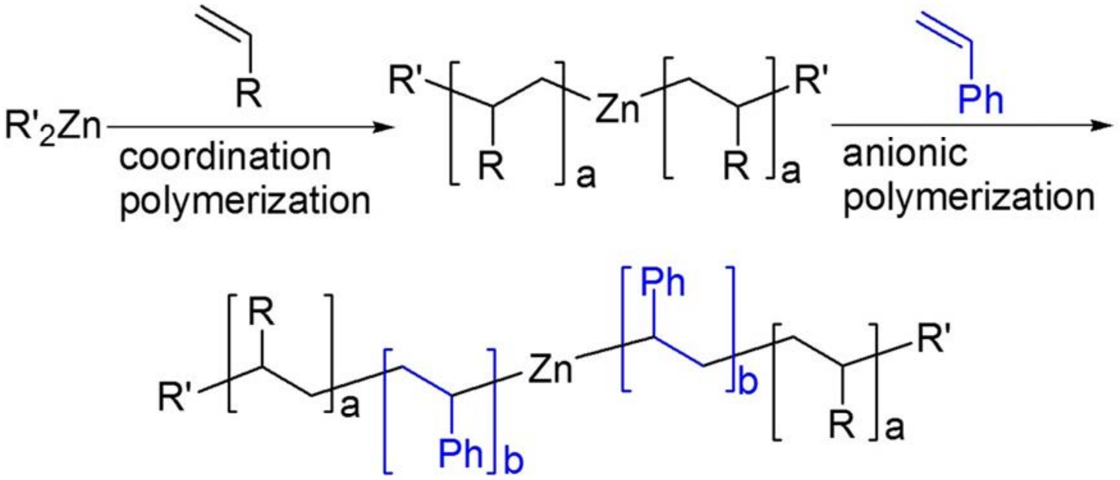
"One-Pot" Block Copolymerization of Olefin and Styrene through "Catalyzed Chain Growth" on Zinc and Anionic Polymerization

전종엽 이분열*

아주대학교 분자과학기술학과

A novel polyolefin-polystyrene block copolymer was prepared from combination of coordination polymerization and anionic polymerization. Polyethylene block was grown on Zinc by various catalysts in terms of "Catalyzed Chain Growth". A fast and reversible exchange of the growing polymer chains between the metal in catalyst and zinc resulted polyethylene units on zinc which was utilized subsequently for anionic polymerization by addition of n-butyllithium and tmdea complex. The molecular weight of each block was tunable and the polymers showed various properties depending on the block length.



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Rational Designs of Sulfur-Rich Polymers as New Cathode Materials for Lithium-Sulfur Batteries

김훈 박문정*

포항공과대학교(POSTECH) 화학과

Rechargeable lithium-sulfur batteries have been considered as one of the most promising electrochemical energy storage systems on account of high theoretical capacity (1,674mAh/g) and the high specific energy (2600 Wh/kg). However, fast capacity fading within initial a few cycles was occasionally witnessed, attributed to the dissolution of polysulfide intermediates into organic electrolytes during charge/discharge cycling, impeding the development of practically viable batteries. In this study, we investigate the development of newLi-S batteries with improved cycle performance by synthesizing sulfur-rich polymers. Porous trithiocyanuric acid (TTCA) crystals having two functional groups of thiol and amine were employed as soft templates for the synthesis. The thiol moieties were particularly aimed to promote ring-opening polymerization of elemental sulfur along pore surfaces. Unique square tube morphology was obtained from the TTCA frameworks by optimizing crystallization solvents, which contain abundant micropores at the surfaces and macropores within the crystals, enabling the implementation of three-dimensionally interconnected sulfur-rich phases after vulcanization. Our Li-S batteries based on the new sulfur-rich macromolecules cell can deliver reversible discharge capacity of 945 mAh/g after 100 cycle at 0.2C with high capacity retention of 92%, as well as stable cycling performance over 450 cycles. These Li-S cells also demonstrated improved rate performance of 1210mAh/g at 0.1C and 730mAh/g at 5C. The markedly enhanced rate performance of our Li-S cells was rationalized by facilitated fast Li+-ion transport in sulfur-rich polymers along the organized amine moieties in TTCA ring.

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Fabrication of conductive inks with carbon black and carbon nanotubes for inkjet printer

김용준 신관우[1,*] 권오선[*] 김희주[2]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정 [2]서강대학교 화학

Paper based applications such as paper based digital microfluidic chip, paper display, paper battery and paper bio-sensor are fabricated with some advantages simple, low-cost, easy and portable [1]. Many researchers usually use metallic inks for the conductive electrodes in that applications. However the metal ink needs curing temperature and time, but also need organic solvent for dispersant of metal nanoparticles. To solve the problems, some people use carbon materials for inks which have dispersion effect in water. In my research, I can print water based carbon material inks such as carbon black and carbon nanotubes for the epson inkjet printer. By using these inks, I can fabricate the electrode on normal paper and photopaper substrate which have higher conductivity and stability than previous work [2]. So I can get the previous conductivity 760Ω/sq. from a minimal printing number is 4 times. Finally, the paper electrodes on paper will be used high sensible and stable paper devises in the office environment.

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Hierarchical Homogeneous TiO2 Structures Composed of TiO2 Nanoparticles and Nanotubes for highly efficient dye-sensitized solar cells

최종민 박태호*

포항공과대학교(POSTECH) 화학공학과

We prepared well-defined hierarchical structures comprising doubly open-ended TiO2 nanotube (NT) arrays decorated with various layers of small-sized TiO2 nanoparticles (NPs) to identify the electron collection mechanisms in homogeneous hybrid structures. We found that competitive electron transport pathways, direct transport through the NT and randomized transport through the NPs, are present in the homogeneous hybrid structures. Photoinduced electrons generated at the small-sized TiO2 NPs directly connected with TiO2 NTs dominantly traveled to the NTs. With an increasing number of TiO2 NP layers, photoinduced electrons are randomly transported through the TiO2 NP layers. Enhanced light harvesting and efficient charge collection (～95%) caused by the increased amounts of dye loading and the direct transport through the NT, respectively, are achieved in a structure with ～1.4 layers of few-nanometer-sized TiO2 NPs, resulting in a power conversion efficiency of 11.3% with a JSC value (22.9 mA/cm2) close to the theoretical value (～26 mA/cm2) of a N719-based dye-sensitized solar cell.

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Unique monotropic phase transition behaviors of diphenylpyrimidine molecule

박민욱 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

A butterfly-shaped diphenylpyrimidine molecule (DPP-6C12) was synthesized by covalently attaching two tridodecyl benzoate tails (6C12) at the both sides of the diphenylpyrimidine (DPP) moiety. Unique phase transition behaviors of DPP-6C12 and their origins were investigated with the combined techniques of thermal, scattering, spectroscopic, and microscopic analyses. On the basis of the experimental results and analyses, it was realized that a butterfly-shaped DPP-6C12 formed three ordered phases: a plastic crystal phase (PK), a crystal phase (K), and a liquid crystal phase (Φ). By breaking the molecular symmetry and coplanarity of DPP-6C12, peculiar monotropic phase transition behaviors were observed. The stable Φ mesophase was formed either by a slow heating above the metastable PK phase or by an isothermal annealing between TΦ and TK. The stable K phase was only formed by a slow heating from the preordered Φmesophase, and the formation of the K phase directly from the isotropic state (I) was forbidden because the nucleation barrier from I to K was too high to be overcome via thermal annealing. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), BK21Plus Program, Korea

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Phenylboronic Acid-Sugar Grafted Polymer Architecture as Tumor Targetable and Dual-Stimuli Responsive Gene Carrier

김진환 김원종*

포항공과대학교(POSTECH) 화학과

We present herein a cationic polymer structure composed of phenylboronic acid (PBA) and sugar installed polyethylenimine (PEI) and polyethyleneglycol (PEG). The chemical bonding of PBAs with diols in sugar enabled the cross-linking of low molecular weight PEI to high molecular weight, resulting in better interaction with anionic DNA for gene delivery. Inside the cell, the binding of PBA and sugar was disrupted by both acidic endosomal pH and intracellular ATP, followed by effective release of gene contents. This dual stimuli-responsive gene release assisted the polymer to deliver DNA for high transfection efficiency with low cytotoxicity. In addition, PEGylation with PBA moiety facilitated the binding of polymer/DNA polyplexes to sialylated glycoprotein which is overexpressed on the tumor cell membrane, thus provided high tumor targeting ability. Therapeutic application of our polymer was demonstrated as anti-angiogenic gene delivery agent for tumor growth inhibition. Our judicious designed polymer structure based on PBA provides an enormous potential of gene delivery agent for effective gene therapy in a stimuli-responsive, tumor targetable manner.

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Facile synthesis of 2D polyaniline nanosheets on ice surfaces

최일영 박문정[1,*]

포항공과대학교(POSTECH) 첨단재료과학부 [1]포항공과대학교(POSTECH) 화학과

Polyaniline (PANI) has widely been studied as one of promising conducting polymers for uses in a range of electrochemical devices. Good environmental/chemical stability, high electrical conductivity, and easy of synthesis have been highlighted as desirable characteristics of PANI towards future electronic materials. Decades of research on PANI have further revealed that the electrical properties of PANI can be largely tailored by changing the dimensionality of nanostructures. This imprinted the importance of developing 2D morphologies to achieve enhanced conductivity, especially along desired directions, towards their applications in high density integrated electronic devices. Despite their positive aspects, successful fabrication of 2D PANI nanostructures with improved properties is in its infancy because of the difficulties in controlling surface and interfacial properties. Here, we present a facile synthesis of 2D PANI nanosheets via chemical oxidative polymerization using ice as a template. The ice offers unique surfaces of water molecules that are arranged in layers of hexagonal rings, facilitating hydrogen bonding interactions with aniline monomers in an organized manner. The easy removal of ice also enables the attainment of template-free PANI nanosheets in tens of nanometers thickness. Notably, the ice-templated PANI nanosheets revealed two orders of magnitude higher electrical conductivity than conventional PANI thin films prepared by electrochemical deposition methods. The origin of the improved electrical properties of the PANI nanosheets was found in a unique edge-on π-stacking, attributed to ordered hydroxyl groups at the ice surfaces. Our work should open a new chapter in advancing organic electronics upon putting forward a new methodology.

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Low Temperature High-Performance Solution-Processed Oxide Electronics for Large Area Electronics

김명길

중앙대학교 화학과

The flat panel display technology is one of the most successful examples of large area electronics. This rapidly emerging technology expands to diverse new directions, for example, transparent flexible/stretchable displays, radio-frequency identification (RFID) tags, conformal sensor arrays, and solar cells. To be maximally useful, large area electronics require high performance electronic materials, cost-effective fabrication processes, facile scaling up of substrate size, and new functionality. Solution processed metal oxide electronics could potentially meet the requirements of commercial large area electronics, such as high-throughput fabrication processes and a choice of materials with appropriate electrical performance characteristics. However, this area still faces several challenges, such as low performance, high annealing temperatures, and the inability to fine-tune intrinsic properties. An intensive study of interface optimization, novel fabrication concepts, and new materials development can addresses critical issues in solution processed metal oxide semiconductor electronics. In this talk, I will present that new material designing principle afford the development of high performance amorphous metal oxide semiconductor material (a-$ZnIn_4Sn_4O_{15}$), which achieve high field effect electron mobilty up to ~90 $cm^2V^{-1}s^{-1}$. Also compared to the high processing temperature ($T_{anneal} > 400\ ^oC$) of conventional sol-gel precursors, the low temperature processable novel precursor design concepts of combustion precursors dramatically reduce the processing temperature as low as 200 ^oC. Finally, electronically functional metal oxide nanocomposites enabled fine tuning of intrinsic material properties in solution-processed metal oxide semiconductor-based large area electronics. Overall, the significant progresses of material, precursor and processing concept could bring the next generation large area electronics into our daily life earlier than our expectation.

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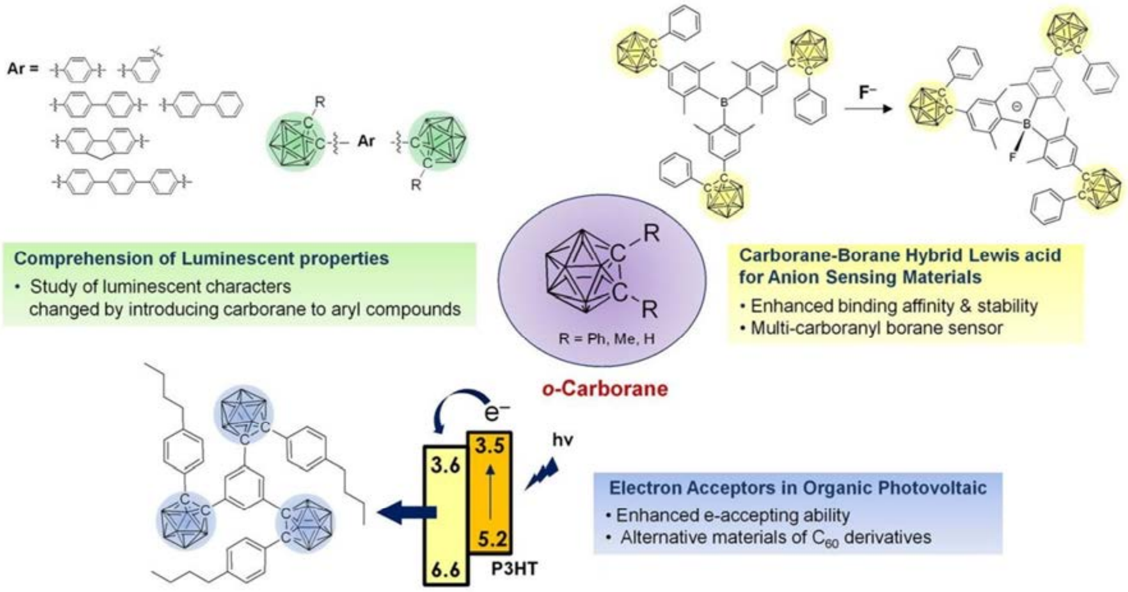
Photonic Materials based on Carborane Cluster

이강문

강원대학교 화학과

This research provides various synthetic approaches to the development of novel photonic materials possessing enhanced response based on Lewis acidic properties of *o*-carborane cages. Firstly, the *o*-carborane cages which possess high electron-withdrawing ability and high stability were combined with the triarylborane sensors so as to increase both the Lewis acidity. A triarylborane bearing three carborane cages on the aryl groups was prepared and a UV-vis titration experiment carried out in THF/H_2O (9/1 v/v) showed that it binds fluoride ions with a quietly high binding constant. Secondly, we could observe the unprecedented electron-accepting properties of a 1,3,5-tris-*o*-caboranyl benzene compound, together with DFT calculations. These would show a possibility of a novel concept for electron accepting materials which can be stood in for C_{60} derivatives via quenched photoluminescence of a P3HT by doping with this *o*-carboranyl benzene. Finally, p-terphenyl, biphenyl and fluorene based carborane compounds are designed and synthesized. All compounds demonstrated that introducing the carborane cages can gives rise to strong π-π^* transition band assigned by aggregation-induced emission on soild and film states. TD-DFT calculations showed that introducing the *o*-carborane cages induces the narrowing of the energy gap between the S_1 and the closest triplet state, from which the facilitated S-T states mixing leads to a sufficiently non-radiative decay. These results indicated that carboranyl compounds could be applied as delayed fluorescent materials of a novel concept. Consequently, carborane based new photonic materials will be first pursued and then the characteristics of such materials can be commonly applied to the photonic devices.


Ar =
R
Ar
R
F⁻
B
F
Comprehension of Luminescent properties
• Study of luminescent characters changed by introducing carborane to aryl compounds
R
C
C
R
R = Ph, Me, H
o-Carborane
Carborane-Borane Hybrid Lewis acid for Anion Sensing Materials
• Enhanced binding affinity & stability
• Multi-carboranyl borane sensor
e⁻
hν
3.6
3.5
5.2
6.6
P3HT
Electron Acceptors in Organic Photovoltaic
• Enhanced e-accepting ability
• Alternative materials of C60 derivatives

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Benchmarking metal and metal oxide promoters for oxygen evolution reaction in $Li-O_2$ cells

변혜령

RIKEN, Byon Initiative Research Unit

Despite high theoretical capacity, a $Li-O_2$ cell has suffered from huge oxidation potential polarization on carbon-based positive electrode for charge (>4.2 V vs. Li/Li+), due to sluggish decomposition of non-conductive discharge product, lithium peroxide ($Li_2O_2 \leftrightarrow 2Li^+ + O_2 + 2e$-) [1]. Such high potential triggers side reactions such as degradation of electrolyte and carbonaceous electrode, which results in poor cycle-ability [1]. To mitigate this problem during oxygen evolution reaction (OER), solid-state metal or metal oxide nanoparticles (indicated as promoters), which have been widely employed as catalysts in aqueous media, were introduced to the electrode [2]. However, the specific role of promoters in the $Li-O_2$ battery is little known due to complication from accompanying parasitic side reactions [3]. In addition, reasonable comparison of promoters' activities is not feasible under different performance conditions when various reports were referred [2]. Therefore, to gain a reasonable assessment of their activities in the $Li-O_2$ cell and an understanding of the promoters' role, it is necessary to examine $Li-O_2$ cells with these promoters under the same condition and analyze their reaction processes in detail. Here I present diagnosis of the true role of promoters, representative of platinum (Pt), gold (Au), palladium (Pd), ruthenium (Ru), cobalt oxide (Co_3O_4) and nickel oxide (NiO), for OER in $Li-O_2$ cells.Pt, Au, Pd, Ru, Co3O4 and NiO nanoparticles were synthesized via wet chemistry and loaded on carbon nanotube (CNT) with around 40 wt%. These composites were used as the positive electrode. The $Li-O_2$ cells containing these promoter (metal or metal oxide nanoparticles)/CNT combinations (1.2 mg of CNT) were examined using galvanostatic mode under the same operating conditions (0.06 mA, 25 ^{o}C).The promoter/CNT electrodes show reasonably lower charge potentials than the promoter-free electrode for the 1st charge. Through in situ gas analysis of online electrochemical mass spectroscopy (OEMS) and ex situ chemical analysis of X-ray near-edge fine structure (XANES) spectroscopy, the evolved gas amount and remaining product after charge could be correlated, which accounted for the true reaction occurring for each promoter. References(1) (a) G. Girishkumar, B. McCloskey, A. C. Luntz, S. Swanson and W. Wilcke, J. Phys. Chem. Lett., 1, 2193 (2010); (b) P. G. Bruce, S. A. Freunberger, L. J. Hardwick and J.-M. Tarascon, Nat. Mater., 11, 19 (2012).(2) (a) Y. ?C. Lu, H. A. Gasteiger and Y. Shao-Horn, J. Am. Chem. Soc., 133, 19048 (2011); (b) Z. Peng, S. A. Freunberger, Y. Chen and P. G. Bruce, Science, 337, 563 (2012); (c) F. Li, D. ?M. Tang, Y. Chen, D. Golberg, H. Kitaura, T. Zhang, A. Yamada and H. Zhou, Nano Lett., 13, 4702 (2013); (d) R. Black, J.-H. Lee, B. Adams, C. A. Mims and L. F. Nazar, Angew. Chem. Int. Ed., 52, 392 (2013).(3) B. D. McCloskey, R. Scheffler, A. Speidel, D. S. Bethune, R. M. Shelby and A. C. Luntz, J. Am. Chem. Soc., 133, 18038 (2011).

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Controlled Synthesis and Therapeutic Applications of Plasmonic Core-Petal Nanostructures

Amit Kumar 남좌민*

서울대학교 화학부

Metal nanostructures with highly branched morphologies are an interesting and useful new class of nanomaterials due to their plasmonically enhanced optical properties, large surface area and potential as catalytic substrates, sensing probes and building blocks for nanoscale devices. In particular, the surface plasmon-derived photo-induced therapeutic effect and catalysis are highly dependent on their surface nanostructures, but the control of their branching structures is challenging. Here, we introduce a strategy for the controlled synthesis of plasmonic core-petal nanostructures (CPNs) with highly branched morphologies. The fine nanostructural engineering of CPNs was facilitated by gold chloride-induced oxidative disassembly of biopolymer polydopamine corona around spherical Au nanoparticles and successive anisotropic growth of Au nanopetals. We show that CPNs can act as multifunctional nanoreactors that induce protrusion-dependent, controllable photodynamic and photothermal dual therapeutic effects and ROS generation. NIR laser-activated CPNs can be used to induce the effective destruction of cancer cells via the combination of benign plasmonic hyperthermia (~42 °C) and ROS-mediated oxidative intracellular damage. It was also shown that CPNs exhibit very strong surface-enhanced Raman scattering (SERS) signals, and this allows for post-mortem probing of ROS-mediated oxidative structural modifications of DNA, which mutations could be responsible for the apoptotic fate of cancer cells. Here, we have showcased the controlled synergistic plasmon-based catalytic and thermoplasmonic properties of NIR-active branched nanostructures for organic PS-free bimodal PDT-PTT ablation of cancer cells.

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Post-synthetic Transformation of Microporous MOFs to Hierarchical Micro- and Mesoporous MOFs

김용휘 YANG TAO 윤경원 이은성[1] 김기문[1,*]

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With growing interests on metal-organic frameworks (MOFs), post-synthetic modification receives considerable attention to get more control over the materials, as a pre-synthesized highly porous and desirable framework can be chosen for further modification to fine tune the pore environment without disrupting the framework topology. We recently reported the complete exchange of framework-constituting metal ions from microporous frameworks keeping the original framework topology intact. Extending this work, recently we have demonstrated a partial removal of metal ions of MOFs can generate larger pores with preserving the original microporous framework. Here we present a post-synthetic transformation from microporous MOF to hierarchical micro- and mesoporous MOF. This unique transformation is achieved simply by treating microporous MOF, POST-66(Y), with water. This method generates mesopores with a size in the range of 3 to 20 nm while maintaining the original microporous structure. The degree of micro- and mesoporosity can be controlled by adjusting the time and temperature of hydrolysis. This simple method may open up an opportunity to study the properties of nanometer sized guest molecules such as proteins and metal particles in a confined space of MOFs.

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Exceptionally High Proton Conductivity in a Sulfonic Acid-Functionalized UiO-66

방원주 조현아 송정화 이종현 임광수 홍창섭*

고려대학교 화학과

We demonstrate that the facile post-oxidation of a thiol-laced UiO-66-type framework UiO-66$(SH)_2$ enabled generation of the sulfonic acid groups covalently linked to the backbone of UiO-66$(SO_3H)_2$. The oxidized material exhibits a superprotonic conductivity of 8.4×10^{-2} S cm^{-1} at 80 °C and 90% relative humidity (RH) and maintains long-term stability in conductivity. This value exceeds that of any proton-conducting MOFs reported to date and is equivalent to the conductivity range of the best performing electrolyte, Nafion.

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발표종류: 분과기념강연, 발표일시: 금 10:00, 좌장: 장준경

Quantitative understanding of the control capacity of life forms over biological functions: Novel stochastic kinetics approach

성재영

중앙대학교 화학과

For quantitative understanding of probabilistic behaviors of living cells, it is essential to construct a correct mathematical description of intracellular networks interacting with complex cell environment, which has been a formidable task. Here, we present a novel model and stochastic kinetics for a vibrant intracellular network interacting with hidden cell environment, employing a complete description of cell state dynamics and its coupling to the system network. Our analysis reveals that various environmental effects on the product number fluctuation of vibrant reaction networks can be collectively characterized by Laplace transform of the time correlation function of the product creation rate fluctuation with the Laplace variable being the product decay rate. On the basis of the latter result, we propose an efficient method for quantitative analysis of the chemical fluctuation produced by intracellular networks coupled to hidden cell environment. By applying the present approach to the gene expression network, we obtain simple analytic results for the gene expression variability and the environment-induced correlations between the expression levels of mutually non-interacting genes. The theoretical results compose a unified framework for quantitative understanding of various gene expression statistics observed across a number of different systems with small number of adjustable parameters with clear physical meanings.

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발표분야: General Oral Presentation
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The folding of single polymer chains in dilute solution

Chi Wu

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It has been predicted in theory that a long linear homopolymer chain can undergo a coil-to-globule transition when the solvent quality changes from good to poor. However, it is extremely difficult to observe such a transition; namely, the intrachain contraction is always spoiled by interchain aggregation. Our laser light scattering studies of the temperature-induced folding of narrowly distributed individual poly(N-isopropylacrylamide) (PNIPAM) linear chains in solution have, *for the first time*, revealed such a transition. Moreover, we found a novel molten globular state between the coil and globular states. The time required for the transition (~10^2 sec) was too short to support a previously suggested high intrachain-knotting inside the globule. Our results also showed that even at the collapsing limit, the globule still contained ~70% of water in their hydrodynamic volume, which is not as “dry” as we thought. Our study was extended to the folding of some PNIPAM copolymer chains. We have demonstrated that after the introduction of second hydrophilic or hydrophobic monomer into the PNIPAM chain backbone, the chain folding could lead to some unique structures, such as a single-chain micelle and an ordered coil state. In this lecture, we also like to emphasize the importance of combining synthetic chemistry with polymer physics.

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The kinetics of loop formation of a single polymer chain in glass-forming liquids

권슬기 성봉준*

서강대학교 화학과

The dynamics of glass-forming liquids has been extensively studied because dynamic behaviors of glass-forming liquids significantly differ from that of ordinary liquids. There are unique dynamic behaviors such as drastic increase of viscosity and spatially heterogeneous dynamics when glass-forming liquids approach their glass transition temperature(T_g). Biological systems such as bacterial cytoplasm and lipid membrane, where various chemical reactions take place, also show the characteristic properties of glass-forming liquids. We investigate the diffusion-controlled loop formation reaction of a single polymer chain, which is relevant to many biological processes, using Molecular Dynamics (MD) simulation and Szabo, Schulten and Schulten (SSS) theory. SSS theory gives the general theoretical solution of looping time by reducing many degrees of freedom of polymer motions to 1D diffusion process with a single timescale along the appropriate reaction coordinate. We find that the end-to-end distance of polymer is a proper reaction coordinate for loop formation reaction. The looping time, the time required for the polymer ends to come close and react, is obtained by both MD simulations and SSS theory at various temperature from 0.5 to 3. We find that as the temperature becomes lower, the looping time calculated by MD simulations deviates from what is predicted by SSS theory, showing large fluctuation. Near the critical temperature, distribution and relaxation of end-to-end distance strongly depend on their initial conditions. Furthermore, the relaxation time of end-to-end distance becomes comparable to the looping time, which means that the looping time is strongly affected by their initial state and therefore the loop formation kinetics cannot be described by SSS theory with a single diffusional timescale in glassy environment.

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IR spectroscopy of mass-to-charge selected peptide and protein ions embedded in liquid helium nanodroplets

Doo-SIk Ahn Ana Isabel González Flórez Gert von Helden*

Department of Molecular Physics Fritz-Haber-Institute of the Max-Planck Society, Germany

Gas phase structures of peptides and proteins have been studied to understand the intrinsicstructural preference by intramolecular interactions without interactions from surroundings such assolvents [1]. IR spectroscopy is one of the most powerful tools to investigate the protein structures.Especially, each peak dictates the hydrogen bondings in proteins as a function of frequency shiftand intensity. To get the detailed vibrational signatures, cooling of target ions are necessary toremove thermal broadening factors, but it is still challenging for large biomolecular ions [2].

Liquid helium nanodroplets are an ideal cryostat for spectroscopic applications due to theisothermality at 0.38 K and the transparency from far IR to deep UV [3]. To chill the largebimolecular ions by liquid helium nanodroplets, we have developed the pulsed liquid heliumnanodroplet beam coupled with electrospray ionization source and linear hexapole ion trap [4,5].Peptide and proteins ions generated via electrospray ionization are selected/accumulated in thehexapole linear ion-trap. Mass-to-charge selected ions in the ion-trap are captured by liquid helium nanodroplets and are rapidly cooled via evaporative cooling. Further downstream, the ion-doped helium nanodroplets are interrogated by IR radiations. IR spectra of peptide/protein ions arerecorded by monitoring of the intensities of ejected ions as a function of wavelength. All IR spectrawere obtained by using IR Free Electron Laser facility at Fritz-Haber-Institute (FHI-FEL).

In this talk, we will present the recent experimental results and discuss about the role ofpermanent charge(s) on the conformations of peptides and proteins in the gas phase. Specifically,1) IR spectrum of protonated Leu-Enkephalin and its modulation by complexation with 18-crown-6and dimer-formation. 2) charge-state dependent IR spectra of protonated Ubiquitin andCytochrome C. Theoretical calculation results will be shown to support experimental findings aswell.

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일시: 2015년 4월 15~17일(수~금) 3일간
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발표코드: **PHYS.O-5**
발표분야: General Oral Presentation
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Atomic layer deposition of NiO in porous chromium terephthalate MIL-101

정명근 한상욱 박은지 이주하 김보라 김승연 박기정 김일회 김영독*

성균관대학교 화학과

NiO was immobilized on the porous chromium terephthalate MIL-101 via atomic layer deposition (ALD), in which bis(cyclopentadienyl)nickel ($Ni(Cp)_2$) and oxygen were used as metal precursor and oxidizing agent, respectively. NiO-loaded MIL-101(Cr) with various ALD cycles were characterized by transmission electron microscopy (TEM), N_2 and Ar isotherm, X-ray photoelectron spectroscopy (XPS), inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and thermal gravimetric analysis (TGA). It was confirmed that the deposited NiO was distributed inside internal cages as well as on the topmost surface of MIL-101(Cr). The deposition of NiO enhanced a thermal stability of MIL-101 compared to that without NiO and provided a catalytic activity for CO oxidation. In conclusion, we suggest that ALD can be a useful technique for enhancing chemical competency of metal-organic-framework (MOF) and providing new functionality to them.

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Superhydrophobic surface with photocatalytic activity under UV and visible light irradiation

이주하 박은지 정명근 한상욱 김보라 김승연 박기정 김일희 김영독*

성균관대학교 화학과

Surface which is superhydrophobic and photocatalytically active at the same time was prepared by mixing polydimethylsiloxane (PDMS)-coated SiO_2 with nitrogen-doped TiO_2 (N-TiO_2) nanoparticles and distributing the mixture on a flat slide glass with PDMS adhesives. When the relative amount of PDMS-coated SiO_2 was 50% or even larger except 100%, the surface showed a highly stable superhydrophobicity with a water contact angle of 155° and photocatalytic activity for degradation of methylene blue in aqueous solution under UV and visible light irradiation. The surface consisting of PDMS-coated SiO_2 and N-TiO_2 with a ratio of 5:5 was also photocatalytically active for decomposing 2-methylisoborneol which is water contaminant in the presence of UV and visible light.

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Direct Observation of Ultrafast Exciton Dynamics in Helical π-stacks of Self-assembled Perylene Bisimides Using Femtosecond Broadband Fluorescence Upconversion Spectroscopy

성주영 김동호*

연세대학교 화학과

The discovery of molecular self-assembles in nature such as light harvesting complexes in plants and several kinds of bacteria and algae, has captured the imagination of many researchers, inspiring numerous works to fabricate functional aggregates. Moreover, advance in supramolecular chemistry and molecular nanoengineering has paved the way to devise tailor-made artificial photon processing materials for future application of molecular assemblies. The fact that the performance of the electronics and photonics depend strongly on the optical properties of these materials has driven the need for a more fundamental understanding of exciton transport in molecular assemblies.We have sought a more definitive evidence of exciton dynamics in H-aggregates of planer π-conjugated molecules through broadband fluorescence upconversion spectroscopy. Here, for the first time, we have obtained transient fluorescence from Frenkel state of π-π stacking aggregates. By recording trace of the vibronic peak ratio in transient fluorescence spectra, the initial exciton delocalization size and localization dynamics are directly unraveled. This comparative study on a simple PBI dimer and the more realistic model of device constituent elements, extended PBI aggregates suggests the possibility of the long range energy transfer in the artificial photon accessing materials, which occurs in a coherent manner. Therefore, we think that our current work about exciton dynamics of the PBI aggregates would not only give an insight into future experimental and theoretical study of molecular aggregates but also set a stage for the use of molecular aggregates in the field of molecular materials.

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발표코드: **PHYS.O-8**

발표분야: General Oral Presentation

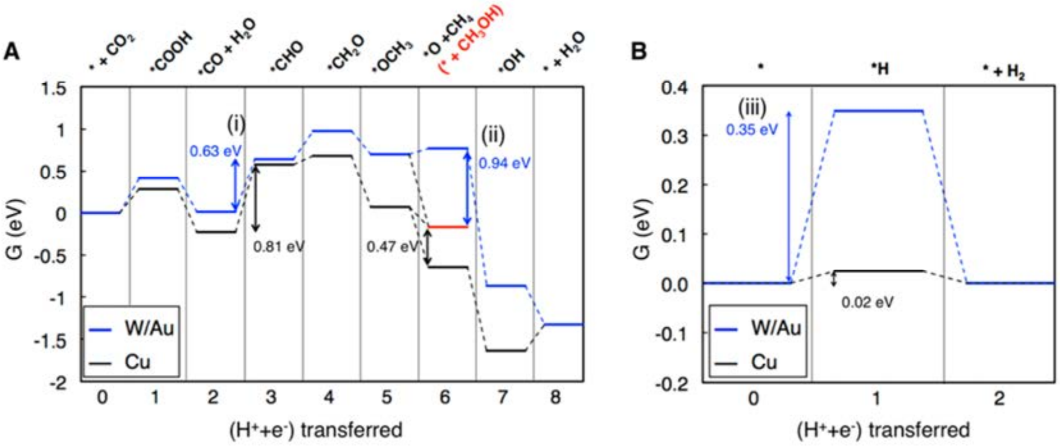
발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 권오훈

Selective Heterogeneous CO_2 Electroreduction to Methanol

백서인 정유성[1,*]

한국과학기술원(KAIST) EEWS [1]한국과학기술원(KAIST) EEWS 대학원

Catalytic electroreduction of carbon dioxide to useful chemical feedstocks is an environmentally and technologically important process, yet the low energy e?ciency and di?culty in controlling product selectivity are great challenges. The reason for part of the latter is that there are presently no catalystdesign principles to selectively control CO2 electroreduction toward a desired product. In this work, as a ?rst attempt, we suggest combining a few criteria (CO binding energy, OH binding energy, and H binding energy) that can be collectively used as activity- and selectivity-determining descriptors to preferentially produce methanol over methane from CO2 electroreduction. We then apply these concepts to near-surface alloys (NSAs) to propose e?cient and selective CO2 electrochemical reduction catalysts to produce methanol. The W/Au alloy is identi?ed as a promising candidate to have increased catalyst e?ciency (decreased CO2 reduction overpotential and increased overpotential for unwanted hydrogen evolution) as well as improved product selectivity toward methanol, in comparison to conventional Cu catalyst.



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Effect of Solution Chemistry and Humic Acid on Dispersity and Sedimentation of Carboxyl-modified Carbon Black Nanoparticles in Aqueous System

박소연 한요셉 황국화 김동현 박선영[1] 김현중[*]

전북대학교 자원·에너지공학과 [1]국립환경연구원 위해성평가연구과

In this study, the dispersion and aggregation behavior of carbon black nanoparticles (CB-NPs) functionalized by carboxyl group was investigated by examining the changes of sedimentation and hydrodynamic diameter of CB-NPs over time as well as the zeta potential. CB-NPs suspension was prepared by adding CB-NPs into NaCl and $CaCl_2$ solution, and the initial concentration of CB-NPs suspension was kept as 10 ppm. Ionic strength range was 0.1 to 10 mM for NaCl and 0.01 to 1 mM for $CaCl_2$ respectively. Also, the effect of humic acid investigated at the same solution condition.Figure 1 shows the change of sedimentation and hydrodynamic diameter of CB-NPs over time and zeta potential at pH 6.0 and the absence of humic acid condition. In NaCl solution, the size of CB-NPs rapidly increased and the relative absorbance of CB-NPs suspension rapidly decreased over time at 10 mM. In $CaCl_2$ solution, the size of CB-NPs remained constant and the relative absorbance of CB-NPs remained almost constant over time at 0.01 to 1 mM. Zeta potential value decreased with increase ionic strength for NaCl and increased with increase ionic strength for $CaCl_2$. Figure 2 shows the change of sedimentation and hydrodynamic diameter of CB-NPs over time at pH 6.0 and the presence of humic acid condition (1 and 5 ppm). In both NaCl and $CaCl_2$ solution the size of CB-NPs and the relative absorbance of CB-NPs suspension remained almost constant over time at all ionic strength range. Based on these results, CB-NPs were found to be well dispersed below 5 mM ionic strength for NaCl and 1 mM ionic strength for $CaCl_2$ at the absence of humic acid, and at all ionic strength range at the presence of humic acid (1 and 5 ppm humic acid).

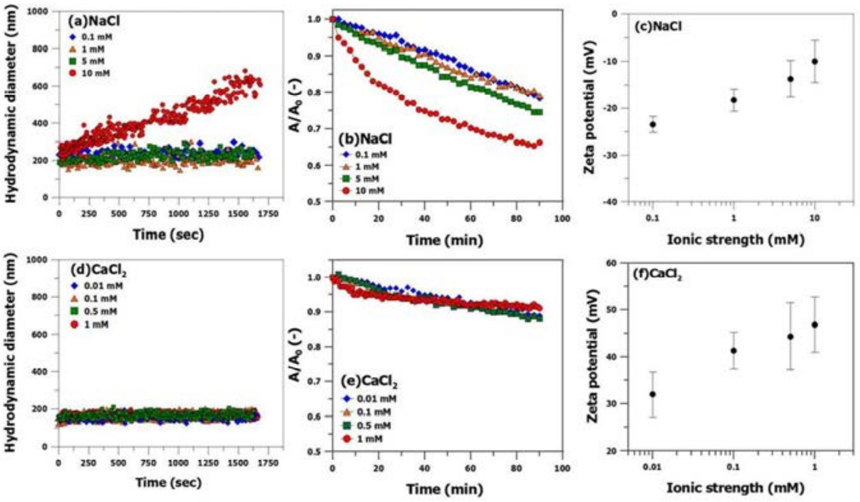

Fig. 1. Dynamic light scattering of CB-NPs in (a) NaCl solution and (d) $CaCl_2$ solution at pH 6.0. Sedimentation plots for CB-NPs in (b) NaCl solution and (e) $CaCl_2$ solution at pH 6.0. Zeta potential for CB-NPs as a function of different ionic strength in (c) NaCl solution and (f) $CaCl_2$ solution at pH 6.0.

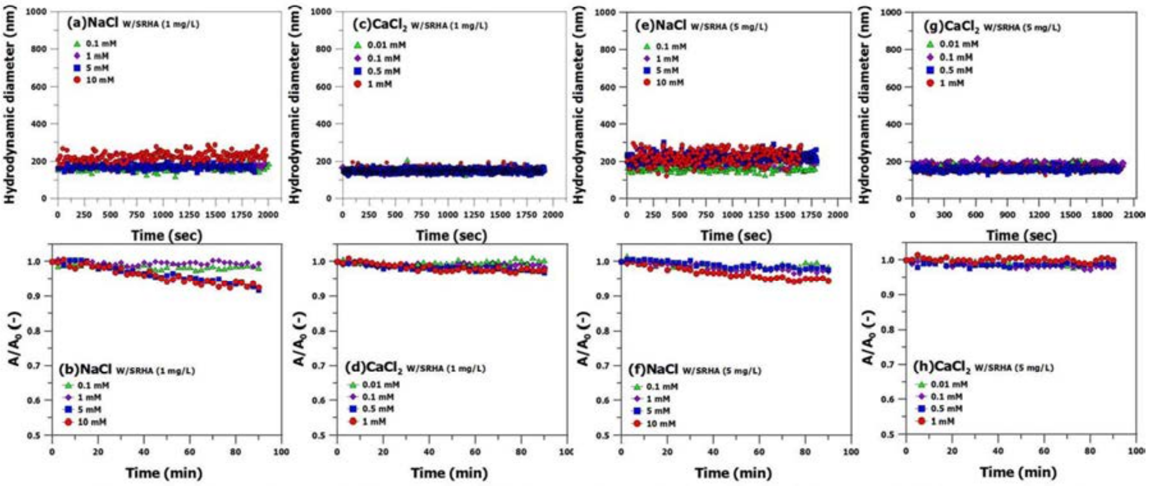

Fig. 2. Dynamic light scattering of CB-NPs in (a) NaCl solution and (c) $CaCl_2$ solution at pH 6.0 and humic acid concentration of 1 ppm and in (e) NaCl solution and (g) $CaCl_2$ solution at pH 6.0 and humic acid concentration of 5 ppm. Sedimentation plots for CB-NPs in (b) NaCl solution and (d) $CaCl_2$ solution at pH 6.0 and humic acid concentration of 1 ppm and in (f) NaCl solution and (h) $CaCl_2$ solution at pH 6.0 and humic acid concentration of 5 ppm.

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State-dependent dispersion of molecules by pulsed optical standing waves

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We report the state-dependent transverse acceleration of CS_2 molecules with pulsed optical standing waves. The steep gradient of the standing wave potential imparts far stronger optical dipole forces on the molecules than propagating pulses. The wild velocity changes due to the standing waves of various intensities are well reproduced in numerical simulations using the effective polarizability depending on the molecular rotational states. The analysis based on the state-dependent effective polarizability can be a cornerstone of developing a new technique of state selection for both polar and nonpolar molecules.

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발표분야: Oral Presentation of Young Analytical Chemists

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장기저장된 폴리우레탄계 복합화약의 특성 분석

이소정 조은소리 권국태 김진석[1,*]

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부

고가의 정밀유도무기는 실전 배치되면, 오랜 기간 동안 개봉하지 않고 운용된다. 유도무기 내부에 있는 화학물질로 구성된 화약은 시간에 따라서 점점 특성이 변하게 되며, 특히 고분자 물질로 구성된 복합화약의 경우 고분자의 분자량이 변하여 복합화약의 기계적특성이 점점 변하고, 이에 따라서 화약의 각종 특성이 변하게 된다. 화약의 주요 특성으로는 성능특성, 민감도특성 및 열적특성을 대표적으로 들 수 있다. 본 연구에서는 약 35 년 이상 장기 저장된 공대지 유도미사일 내부의 주조형복합화약 3 종에 대하여 구성성분, 민감도 특성 및 열적특성을 비교분석한 연구결과다. 3 종의 화약 중 1 종은 고분자의 노화가 많이 진행되었음을 확인 할 수 있었고, 속감도에서도 민감한 결과를 나타내었다.

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발표종류: 구두발표, 발표일시: 금 10:02, 좌장: 이영복

Fabrication of Modified Electrodes Based on Au_{25} Nanoclusters for Electrochemical Sensing Applications

장미 이동일*

연세대학교 화학과

Thiolate protected Au_{25} nanoclusters (NCs) have been the focus of intense research because they exhibit unique electrochemical and optical properties with excellent stability. Previous studies revealed that Au_{25} NCs showed excellent electrocatalytic activity toward the oxidation of dopamine, ascorbic acid and uric acid. Au_{25} NCs with these electrochemical properties can be utilized in a variety of electrochemical applications. In this study, we examined several matrices for the immobilization of Au_{25} NCs on electrode. Sol-gel technology has been commonly used for the encapsulation of a variety of materials including gold nanoparticles. Au_{25} NCs were immobilized into (3-mercaptopropyl)-trimethoxysilane (MPTMOS) network via thiol linkers to form Au_{25} sol-gel electrode (Au_{25}SGE). Cyclic voltammograms of Au_{25}SGE exhibited stable, well-defined and reversible redox peaks of Au_{25} NCs. In addition, enzyme sol-gel electrodes prepared by immobilizing glucose oxidase (GOx) on Au_{25}SGE showed electrocatalytic activity toward the oxidation of glucose. In another study, we explored the possibility of using cationic polymers, for example chitosan and polyethylenimine (PEI), to immobilize Au_{25} NCs. Whereas the redox peaks of Au_{25} NCs in chitosan were not well-resolved, they became clearly resolved by the addition of an ionic liquid, for example 1-decyl-3-methylimidazolium tetrafluoroborate ($DMImBF_4$). The electrochemical sensing properties of Au_{25} NCs immobilized in these matrices are also presented.

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발표분야: Oral Presentation of Young Analytical Chemists
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Fluorescent-free Immunoassay on Nanobiochip by Wavelength Dependent-enhanced Dark Field Microscopy

이승아 박근영[1] 주소영 강성호*

경희대학교 응용화학과 [1]경희대학교 화학과

Highly sensitive fluorescent-free detection on gold-nanopatterned sandwich immunoassay chips was investigated by a wavelength dependent-plasmon resonance scattering (PRS) technique. Individual silver nanoparticle (SNP) conjugated-target protein molecules on the nanobiochip were selectively detected by the wavelength dependent-enhanced dark field illumination. With the enhanced dark field spectral imaging technique, we observed label-free cardiac troponin I as a model target molecule on 100 nm and 500 nm gold spots by monitoring changes in the plasmonic resonance based on wavelength dependence. Quantitative analysis as a function of increasing PRS intensity was possible in the range of 85 aM - 35 fM through enhanced dark field microscopy. We also showed that the PRS signals from the SNPs (blue color) and the gold spot (yellow color) could be clearly distinguished by using the color camera. The wavelength dependent-enhanced dark field illumination method allows us to selectively detect target biomolecules at the single-molecule level for next generation biochips.

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Novel One-Capillary Dual-Wavelength Nonaqueous Capillary Electrophoresis for Simultaneous Analysis of Various Synthetic Organic Dyes

박문희 구민정 강성호[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Dual-wavelength nonaqueous capillary electrophoresis (DW-NACE) was developed for simultaneous analysis of seven synthetic organic dyes [i.e., crystal violet (CV), methyl violet blue (MVB), methyl violet B base (MVB), rhodamine 6G (R6G), rhodamine B Base (RBB), nile blue A (NBA), and methylene blue (MB)] at different emission wavelengths in a single-capillary. All synthetic organic dyes were simultaneously injected, detected, and quantitatively analyzed using two lasers (543 nm laser and 635 nm laser) within 15 min in the dynamic ranges as follow: CV, MVB, MBB (0.5 - 50 μM), R6G (0.05 - 5 nM), MB (0.02 - 10 pM), NBA (0.006 - 10 pM), and RBB (0.4 - 1000 fM). In particular, the limit of detection (LOD, *S/N* = 3) in the RBB was 0.4 fM, which was 2 x 10^5 times lower than the LOD obtained from previous nonaqueous micellar electrokinetic chromatography methods. This novel method shows the feasibility of fast high-throughput screening of various synthetic organic dyes.

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장소: 일산 KINTEX

발표코드: **ANAL.O-5**

발표분야: Oral Presentation of Young Analytical Chemists

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Sub-diffraction limited resolution of nanoparticles by wavelength-modulation plasmonic scattering nanoscopy

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Sub-diffraction limited resolution of Nanoparticles (NPs) was achieved with wavelength-dependent enhanced dark-field (EDF) illumination. Diffraction limited and color blended adjacent EDF images of gold nanoparticles (GNPs), gold nanorods (GNRs), and silver nanoparticles (SNPs) were modulated at their specific localized surface plasmon resonance wavelengths. The point spread functions of NPs were approximated as symmetric two-dimensional (2D) Gaussian functions and fitted with least-square algorithm to resolve the central coordinates (x, y). The Cram?r-Rao lower bound (CRLB) based localization precisions of GNPs, GNRs, and SNPs were measured as 2.5 nm, 5.0 nm, and 2.9 nm, respectively. According to the resolved coordinates of NPs and the corresponding localization precisions, sub-diffraction limited images were rendered. This novel method was applied in a live single cell and provided remarkable sub-diffraction limited images of NPs.

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Evaluation of UV-curing behaviors for acrylate polymer by real-time FT-IR

박재홍 남궁현*

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Real-time FT-IR spectroscopy enables us to monitor the change of functional groups involving in the polymerization. By detecting the conversion of monomers into polymer as well as unreacted groups in curing polymer, the curing behaviors could be readily observed and characterized. We have developed the optimal FT-IR system consists of an ATR, a mercury xenon UV-lamp, and a FT-IR spectrometer. With the real-time FT-IR spectroscopy, we investigated the characteristics of the curing kinetics of the UV-cuable acrylate. It is found that the proper vibrational band indicating curing process of the acrylate was determined at the 810 cm^{-1}, out of plane, C-H bending in $H_2C=CH-$ group. The curing kinetics of the polymerization was phenomenologically described as a compressed exponential function without physical interpretation. Using this empirical modeling, UV-curing behaviors of the acrylate resin were evaluated with varying photo-initiator concentration. Analysis on the curing behaviors allows us to specify relationship of photo-initiator concentration, curing rate of the polymer, and amount of residual with various UV-curing environments.

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Electrocatalytic Conversion of Carbon dioxide Using Atomically Precise Metal Nanoclusters Modified Electrodes

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Conversion of carbon dioxide (CO_2) an unintended byproduct from energy generation and fuel consumption has become the most important worldwide issue. Hence, efficient conversion of CO_2 to valuable chemicals such as syngas, CO, formate and methanol remains one of the challenges for CO_2 utilization. Of the diverse approaches of CO_2 conversion, electrocatalytic reduction of CO_2 has received much attention because it can be easily designed for a continuous process at room temperature. However, the electrode materials such Cu and Ag currently employed in the electrocatalytic reduction of CO_2 exhibit large overpotential and low current density, which makes it difficult to develop carbon neutral process from electrocatalytic methods. In this poster, we report that atomically precise metal nanoclusters for example, $Au_{25}(SR)_{18}$ where SR is thiolate, can be effectively used as homogeneous and heterogeneous catalysts. CO_2 reduction potential was found to be -2.0 V vs. NHE at a glassy carbon electrode in CH_2Cl_2, which decreased significantly in the presence of Au_{25} nanoclusters and more overpotential decreasing was observed by introducing an ionic liquid as co-catalysts. Various types of nanoclusters prepared by doping with foreign metals such as Pt, Pd and Cu offer special advantages in the development of electrocatalysts. The preparation and effects of doping in the electrocatalytic reduction reaction are presented. Au_{25}-based modified electrodes were also found to be an efficient heterogeneous catalyst for the reduction of CO_2. The electroreduction of CO_2 was found to start at -1.2V at glassy carbon electrode in aqueous media and positively shifted to -0.9 V at the modified electrode, indicating the electrocatalytic effect of Au_{25} nanoclusters.

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Optimization and Application of APCI Hydrogen?Deuterium Exchange Mass Spectrometry (HDX MS) for the Speciation of Nitrogen Compounds

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A systematic study was performed to investigate the utility of atmospheric pressure chemical ionization hydrogen?deuterium exchange mass spectrometry (APCI HDX MS) to identify the structures of nitrogen-containing aromatic compounds. First, experiments were performed to determine the optimized experimental conditions, with dichloromethane and CH3OD found to be good cosolvents for APCI HDX. In addition, a positive correlation between the heated capillary temperature and the observed HDX signal was observed, and it was suggested that the HDX reaction occurred when molecules were contained in the solvent cluster. Second, 20 standard nitrogen-containing compounds were analyzed to investigate whether speciation could be determined based on the different types of ions produced from nitrogen-containing compounds with various functional groups. The number of exchanges occurring within the compounds correlated well with the number of active hydrogen atoms attached to nitrogen, and it was confirmed that APCI HDX MS could be used to determine speciation. The results obtained by APCI HDX MS were combined with the subsequent investigation of the double bond equivalence distribution and indicated that resins of shale oil extract contained mostly pyridine type nitrogen compounds. This study confirmed that APCI HDX MS can be added to previously reported chemical ionization, electrospray ionization, and atmospheric pressure photo ionization-based HDX methods, which can be used for structural elucidation by mass spectrometry.

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Global phosphopeptide enrichment by grating phospho-specific antibodies into online mHFER-nanoLC-ESI-MS/MS

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Phosphoprotein, one of post translational modifications, is involved in cellular processes such as cell proliferation, cell signaling, and apoptosis. Mass spectrometry in phosphoproteomics is commonly utilized due to accuracy, sensitivity, and precision. However, phosphoproteins in MS analysis have several limitations due to low abundant and low ionization efficiency caused by negatively charge ion of phosphates in general MS analysis with a positive acquisition mode. Although conventional enrichments (e.g., SCX, IMAC, and TiO_2) in phosphoproteome has been widely used, a large amount of proteins (above 500 ug) is inevitably required for next shotgun analysis. Herein, we introduce a new strategy for enrichment of targeted phosphopeptides whereby that enables the identification of phosphopeptides and their sites of phosphorylation with the smallest sample amount (~1 ug). To this end, we newly developed the concept of coupling online microbore hollow fiber enzyme reactor (mHFER) with phospho-sepcific antibodies (pAbs) to selectively enrich targeted phosphopeptides from protein complex mixture. In pAbs-based online phosphopeptide enrichment with mHFER, tryptic peptides obtained from MCF7 were mixed with pAbs, and then followed by the mixture was injected into online mHFER-nanoLC-ESI-FT orbitrap-MS/MS. The peptides having no-affinity with pAbs were washed out during flow-through in the mHFER (10 kDa in MW cutoff), and the remaining phosphopeptides eluted subsequentially from mHFER by tryptic digestion were subjected to online shotgun analysis. As a result, we found that pAbs-based online mHFER is highly selective, precise, and suitable for phosphopeptide enrichment, compared to that of conventional mothods.

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Application of isotope-coded carbamidomethylation for absolute quantification of human serum BNP-32 using a nanoLC-ESI-MS/MS

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Brain natriuretic peptide-32 (BNP-32) is widely known as an essential biomarker in congestive heart failure (CHF). N-terminal proBNP, a precursor form of BNP-32, is more abundant than that of cardiac troponin T, when exposed to the extraordinary left ventricle-ejection fraction (LV-EF) caused by CHF. In spite of determination of BNP-32 in human serum is essential for precise determination of CHF, it is still challenges, due to its low abundance in human serum (100 pg/mL) and higher variation in measuring targeted BNP-32 using an immunoassay. Here, we applied a novel and simple isotope labeling method, named as isotope-coded carbamidomethylation (iCCM), to the quantification of the human BNP-32. In iCCM, two aliquots of BNP-32, having two cysteine residues, was denatured with a reducing buffer (50 mM ammonium bicarbonate contained with 10 mM dithiothreitol) and then alkylated separately with each of iodoacetamide (IAA) as carbamidomethylation (CM) and its isotope (IAA-13C2, D2), thereby leading to the mass difference of 8 Da between CM- and iCCM-labeled BNP-32. To evaluate the efficiency of iCCM approach, the CM- and iCCM-labeled BNP-32 standards were pooled at five different mixing ratios and then introduced into nanoLC-ESI-MS/MS. As a result, the mixing ratios of CM-/iCCM-peptides were dramatically matched with their expected ratios with good linearity (R2=0.9999). The developed iCCM strategy is an alternative tool for quantification and early diagnosis of BNP-32 in CHF patients.

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Top-down and bottom-up lipidomic analysis of lipoproteins from rabbits by FlFFF and mass spectrometry

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Lipidomic analysis from lipoproteins requires separation of high-density lipoproteins (HDL) and low-density lipoproteins(LDL), followed by mass spectrometry (MS). In a separation technique of flow field-flow fractionation (FlFFF), particles attain different equilibrium heights based on their sizes and smaller particles at the higher equilibrium height elute faster than larger particles, having a higher velocity in the flow-driven laminar flow. As the size of HDL is smaller than that of LDL, separation of lipoproteins from plasma is easily achieved by FlFFF in their intact forms. The bottom-up lipidomic analysis of lipoproteins is carried out by FlFFF for fractionation of lipoproteins, lipid extraction, and analysis by liquid-chromatography-mass spectrometry (LC-MS). Although bottom-up method can provide an extensive library of lipids, it requires tediously long preparation or analysis time, which is extremely inconvenient when the sample set is large. For analysis of targeted lipids from lipoproteins, top-down approach of on-line FlFFF-MS can shorten the analysis time as neither of off-line FlFFF nor lipid extraction is required and still provides highly accurate analysis. In this study, a comprehensive lipidomic analysis of lipoproteins from pooled serum samples of rabbits with metabolic conditions were investigated by the bottom-up approach using multiplexed hollow fiber FlFFF (MxHF5) for separation and collection of lipoproteins, followed by nanoflow LC-ESI-MS/MS for lipid analysis. Based on the result from bottom-up method, lipid species showing significant differences between groups of rabbits were selected and quantified by individual samples in top-down chip-type asymmetrical FlFFF-ESI-MS/MS.

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Evaluating the Effect of Cross-linking Agent Content and Polymerization Methods on Molecular Weight and Structure of Branched Cationic Polyacrylamide Copolymer by Frit-inlet Asymmetrical Flow Field-Flow Fractionation &Multi-angle Light Scattering

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Polyacrylamide (PAM) consists of acrylamide monomers, which form long-chain polymers by free radical polymerization, and it is widely used as flocculant in waste water treatment and oil removals. For higher efficiency in flocculation, molecular weights, structures, and charge densities of PAM must be taken into consideration. For negatively charged particles in waste water, branched cationic PAM has been reported to be more efficient flocculant than linear one as branched one has lower viscosity and higher solubility than linear polymers. In this research, effect of different amount of crosslinking agent and different kinds of polymerization methods on absolute molecular weight and structure of branched cationic PAM copolymers were investigated. Different amount of crosslinking agent determines the number of branches per polymer molecule, which eventually affects the structure and molecular weight. As the amount of crosslinking agent increases, polymers are predicted to be more compact in sizes. Two different polymerization methods, solution and emulsion polymerization, affect the chain length of polymer, which changes the molecular weight and RMS radius of the copolymer. Changes in molecular weight and RMS radius by the content of crosslinking agent and different polymerization methods were analyzed by frit-inlet asymmetrical flow field-flow fractionation (FIAF4)-multi-angle light scattering (MALS).

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Lipid Profiling of Diabetic Rat Muscle tissues under Physical Exercises using Nanoflow LC-ESI-MS/MS

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Lipids are responsible for various biological functions such as constituents of cell membrane and participants in cell signaling, and they are relevant to the development of various human diseases such as diabetes. As diabetes develop, general lipids profile is likely to alter from that of healthy control. Exercise has been reported as one of the major factors that alters the lipids profile in many types of diseases. Thus, lipidomic research on the change in the abundance of lipid species induced by exercise is important in revealing the correlation between diabetes and exercise.In this research, the gastrocnemius and soleus muscles of skeletal muscles from the lower leg were selected to investigate the effect of exercise on healthy controls and diabetic models. While gastrocnemius is mainly composed of white muscle that contracts lower leg rapidly and powerfully by anaerobic bursts of activity, and soleus is a red muscle that contracts for longer period of time with little force by aerobic bursts of activity. Lipids in gastrocnemius and soleus skeletal muscles from four groups of rats - healthy controls, healthy controls under exercise, diabetic models, and diabetic models under exercise - were investigated to discover the lipid species showing significant differences between healthy and diabetic rats, and to evaluate how exercise changes the profile of lipids from healthy and diabetic rats. Lipids in two different muscles were extracted from pooled samples in each group using the modified Folch method with MTBE/MeOH, and characterized by nanoflow liquid chromatography electrospray-ionization tandem mass spectrometry (nLC-ESI-MS/MS). A total of 245 and 252 lipid species from gastrocnemius and soleus muscles, respectively, were identified and analyzed quantitatively.

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Effect of Incubating Microbial Species in Freshwater on Dissolved Organic Matters by Flow Field-Flow Fractionation

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Dissolved organic matters (DOM) and particulate organic matters (POM) are organic substances that are generated by microbial metabolism in the environment and are widely distributed in soil and freshwater. There have been a number of studies that adopted various methods to analyze and characterize organic matters. Among different kinds of organic matters, biodegradable organic matters (BOM) are fraction of organic matters that are ingested and metabolized by microbial species. In this study, asymmetrical flow field-flow fractionation (AF4) was utilized to analyze biodegradable DOM (BDOM) and POM (BPOM) in forest stream, agricultural stream, and Bamseom in Korea and characterize the change in organic matters caused by incubating microbial species in each sample. Since humic and fulvic substances, which best represent the organic matters in most of the freshwater, are sensitive to change in ionic strength of the carrier solution used in AF4, it is important to optimize the condition of the carrier solution to obtain reproducible result. Also the retention of organic matters during analysis is affected by the type of membrane material used. In this experiment, by examining the result of changing ionic strength of carrier solution and membrane material, the best carrier solution and membrane material for fractionation were selected.Two different signals, protein-like and humic-like signals, were selected to characterize two types of fluorophores in each sample. After the fractogram of each sample is obtained, peak areas of before- and after-incubation samples are compared to see the degree of degradation of each kind of organic matters by the microbial species.

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High Speed Subcellular Organelle Fractionation by Flow Field-Flow Fractionation

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Subcellular organelles have their own specific roles in cells. When organelles malfunction in cells, activities of proteins in cells can be affected, causing organelle related diseases. Researches on discovering biomarkers of disease by separating organelles have attracted increased attention in biological research fields. Therefore, in subcellular organelle studies, fractionation of organelle is a fundamental and crucial stepUsually, separation of subcellular organelles is conducted by centrifugal methods but even though procedures are relatively simple and easy to carry out, the methods can be time-consuming as they require additional purification processes due to the low efficiency in purification. Besides centrifugal methods, fractionation of subcellular organelles can be conducted by fluorescence activated sorting or affinity purification methods. However, these methods usually require relatively complex preprocessing steps. Flow field-flow fractionation (FlFFF) is an elution method based on size-separation. In this study, FlFFF was attempted to fractionate the various cell organelles in a short period of times without any complex pre-processing steps. Separation of organelle was carried out in a steric mode of FFF and completed within 15 minutes. Organelles in each fraction were confirmed with different methods of scanning electron microscope (SEM) for observe and compare the particle sizes and western blotting to identify organelle markers. Lastly, by using nanoflow liquid chromatography and tandem mass spectrometry, subcellular proteins from each fraction was analyzed.

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Profiling of phosphoproteome from respiratory syncytial virus-inducedsera using phospho-specific antibodies in combination with online mHFER nLC-ESI-FT orbitrap-MS/MS

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Respiratory syncytial virus (RSV) is a major pathogen of infants and young children, and its infection annually results more than 300,000 deaths worldwide. Although the proteomic study for treatment of disease caused by RSV has been reported, discovering biomarker of RSV is not fully evaluated. To unveil a biomarker from RSV-induced samples, we carried out the profiling of phosphoproteome in RSV-induced sera. Phosphoprotein, one of post translational modifications, is relevant to many human diseases and bioresponses. In order to profile phosphoproteome from RSV-induced sera, phospho-specific antibodies (pAbs) with online microbore hollow fiber enzyme reactor (mHFER, M.W. cut off 10 kDa) was utilized for phosphopeptides enrichment. RSV-induced mouse sera (3days and 7days) and control (0 day) were digested with trypsin and proteolytic peptides from each mouse serum (0day, 3days, 7days) were reacted with pAbs for 1 hour at 4℃. The resulting mixture was introduced into online mHFER-nLC-ESI-MS/MS. Both of ordinary peptides and phosphopeptides having no affinity with pAbs will be first eluted during flow-through run, and the remaining phosphopeptides in mHFER were simultaneously released by trypsin. Consequently, phosphopeptide enrichment utilizing pAbs-based online-mHFER facilitates for understanding cell signaling in RSV infection pathway and contributing development of therapeutic agent.

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Highly active graphene based Ni-Pd binary alloyed catalysts for electrooxidation of ethanol in an alkaline media

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전남대학교 화학과

Highly active graphene (G)-supported NixPd100-x binary alloyed catalysts (BACs) were prepared with the variation of Ni and Pd metals loading, through a facile chemical reduction method and used as an anode catalyst for ethanol oxidation reaction (EOR). The X-ray diffraction reveals that the NixPd100-x/G catalysts were homogeneously alloyed and Ni was present with the oxidized form. The transmission electron microscopy images also suggest the alloyed formation with different shapes of metal nanoparticles (NPs). The electrochemical properties of the catalysts were evaluated using cyclic voltammetry (CV) and chronoamperometry (CA) in 1 M KOH electrolyte. The higher catalytic activity for EOR was observed in Ni50Pd50/G. Among all NixPd100-x/G BACs, the Ni50Pd50/G catalyst showed highest onset potential (?0.8 V) with long term stability. The overall parameters of EOR study were determined that the Ni50Pd50/G was more favorable in various ethanol concentration and scan rate.

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An amerometric biosensor for Virus Proteins

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In this presentation, we demonstrate a sandwich assay platform involving aptamer-protein-antibody complex for the electrochemical detection of virus protein onto a gold nanoparticle modified electrode surface. Our attempt was to achieve viral protein (e.g. H5N1) sensing through the measurement of associated current resulting from the enzymatic reaction between alkaline phosphatase conjugated to anti-H5N1 adsorbed onto aptamer/H5N1 surface complexes and the substrate, 4-amino phenyl phosphate (APP).Cyclic and differential voltammetry methods were used to characterize the detection method.

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Separation of differently sized gold nanorods using gel electrophoresis

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본 포스터에서는 불균일하게 크기가 분포되어 있는 금 나노로드 콜로이드 용액으로부터 균일한 크기의 나노로드를 젤 영동법으로 분리하기 위해 젤 매트리스 및 계면활성제 농도를 변화시켜 분리법을 최적화시키고자 하였다. 이와 함께, 항체로 코팅된 금나노로드 입자를 크기별로 분리하는데 최적화된 방법을 적용하였다. 젤 영동 분리 실험 결과를 전자투과현미경(TEM) 이미지와 UV-vis 분광법을 이용하여 확인하였다.

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Structural characterization of MAS NMR as a cathode material for lithium ion battery

안지은 김민지 하지원 이영일*

울산대학교 화학과

$LiCoO_2$ is generally used as the cathode material, however, it has the thermal instability, poor rate performance, and the toxicity and high cost. As alternative $LiCoO_2$, $xLi_2M'O_3*(1-x)LiMO_2$ electrode materials (M′= Mn, Ti and M = Mn, Ni, Co) have attracted much attention due to its high rate performance and improved safety. In this work, structural investigations of $LiNi_{0.8}Co_{0.1}Mn_{0.1}$, $LiNi_{0.8}Co_{0.15}Mn_{0.05}$, $LiCo_xAl_yO_2$ cathode materials has been performed by ^{7}Li , ^{27}Al and ^{59}Co MAS NMR.

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Characterization of bleached human hair by FT-IR microspectroscopy and Chemical imaging

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The FT-IR imaging method enables chemical imaging by combining the spectral and spatial information. The chemical images consist of chemical information from all pixels covering the measuring areas at the same time. It also useful method of analysis for human hair, with the ability to analyze the central core, cortex, of cross sectioned hair. We studied bleaching of the hair, and checked chemical effects as a function of position in the hair cross section. Many researchers observed the surface of hair using SEM, and now it is well known that cuticle layers lift and break. The transformation due to breakage of a specific chemical group was observed and spatially characterized. In this study, the products from disulfide oxidation of the amino acid cystine are sulfonic acid of cystine, cystine monoxide, and cystine dioxide. We observed the cystine monoxide band from the products of disulfide oxidation of the amino acid cystine that is also associated with hair damaging. By spectrally mapping infrared functional groups, the images of the damaged location can be obtained from bleached hairs.

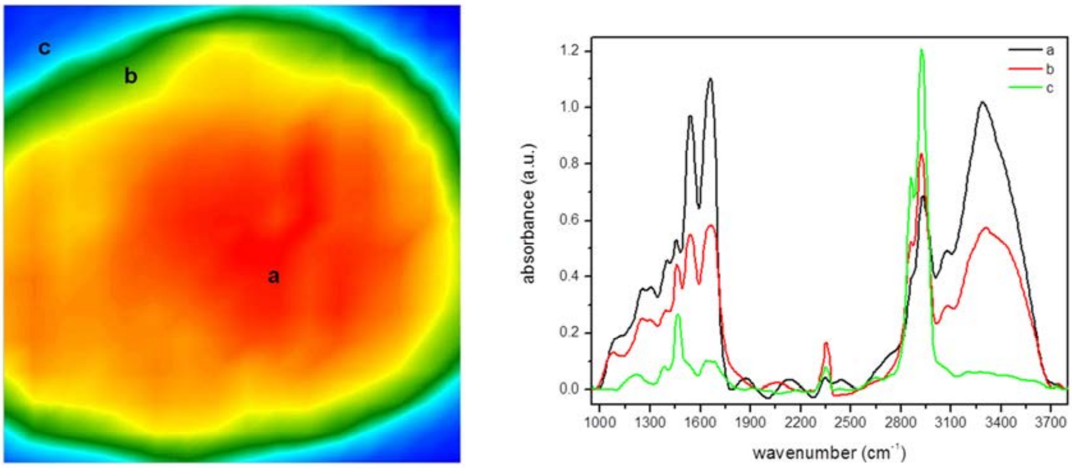

Figure 1. Chemical image and FT-IR spectra of cross-sectioned human hair.

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The Development of Combined System with Parabolic IR Emitter and Pyroelelctric sensor within Bandpass Filter for Open Path Remote Analysis

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화재 시 화염과 더불어 독성 가스가 발생하며 이 가스를 현장에서 분석할 때 여러 가지 방식이 사용되고 있다. 기존 방식은 발생가스를 직접 샘플링하여 실험실에서 측정하는 방법이 주로 사용되었으나, 샘플링 등의 절차에서 발생되는 분석오류를 줄이기 위해 현장에서 샘플링없이 직접 측정하는 방식이 요구되고 있다. 화재 현장의 경우 화재 위험 반경에 때문에 근접 분석이 어려워 원거리에서 측정하여야하며, 현재 사용하는 원거리 분석 장치(Passive Open Path FT-IR)의 장비 크기 및 이동 문제로 현장 접근성에 어려운 단점이 있다. 따라서 원거리 분석을 용이하게 하기 위해 센서의 크기를 최소화하고 측정자의 위험을 최소화하기 위해, 무선 통신을 통하여 가스를 모니터링하도록 개발하였다. 원거리 측정을 위하여 고 감도 Pyroelelctric sensor 와 Silicon nitride 소재로 한 Parabolic 적외선 광원으로 구성하였으며, 무선 통신은 blue-tooth 통신으로 구성하였다. 이러한 장비를 사용하여 CO 등 화재 관련 데이터를 정량 분석한 결과 상관계수(R2)가 0.9 이상의 높은 선형성을 확인하여 원거리 측정의 가능성을 입증하였다.

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Simultaneous Analysis of NSAIDs in Aqueous Sample by Dispersive Liquid-Liquid Microextraction (DLLME) and LC/MS

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Dispersive liquid-liquid microextraction (DLLME) may be utilized as a green chemistry approach to reduce the consumption of hazardous organic solvents in the chemical analysis. A simple and efficient sample preparation method was developed using DLLME prior to LC/MS analysis for simultaneous extraction and determination of trace amounts of Non-Steroidial Anti-Inflammatory Drugs (NSAIDs) including indoprofen, ketoprofen, naproxen, diclofenac, ibuprofen, mefenamic acid, tolfenamic acid from an aqueous sample. Optimal dispersive solvent and extraction solvent were chosen acetonitrile and chloroform, respectively. Simultaneous chromatographic separation of seven NSAIDs by HPLC/MS system was achieved on an Eclipse XDB-C18 (2.0 mm i.d. × 150 mm length, 5 ㎛ particle size) column using isocratic elution with 0.1 % formic acid and methanol (30:70).

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Chemical Speciation Applied Supercritical Fluid Chromatography-atmospheric Pressure Photon Ionization Hydrogen/Deuterium Exchange (HDX) Mass Spectrometry for Structural Anaylsis

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For comprehensive complicated mixture, structural identification is a very important for mass spectrometry analysis of poly aromatic hydrocarbon compounds. Hydrogen/Deuterium Exchange (HDX) technique has been used for structual interpretation in proteins, peptides, metabolites, antibiotics and petroleomics. However, HDX technique is limited because expensive deuterium solvent is used a lot and hence coupling to high performance liquid chromatography (HPLC) has been limited. In this study, HDX tendency of 21 standard compounds including polar heteroatoms at the molecular level was identified by combination of HDX in the process of atmospheric pressure photo ionization (APPI) and Supercritical fluid chromatography-Mass Spectrometry (SFC-MS). SFC utilizes supercritical carbon dioxide, methanol as mobile phase and offers a faster runtime in comparison with HPLC which is used aprotic solvents. In other words, mobile phase only a little of deuterated methanol is needed when HDX is applied to SFC. 0.3 mL of CH3OD for deuterium exchange was just used during all chemicals was eluted in 9 minutes. Overall, HDX SFC-MS was successfully applied to nitrogen-containing compounds preliminary to analysis of heavy crude oils for structual elucidation. Therfore, these results are examples of using powerful separation technique and we expect that this developed technique will be carried out to study crude oils and metabolites where a many unknown compounds have to be determined.

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Electrochemical and HPLC analysis of anticancer drugs

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본 포스터는 서로 섞이지 않는 두 전해질 (수용성 액체/유기성 액체) 계면에서 항암제가 전이하는 반응에 따라 전류 값의 변화를 측정하는데 기초를 둔 항암제 검출용 전기화학 센서 개발에 관한 연구 결과를 나타냈다. 수용성 액체와 유기성 액체 사이에 계면을 형성하고 전압을 걸어주었을 때, 물에 존재하는 약물 이온이 유기용액으로 전이하는 정도에 따라 전류의 변화가 일어나는 것을 순환전압전류법과 시차펄스 전위법을 사용하여 분석하였다. 또한, 항암제를 검출한 전기화학적 데이터와 HPLC 로 분석한 결과를 비교분석하였다.

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The Quantification and Characterization of N-linked Glycans by Capillary Electrophoresis UV-Visble Spectroscopy and Capillary Electrophoresis Mass Spectrometry

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창원대학교 화학과

Glycosylation is attaching the oligosaccharides to proteins or peptides by post-translational modification processing. Various investigations concerning quantitative glycan analysis have been performed because of the importance of the oligosaccharide moieties on glycoproteins that affect a wide range of protein functions such as cellular recognition processes.Presently, capillary electrophoresis (CE) has become an accepted technique for the analysis of the biomolecules. The biomolecules can be separated by CE with high speed and resolution. In this study, the quantitative analysis of N-linked glycans of the glycoprotein has performed in UV-Visble spectroscopy with 2-amino benzamide (2-AB) labeling techniques. The structural analysis of N-linked glycans was characterised by capillary electrophoresis tandem mass spectrometry (CE-MS/MS)Key WordsCapillary electrophoresis, Mass spectrometry, UV-Visble spectroscopy, 2-AB labeling and N-linked glycan

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Carboxyl Modification of Peptides with Linear Aliphatic Diamines for Increasing Charge States

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Mass spectrometry has been used usually in protein identification. Especially mass spectrometry played a significant role in the analysis of peptides sequence, as well as posttranslational modification (PTM) analysis. However, analysis of PTMs, such as phosphorylation and glycosylation, is difficult with collision-induced dissociation (CID) by the loss of modification residues. The CID and electron-transfer dissociation (ETD) are complementary each other to interpret the PTMs. But ETD is particularly ineffective for the dissociation of tryptic peptide in doubly and singly charge states.In this study, we have tested carboxyl modification of peptides as a method for increasing the charge states of peptides in electrospray ionization with tandem mass spectrometry (ESI-MS/MS). The carboxyl-reactive crosslinker reagent 1-[Bis(dimethylamino)methylene]-1H-1,2,3-triazolo[4,5-b]pyridinium 3-oxid hexafluorophosphate (HATU) is used to crosslink the carboxylic acid group of the peptide angiotensin II and the tryptic digested albumin peptides to linear aliphatic diamines such as ethane-1,2-diamine, butane-1,4-diamine, and hexane-1,6-diamine.As a result, the carboxyl modified peptides increased the most abundant charge state compared to native peptides. The longer crosslinkers effectively increased the most abundant charge state because of the reduction of the charge repulsion in the peptides.Key WordsPeptide, Carboxyl modification, ETD, Mass spectrometry, HATU, and Linear aliphatic diamines

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An EWOD (electrowetting-on-dielectrics) platform for detection of chemical and biological warfares

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서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Electrowetting-on-dielectrics (EWOD) devices actuate droplets of volumes up to several microliters using the principle of modulating the intersurfacial tension between an electrode coated with a dielectric layer and a liquid droplet. In this study, we have sought to perform sample preparation for MALDI-TOF detection of chemical and biological warfares using EWOD technology. In this study, electrodes were patterned on the paper with a conducting material and then its surface was coated with a dielectric layer of parylene-C and covered with a Teflon AF thin film to increase hydrophobicity on the surface of the chip. Application of voltage potential to the electrodes reduces the solid-liquid interfacial tension, so resulting in movement of a droplet through a series of electrodes. This result is expected to help one achieve the automation of the detection of chemical warfares. In the poster-session, the detailed experimental setup and the results will be presented.

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MALDI-TOF Quantitative Analysis of Polymeric guanidine-containing Biocide ingredients in commercial products

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서강대학교 화학과

Guanidine-containing polymeric ingredients, such as polyhexamethylene guanidine (PHMG) and poly hexamethylene biguanidine (PHMB), possess antiseptic, antibacterial activity and therefore are able to prevent the growth of bacterial, mold, and any microbe. Due to this reason, these biocidal ingredients are used in commercial products such as wet wipes, humidifier disinfectants, contact lens cleansers, and cosmetic removers. Recently, it was reported that long-term exposure to guanidine-containing polymeric biocides can cause pulmonary disease when it is inhaled in a form of droplets. For this reason, the necessity to qualitatively and quantitatively analyze these compounds has been addressed. In the present study, we developed a sample purification and enrichment procedure for the analysis of these PHMG and PHMB, and the pre-processed sample was analyzed using MALDI-TOF mass spectrometry. And, we proved for quantitative analysis of PHMG and PHMB by applying the internal standard method. We have tested several internal standards which were chosen based on the similarity to PHMG; internal standard using 13C-guanidine substituted PHMG shows different distribution in comparison with normal PHMG which can overcome the peak overlapping. The developed method is expected to provide a useful protocol for the quantitative analysis of guanidine-containing polymeric biocides use in commercial consumer products.

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TEMPO-assisted FRIPS MS analysis of a peptide with three or more disulfide bonds

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We characterized the small proteins of insulin (51 amino acids, 5,733 Da) using FRIPS (free radical initiated peptide sequencing) mass spectrometry. Insulin consists of two segments, A-chain and B-chain, which are linked together by a multiple disulfide bonds, TEMPO-assisted FRIPS MS approach is reported to selectively cleave the disulfide bond. However, it is not reported yet whether or not it is applicable for peptides/proteins with multiple disulfide bonds. In the present study, we applied the TEMPO-assisted FRIPS approach to the insulin to see how multiple disulfide bonds affects the fragmentation behavior of peptides with multiple disulfide bonds. In our preliminary results, it was found that with TEMPO-assisted FRIPS can provide more detailed structural information of insulin without the reduction of disulfide bonds than the conventional CID could do. In the symposium, we will discuss the potential use future direction of the current research.

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Radical-based peptide fragmentation MS

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The bottom-up MS approach is most widely applied to identify and characterize proteins. However, there exists a weakness that the sequence coverage is rather low. To achieve a better sequence coverage, the middle-down MS approach has been suggested as a complementary tool, which is run in parallel with the bottom-up MS. With this information, we have sought to extend the TEMPO-assisted FRIPS (free radical initiated peptide sequencing) MS approach to the middle-down MS of proteins. As a preliminary study, first, we have explored the possibility of characterizing a relatively large peptide of melittin of ~3 kDa using TEMPO-assisted FRIPS MS, which showed extensive backbone fragmentations. Motivated at the promising results for melittin analysis, we applied the FRIPS methods to peptides produced by Lys-N digestion of BSA. As Lys-N cleaves at N-terminal side of lysine amino acid, it is expected that a longer peptide sequence can be obtained compared with the trypsin digestion that are mostly used in the bottom-up method. For the longer peptides, it was revealed that extensive a, c, x, and z-type fragments were generated in FRIPS MS. Further details of our study will be presented in the symposium.

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Colloidal Carbon Black Nanoparticles & Graphene Oxide Embedded Thin Sol-Gel Film for Dye Molecule Analysis of Handwriting Inks by Laser Desorption/Ionization Mass Spectrometry

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Colloidal carbon black nanoparticles were used as a matrix for matrix-assisted laser desorption/ionization(MALDI) analysis of Handwriting ink dye mollecules. For the application of the analysis method of forged document using the surface-assisted laser desorption/ionization(SALDI) similar to MALDI, we conducted a research to use the Spraying Method of Carbon Black nanoparticles to enhance the detection sensitivity of dyes such as Methyl volet, Crystal violet,Rhodamine B and other 12 dyes on paper and real inks on paper of handwriting. This research focused on the chemical properties of the OMR card marker as a Carbon Black colorant. Through material analysis of these colorant and real-application test, we selected the collidal Carbon Black ink from the appropriate manufacturer. And we investigated the good concentration needed for optimum condition when applying the Carbon Black colorant. Depending on the organic dye, the optimum detection sensitivity appeared within the range of 1 μg/mL - 100 μg/mL. Through the comparison of results, we found this method to be more reliable than the Matrix agents such as HABA(2-(4-Hydroxyphenylazo)benzoid Acid). On the other hand, Graphene oxide (GO) has been widely used more recently for a matrix of laser desorption/ionization (LDI) mass spectrometry of small molecules because GO has relatively lower matrix noise than conventional MALDI matrixes such as DHBA(2,5-dihydroxybenzoic acid). However, use of carbon-based materials is not desirable for time-of-flight (TOF) mass spectrometers since carbon nanomaterials stick to TOF electronics and therefore cause the instability of the MS operation. In order to overcome this issue, we applied GO embedded sol-gel film substrates for LDI MS of extracted ink dye samples of handwriting. Our results showed that the GO sol-gel film matrix substrate produced a much lower background noise than the aqueous GO particle matrix. This suggests that ablated carbon materials were significantly reduced when using the sol-gel film substrates. In addition, GO-embedded sol-gel film produced very clear and intense profiles of synthentic ink dye molecules in the region of m/z 0 - 1000

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Ion-pairing reversed phase chromatography with inductively coupled plasma atomic emission spectrometry for the elemental speciation of As

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The toxic and biological effects of arsenic species vary with the different chemical forms in a sample. In the past study, two kinds of separator columns were used for the separation of arsenic species in a seaweed, and the separation chromatograms were completely different for the five arsenic species. Anion separator column (AS-7 column) could not separate the five arsenic species while the other column (PRP-X100 column) separated them in a seaweed. The two columns could separate five arsenic species in standard solutions. The matrix in a seaweed made an adverse effect on the separation of the arsenic species when the AS-7 column was used.In this work, ion-pairing reversed phase column was investigated for the arsenic speciation in a seaweed. The different chemical species of As elements were separated by ion-pairing reversed phase chromatography, then, the separated species are selectively detected by inductively coupled plasma atomic emission spectrometry.

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Micro-headspace in-tube microextraction coupled with capillary electrophoresis

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In conventional headspace (HS) extraction, analytes evaporated from a sample donor phase in a sealed vessel can be enriched to an acceptor phase often in a liquid form or a sorbent coated on a fiber. The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus an acceptor of small volume is preferred and a single acceptor drop of small volume hanging to the capillary tip has been used in HS extraction for capillary electrophoresis (CE) [1]. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME)/CE using a liquid plug inside a separation capillary as an acceptor in place of the drop [2]. Here, we present micro-headspace (?HS) ITME/CE, a simple but easy way of conducting HS extraction of a small volume sample for subsequent CE analysis. Instead of using a sealed vessel to prepare a HS, a ?HS of a volume much smaller than 1 ?L was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor. Futhermore, ?HS-ITME-CE was performed using the acceptor plug remained in the capillary. Due to the small volumes of the ?HS and acceptor plug, it was possible even for a small volume donor to retain a high ratio of the donor and acceptor volumes for high enrichment factors. All steps of ?HS-ITME-CE were carried out automatically using a commercial CE instrument without any modification. Therefore not only the sample volume could be dramatically reduced, but also the need for a special apparatus was eliminated.

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Optimization of electroactive polymer modified biosensors

김은미 이혜진*

경북대학교 화학과

본 포스터에서는, 탄소 기반 전극을 이용한 바이오센서의 경우 생물질 검출용의 탐침용 리간드 물질(항체 또는 앱타머)을 전극 표면에 도입하기 위해 탄소 표면을 전처리하거나 또는 여러번의 화학적 처리 과정을 사용해야하는 단점을 보완하기 위해 전기적 활성을 갖는 도파민고분자로 코팅한 결과를 나타내고자 하였다. 탄소 기반 센서 표면에 도파민 도입 및 생물질 리간드 고정과 이들을 도입한 바이오센서의 전기화학적 활성에 대해 순환전압전류법과 시차펄스전위법을 이용하여 분석한 결과를 나타내었다.

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Selectivity Comparison Studies for Calcium Ion Sensing at Liquid/gel Interfaces

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본 포스터는 서로 혼합할 수 없는 않은 수용성 액체/ 유기 젤 계면에서 전압을 주사할 때 수용액 안에 존재하는 칼슘 이온이 젤안에 도포된 선택적 이온운반체에 의해 이동하는 반응에 따라 전류값이 변화함을 측정하는 센서 개발에 대해 나타내었다. 이를 이용하여 칼슘이온을 검출할 때 선택성을 증대시키기 위해 두 가지 이온운반체 (예: calcium ionophore Ⅱ와 calcium ionophore A23187)를 사용하였는데, 이들 각 운반체의 칼슘 이온 선택성에 대해 순환전압전류법과 시차펄스전압전류법을 이용하여 조사하고 그 결과를 비교 분석하였다.

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NMR Structural Analysis of Antimicrobial peptides, LPcin analogs with Enhanced Activities in aligned samples

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Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of bovine proteose-peptone PP3. LPcin analogs were designed and modified to enhance antibacterial activity using mutation, sequence shuffling for better amphipathic characteristics. It helps to improve interacting with bacterial membranes. Three candidates with enhanced antibacterial activity were selected among 12LPcin analogs, the name of LPcin-YK1, LPcin-YK2 and LPcin-YK3 respectively. LPcin-YK1 and LPcin-YK3 has shorter amino acids at C-terminus, LPcin-YK2 has same number of amino acids but several amino acids were substituted for better amphipathic characteristics. To understand the correlation between their structures and antibacterial mechanism, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using various biophysical techniques.We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with many biophysical techniques such as Ni-NTA affinity chromatography, dialysis, CNBr chemical cleavage and reversed-phase semi-prep.HPLC. To verify the purified peptides, we performed Tris-tricine PAGE, MALDI-TOF MS and CD spectrometry. In order to investigate the structures and dynamics, we use various 1D and 2D NMR techniques using micelle and especially bicelle samples to the closest anionic membrane environments.In here, we will present not only the optimization of high-yield expression and purification, but also solution and solid-state NMR experiments to elucidate the correlation between structure and antimicrobial activity. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra and PISA Wheel pattern were also underway.

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인-질소 클러스터 화합물의 질량분광 실험연구(Mass Spectrometric Stydy on Phosphrorus Nitride Clusters)

배광태 고은미 조수경*

국방과학연구소 국방고등기술원

고에너지물질 연구 분야에서는 고질소 함유 화합물을 개발하는 작업에 많은 노력을 기울이고 있다. 이들은 자체적으로도 많은 활용성이 있지만, 폴리질소를 합성하는 전구체로 활용할 수 있어 이들 물질의 합성 뿐 만 아니라 분해 매카니즘을 확인하는 작업도 매우 중요하다. 본 연구에서는 폴리질소계 화합물을 합성 할 수 있는 방안으로 인-질소 클러스터 화합물을 레이저로 이온화하여 질소만으로 구성되는 분해물을 형상하는 매커니즘을 조사하였다. 비행시간 질량분광기에 인-질소 클러스터 화합물에 대한 MALDI 및 LDI 실험을 수행하였으며, 실험 조건에 따른 분해 패턴을 분석하였다.

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Development of home-built solid-state NMR probes for specific purposes

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The solid-state NMR spectroscopy has been widely used for various insoluble materials like industrial polymers and biological samples. Also, solid-state NMR analysis of membrane protein on a membrane-like environments, such as lipid bilayer and bicelle, is especially valuable for their structure and function relationship. However, most of biological proteins on lipid bilayers have high dielectric property due to containing large amounts of lipids, water, and salts as well as probe efficiency are decreased cause of their electrical properties of lossy samples. Therefore, specific probe with high efficiency is required to study biological samples by using solid-state NMR. Also solid-state NMR methodologies for structural study of membrane protein in bicelle could be used for the in-situ analysis of liquid crystalline materials in LCD panels as well as Li materials in Li ion batteries. Here, we present the optimized design, construction and efficiency of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil for structural study of membrane protein in bicelle. The 1H-15N 2D SAMPI-4 spectra from a single crystal and membrane proteins oriented in bicelles were successfully obtained by using these solid-state NMR probes. We also present the development of a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a solenoidal coil for analysis of industrial materials. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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Electrochemical Immunoassay for detecting Hippuric acid (HA) on the Carbon included Screen Printed Nickel Electrode(SPNE)

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단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring of exposure to toluene is very important in occupational health care. In this work, we are using electrochemical immunoassay system that several advantages such as simple instrumentation, relatively low cost, miniaturization, portability, disposability and fully automation. The system was comprised with immobilization of Fe-HA on the Carbon included SPNE. We made electrode that marked Fe-HA on the carbon included SPNE. The surface morphology of the immobilized Fe-HA on the carbon included SPNE was examined by scanning electron microscopy (SEM). Hippuric acid (HA) has been detected competitively on the interaction of free HA and pentacyanoferrate-(4-aminomethylpyridine-hippuric acid) (Fe-HA) to its antibody on the Carbon included SPNE. This system generated electric signals proportional to free HA concentration. The electrical signal was measured by Cyclic voltammetry(CV) technique. The resulting currents were linearly related with the concentration of HA. The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.

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Development of indicator solution for the measurement of pH from the fat and oils

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단국대학교 화학과

CDR-Foodlab device has been used for checking the pH value in Fat and Oil. To operate CDR-Foodlab device, we need to use the kit with indicator solution. However the indicator solution, which received from company, is expensive. So to make similar product with indicator solution of company, we used various indicator. The components of indicator solution of company were analyzed by UV, IR and GC-MS. We chose various indicator compared with indicator solution of company. To check the pH value in a CDR-Foodlab device, we prepared the standard pH solution of 1 to 13. B sample was matched with indicator solution of company. It will be used as a reagent which can replace the existing that is cheap and accurate. 본연구는 2014 년도 교육부 대학특성화사업(CKⅡ) 사업비중 일부 지원받아 수행되었음.

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Dynamic Nuclear Polarization: Sensitivity Enhancement for Multi-molecular Magnetic Resonance Imaging Agents

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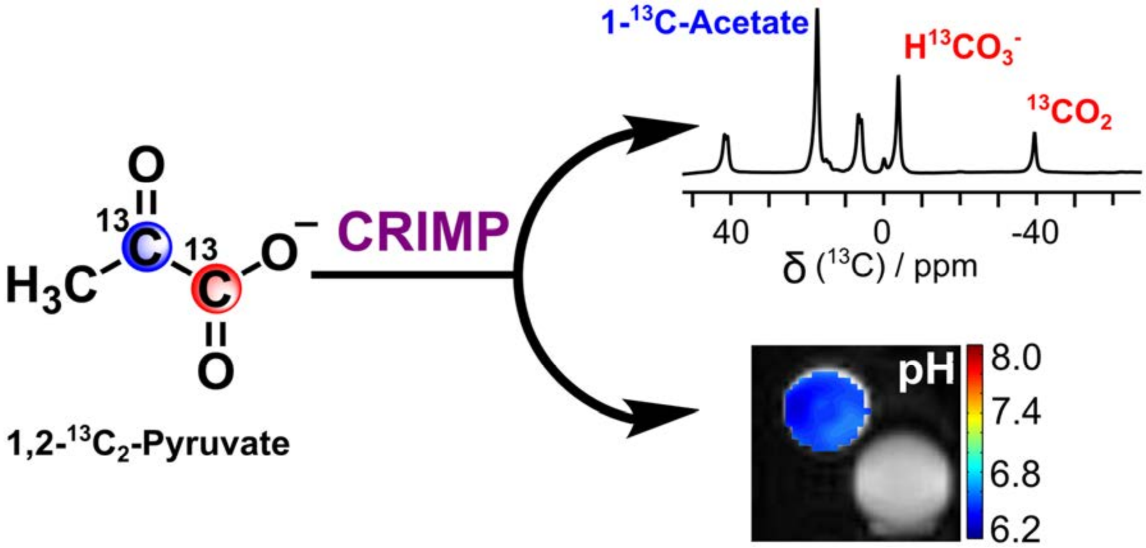
한양대학교 응용화학과

Here we present a novel hyperpolarization method, Chemical Reaction-Induced Multi-molecular Polarization (CRIMP), which could be applied to the study of several *in vivo* processes simultaneously including glycolysis, TCA cycle, fatty acid synthesis and pH mapping. Through the use of non-enzymatic decarboxylation, we generate four hyperpolarized imaging agents from hyperpolarized 1,2-^{13}C pyruvic acid. The CRIMP method is a simple versatile chemical method that can be done without any physical changes to the dissolution pathway or to the polarizer. Many new techniques in the literature including cross polarization, microwave frequency modulation, generating a faster dissolution or injection setup and increasing the magnetic field from dissolution to scanner are all physical methods used to increase hyperpolarization percentages or to increase the T_1 value of hyperpolarized imaging compounds. The new method can potentially be applied to study several in vivo metabolic pathways and multiple biochemical reactions concurrently in real-time.



1,2-$^{13}C_2$-Pyruvate
CRIMP
1-^{13}C-Acetate
$H^{13}CO_3^-$
$^{13}CO_2$
40
0
-40
δ (^{13}C) / ppm
pH
8.0
7.4
6.8
6.2

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Proton-Coupled Electron Transfer Reactions of Metal Nanoparticles Anchored on Metal Oxide Surface

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연세대학교 화학과

Noble metal nanoparticles (metal = Au, Ag, Pd, and Pt) anchored on the surface of semiconductor nanoparticles show catalytic activities for the reduction of azobenzene and CO_2. In azobenzene photocatalytic reduction, the ZnO composite coated with Pd nanoparticles showed the highest reduction activity, followed by Pt, Au and Ag, but the catalytic activity of bare ZnO was found to be negligible. Through the product analysis of the photocatalytic reactions, it was found that azobenzene was reduced to hydrazobenzene via proton-coupled electron transfer reaction. This tendency of metal effect can be elucidated by the proton binding tendency of metals in the composites that controls the proton-coupled electron transfer reaction. Another proton-coupled electron transfer reaction, namely reduction of carbon dioxide, is also performed. In this case, CO_2 reduction experiments were conducted with metal/TiO_2 composite colloids under light (> 320 nm) in aqueous solution (pH 1). The products of CO_2 reduction were analyzed by GC-MS from the headspace and solution of the catalysis reactor and were found to be propane and acetaldehyde.

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Paper Cone Spray Ionization Mass Spectrometry: Simple and Efficient Methods for Solid Sample Analysis

김푸름 차상원*

한국외국어대학교 화학과

The use of the ambient ionization mass spectrometry (MS) have been expanded enormously because of its relatively simple interface and also because of its raw sample analysis capability. Paper spray ionization (PSI) method is the extractive ambient ionization technique that utilizes a triangular shape filer paper as a sampling base as well as an electrospray tip. Active applications of PSI MS include drug monitoring from dried blood spots, food contaminant analysis, and metabolite fingerprinting. In this study, we developed a PSI-based solid sample analysis platform, called paper cone spray ionization (PCSI). Major difference between PSI and PCSI is paper geometry: PCSI uses a triangular pyramid shape or circular cone shape paper base instead of planar triangular shape one. Therefore, a paper base of PCSI can act as a solid sample container and a liquid-solid extraction chamber, as well as an electrospray tip. Analysis of various solid samples and viscous liquid samples such as food powders, animal tissues, and petroleum will be demonstrated in this presentation.

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Differentiation of Ganglioside Isomers by MALDI TOF/TOF Mass Spectrometry

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Gangliosides, acidic glycosphingolipids, have various structural isomers of which sialic acid residue positions are different from each other. Most abundant ganglioside isomers in biological systems are GD1a and GD1b, gangliosides with two sialic acids. In this study, we developed an effective matrix-assisted laser desorption/ionization (MALDI) mass spectrometry (MS) protocol for differentiating GD1a and GD1b isomers. For this purpose, we employed 5-methoxysalicylic acid (5-MSA) as a MALDI matrix because our recent study showed that this matrix induced minimal in-source fragmentation in the ionization of the labile gangliosides, GD1a. In addition, we incorporated salt additives of which cation charge state was +2 in the MALDI sample preparation because this cation could still carry +1 charge after charge neutralization of carboxyl anion group in a sialic acid residue and therefore more information-rich fragment ions could be generated in tandem MS experiments. Our results showed that relative intensities of isomer specific fragment ions were greatly enhanced in tandem mass spectra of GD1a and GD1b by employing doubly-charged cation such as calcium ion instead of singly-charged cation such as potassium ion.

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Analytical Platform Employing Graphitized Carbon Liquid Chromatography-Mass Spectrometry for Glycomic Characterization of Biotherapeutic Glycoproteins

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Monoclonal antibodies (mAbs) represent one of the largest classes of drugs in development due to their great efficacy for treatment of diseases such as cancers and rheumatic therapies. It has been known that glycosylation of protein therapeutics can radically affect their biological activity, plasma half-life, immunogenicity, and stability. Therefore, analysis of glycosylation is crucial for proper characterization of biotherapeutics in order to ensure the quality, safety, and consistency of the product. However, glycan analysis still remains analytical challenge due to its inherent microheterogeneity and diversity including the large number of isomeric structure. Liquid chromatography coupled with mass spectrometry (LC/MS) has become a key technique for rapid glycan profiling with high sensitivity and structure elucidation using tandem MS (LC/MS/MS). LC separation is essential for glycan isomer analysis because MS alone does not distinguish isomeric glycans with same mass. Hydrophilic interaction chromatography (HILIC) and porous graphitized carbon (PGC) combined with LC/MS are widely used for glycan separation. In this study, we have evaluated the chromatographic performance of HILIC and PGC including isomer separation, sensitivity, and quantitation for native and 2-AB labeled N-glycans, respectively. All peaks eluted from LC were further assigned by triple quad (QQQ) MS. We found that higher sensitivity was obtained from 2AB labeled glycans separated by HILIC column while this approach requires additional sample steps including glycan labeling and desalting. On the other hand PGC is a powerful tool in separating isomers of native glycans including neutral and acidic species with minimum sample preparation. Our analytical platform can be used to provide a reference for the column choice and optimized separation conditions for glycan analysis of biopharmaceutical glycoproteins.

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Highly Sensitive Detection of Estradiol in Human Serum Using SERS-based Competitive Immunoassay

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Estradiol (E2) is a biologically active sex steroid hormone that serves as important diagnostic marker in serum of premenopausal and postmenopausal women and in men. Therefore, it is very meaningful to establish highly sensitive and rapid methods for the detection of E2 in human serum. In the past decades, several technologies, including high performance liquid chromatography-mass spectrometry (HPLC-MS), gas chromatography-mass spectrometry (GC-MS) and immunoassays have been developed for the measurement of E2. However, the chromatography methods have lower sensitivity, and need well-trained personnel. Thus, these methods cannot satisfy with the requirements of routine clinical diagnosis. Surface-enhanced Raman scattering (SERS)-based immunoassay using functional nanoparticles has attracted more and more attention due to its higher sensitivity. Herein, we report a SERS-based competitive immunoassay for highly sensitive detection of E2. The method can be applied to detect E2 with good precision at concentrations as low as 0.1 pg/mL. The proposed method has been successfully applied to the determination of E2 for 30 human sera and showed a good correlation compared with the commercially available chemiluminescent microparticle immunoassay (CMIA) kit with good reproducibility. This method has exhibited great potential in the clinical analysis of E2 in human serum.

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Highly Sensitive Detection of Anthrax Marker using SERS-based Competitive Immunoassay

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Anthrax is a highly acute disease caused by the bacterium Bacillus anthracis. In this article, we report a highly sensitive detection technique for pathogenic B. anthracis, based on the use of a surface-enhanced Raman scattering (SERS)-active magnetic sensor. Gold nanoparticles (GNPs) and magnetic beads were used as SERS nanotags and supporting substrates, respectively. Here, an SERS-based competitive immunoassay platform is described for the quantitative evaluation of the anthrax marker. Poly-γ-D-glutamic acid (PGA) capsules were used as a target biomarker for the highly sensitive detection of B. anthracis becausePGAis known to be closely associated with the pathogenesis of B. anthracis infection. The SERS-based competitive assay reveals an extraordinarily high sensitivity for PGA with a limit of detection of ~1.0 ng/mL. This work provides a conceptually new immunoassay prototype for fast and sensitive detection of PGA markers.

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A Microfluidic Chip based Strategy for Biopharmaceutical Glycosyl Modification Analysis

서영숙 안현주*

충남대학교 분석과학기술대학원

Glycosylation plays an important role in ensuring the proper structure and function of most biotherapeutic proteins. However, bioactive glycan modifications add significant complexity to an already-diverse biopharmaceutical glycome. This diversity can greatly complicate glyco-analytical efforts during drug development, production, and regulatory approval. To address this issue, we have developed a novel microfluidic chip capable of online capture, enrichment, and LC separation of phosphoglycans. The chip allows online fractionation of phosphoglycans and non-phosphoglycans onto two different chromatographic runs, with LC gradients and instrumental settings independently optimized for each. Analysis is initiated by injection of glycan mixture onto the two-layer enrichment column. Phosphoglycans are trapped and enriched by the titanium dioxide(TiO_2) layer of the enrichment column, while non-phosphoglycans flow past the TiO_2 layer and are trapped by the PGC layer of the enrichment column. Following enrichment, a water/acetonitrile gradient elutes the non-phosphoglycans from the PGC layer of the enrichment column, which further separates neutral and sialylated glycans. Next, phosphoglycans are eluted from the TiO_2 layer of the enrichment column by injection of a high-pH aqueous elution buffer. We analyzed phosphoglycans selectively by LC/MS chip with a TiO_2-PGC enrichment column. This chip-based strategy for biopharmaceutical glycan analysis increases chromatographic peak capacity, enhances MS sensitivity, and improves glyco-analytical capabilities.

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Observing Platinum Single Nanoparticle Collisions on Copper Ultramicroelectrode by Electrocatalytic Amplification

정승연 권성중*

건국대학교 화학과

Electrocatalytic oxidation of hydrazine occurs at the surface of Pt nanoparticle when it collides onto a Cu ultramicroelectrode (UME). Collision of the single nanoparticle onto a less catalytic electrode surface had observed through a large amplification of the current by electrocatalysis. Pt nanoparticle contacts the electrode, the “blip (or spike)” current response that the current return to the background level was obtained due to the deactivated particles rather than “staircase” response which was described for an Au UME system. The frequency of the current transient was directly proportional to the nanoparticle concentration. And the current transient becomes sharper when the applied potential increases because deactivation rate is rapid. This paper can help us to understand that the interaction between nanoparticles and electrode affects the chemical reaction.

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In Situ Depth Profiling of Plant Metabolites by Nanospray Desorption Ionization (nano-DESI) Mass Spectrometry

이동건 이광빈 전규웅 차상원*

한국외국어대학교 화학과

In nanospray desorption ionization (nano-DESI), one of the extractive ambient ionization methods for mass spectrometry (MS), a steady-state micro-liquid junction formed between two micro-capillaries is used for extracting and dissolving analytes directly from a sample surface at a high spatial resolution. Recently, we have developed nano-DESI MS methods for direct profiling of metabolites from plant tissues in a depth-dependent manner. In the previous study, however, physical removal of plant wax layers was necessary prior to nano-DESI MS analysis, primarily because conventional spraying solvents such as methanol and water could not penetrate the wax layer. In present study, we optimized the nano-DESI spraying solvent system which could allow us to probe metabolites beneath the wax layer without employing any physical removal process. Our results showed that a toluene-containing nano-DESI spraying solvent was the very effective solvent system in terms of spatial resolution of sampling, stability of ion signals, and plant metabolite coverage.

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Synthesis and Characterization of Highly Purified Bimetallic Nanoclusters

김민석 이동일*

연세대학교 화학과

Bimetallic nanoclusters differ from their homometallic nanoclusters in many ways, which has become a topic of increasing interest in recent years. One major area of interest involves the study of $Au_{25}(SR)_{18}$ nanoclusters with bimetallic compositions such as $Pt_1Au_{24}(SR)_{18}$, $Pd_1Au_{24}(SR)_{18}$, $Ag_{1\sim13}Au_{24\sim12}(SR)_{18}$ and $Cu_{1\sim9}Au_{24\sim16}(SR)_{18}$ nanoclusters, where SR is thiolate ligand. Quantum-size of these nanoclusters induce distinctive quantum confinement effects, which result in unique optical and electrochemical properties. Recently we tried to synthesize highly purified Pt- and Pd-doped Au_{25} nanoclusters and clearly defined their optical, electronic, and catalytic properties. In our synthetic method, a mixture of $Pt_1Au_{24}(C_6S)_{18}$ (or $Pd_1Au_{24}(C_6S)_{18}$) and $Au_{25}(C_6S)_{18}$ was produced via judicious control of reaction conditions and size-focusing process. Relatively short complexation time interrupted the appearance of $Au_{25}(C_6S)_{18}$ and increased the production of bimetallic gold nanoclusters. The reaction product was further purified by selective decomposition of $Au_{25}(C_6S)_{18}$ using H_2O_2 and subsequent solvent extraction, resulting in highly pure $Pd_1Au_{24}(C_6S)_{18}$ and $Pt_1Au_{24}(C_6S)_{18}$ nanoclusters. Successful syntheses of $Pd_1Au_{24}(C_6S)_{18}$ and $Pt_1Au_{24}(C_6S)_{18}$ nanoclusters were confirmed by UV-Vis absorption spectroscopy, mass spectrometry and X-ray photoelectron spectroscopy (XPS) studies.

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발표분야: Oral Presentation of Young Analytical Chemists

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Label-free Impedimetric Polytetrabenzidene/Dendrimer Nanocomposite Based Highly Sensitive Immunosensor: Femtomolar Detection of Cardiac Troponin I in Serum

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충남대학교 분석과학기술대학원

A simple and robust but highly sensitive label-free impedimetric cardiac troponin I (CTI) immunosensor was fabricated using a poly-3, 3, 5, 5-tetramethylbenzidine (PolyTMB)/dendrimer (Den) nanoassemble film as anti-CTI antibody immobilizing platform. PolyTMB was electrochemically grown on a gold (Au) electrode by a potential cycling method. Carboxylic acid functionalized third generation poly(amidoamine) dendrimer (Den) and protein A (PA) was then sequentially covalently attached on the PolyTMB and PolyTMB/Den films, respectively. Anti-CTI antibody was then covalently immobilized on the PolyTMB/Den film with controlled orientation. The surface of the immunosensor was characterized using electrochemical quartz crystal microbalance (EQCM), coulometry, scanning electron microscopy (SEM), Fourier Transform Infrared (FT-IR) spectroscopy. The highly sensitive CTI detection was made by monitoring the impedance changes of the immunosensor surface due the anti-CTI-CTI binding, which affect the PolyTMB redox activity. CTI could be selectively detected at a fg/mL level in human serum samples.

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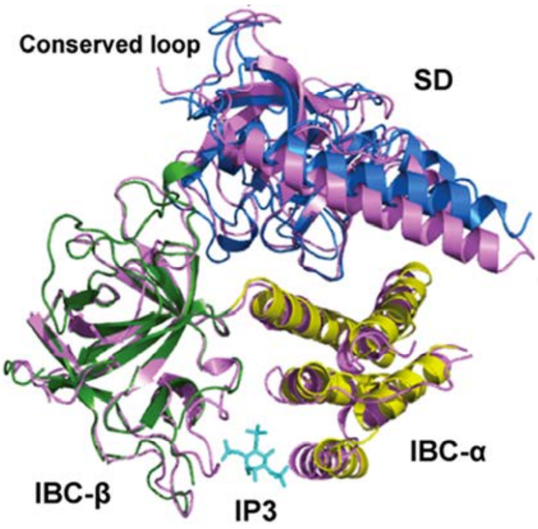
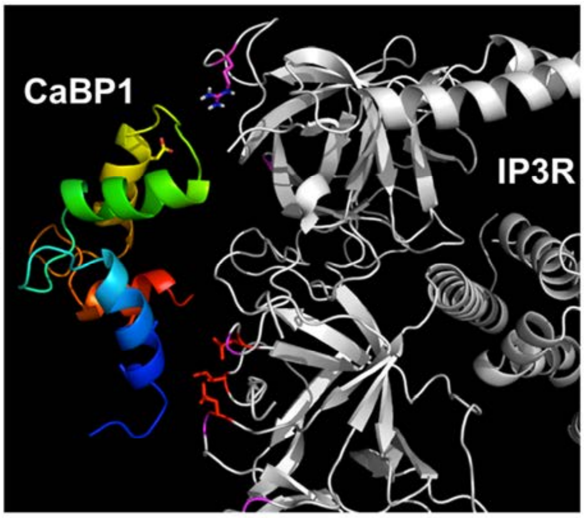
Structural Studies of IP3 receptor: Toward understanding the regulatory mechanism

서민덕

아주대학교 약학대학 약학과, 분자생물학과

Inositol 1,4,5-trisphosphate receptors (IP3R) is an IP3-gated Ca2+ release channel on the ER membrane, and plays a critical role in controlling the cytosolic Ca2+ level of eukaryotic cells. The N-terminal region of IP3R is responsible for binding to IP3 and Ca2+ binding proteins such as Calcium-binding protein 1 (CaBP1) and calmodulin (CaM). In order to elucidate the structural basis for the regulatory mechanism of IP3R, X-ray crystallography and Nuclear Magnetic Resonance (NMR) were employed. Here, we present crystal structures of the N-terminal region (NT) of IP3R1 with (3.6 ?) and without (3.0 ?) IP3 bound. We also employed NMR to investigate the structure of the IP3R:CaBP1 complex in order to understand the regulatory mechanism of IP3R by CaBP1. We used the chemical shift perturbation (CSP) and paramagnetic relaxation enhancement (PRE) data to dock the structure of CaBP1 C-lobe onto the structure of IP3R?NT. The information acquired from these studies would contribute to design new therapeutic treatment for human diseases such as cardiovascular diseases and some kinds of cancers.


Conserved loop
SD
IBC-β
IP3
IBC-α


CaBP1
IP3R

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Quantum Mechanical Effects in Biology

이호재

광주과학기술원(GIST) 화학

Biological systems are complex and condensed. Such environments prohibit most of the quantum mechanical phenomena from surviving to play important roles but classical models work better in the biological systems. In this talk, however, I will present two spectroscopic studies to demonstrate some quantum mechanical effects that may explain ultrafast energy transfer in photosynthesis and migratory birds’ navigation. An ultrafast spectroscopic technique found that there is long-lasting electronic quantum coherence (~300 fs) between pigments inside photosynthetic reaction center. With an aid of theoretical simulation this is understood to be facilitated by proteins tightly surrounding the pigments to enhance energy transfer rates between pigments. A possibility to control some chemical reaction outcomes by a weak magnetic field will also be introduced. This kind of reactions proceeds through so called radical pair mechanism, and it is nominated as a possible mechanism in cryptochrome in their retina that allows birds to feel geomagnetic fields.

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Dynamic polyrotaxane surfaces for the effective control of stem cell differentiations

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Extensive research has been conducted on the regulation of stem cell differentiations by altering physicochemical factors of the contacting materials, including stiffness, microtopography, and three-dimensional mechanical strength. However, the importance of the surface mobility of polymer surfaces in a hydrated state, one of the characteristic properties of polymer surfaces, in controlling stem cell differentiation, is not yet gaining much attention. A simple surface treatment capable of regulating stem cell lineages by changing the molecular mobility has great potential for many biomedical applications because it provides a simple and convenient method of directing stem cell lineage on various material surfaces without changing the bulk properties. In the present study, we report the feasibility of directing stem cell differentiation on supramolecular surfaces that are prepared with a simple surface treatment. The underlying concept that we applied is modulating the morphology of adhering stem cells using a wide range of molecular mobility of polymer surfaces in a hydrated state. Because morphologies of adhering stem cells have been known as an important factor in determining stem cell differerntiation, we hypothesized that a simply deposited supramolecular surfaces capable of changing the adhesion morphology of cells could induce different stem cell differentiation. Polyrotaxane (PRX) is a supermolecule that contains molecularly movable host molecules [e.g., α-cyclodextrin (α-CD)] threaded on a linear guest molecule [e.g., poly(ethylene glycol) (PEG)]. By adopting this threaded macromolecular structure of polyrotaxanes, we developed polymer surfaces with a wide range of surface mobility by simple deposition method. The effect of surface mobility on the differentiation tendency of the adhering stem cell will be introduced.

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Structural study on the Plk4 complexes reveals the molecular basis for scaffold switching in centriole duplication

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한국생명공학연구원(KRIBB) 기능유전체연구센터 [1]한국생명공학연구원 단백체시스템

Polo-like kinases (Plks) are serine/threonine kinases that regulate cell cycle, which commonly contain a canonical catalytic domain and a unique polo-box domain. Polo-like kinase 4 (Plk4) is a master regulator of centriole duplication, whose proper recruitment to centriole is critical for maintaining genomic integrity. The cryptic polo-box domain (CPB) of Plk4 is necessary for the protein function by interacting with the centriolar receptors including Cep152 and Cep192. We found the assembly of Cep152 around the Cep192-encircled daughter centriole and the relocalization of Plk4 from the inner Cep192 ring to the outer Cep152 ring during cell cycle. Crystal structures of the CPB of Plk4 alone and in complex with Cep192- and Cep152-derived fragments revealed that the fragements bind to Plk4 in an opposite orientations and mutually exclusively. Together with the higher binding affinity of Cep152 over Cep192 to Plk4, it accounts for the effective ‘snatching’ of Plk4 from the preformed Plk4-Cep192 complex to the Plk4-Cep152 complex. These results demonstrate that Plk4 is regulated in time and space through ordered interactions of its CPB with two scaffold proteins, Cep192 and Cep152.

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Structural bases for the inhibition of endosomal trafficking by Legionella pneumophila protein VipD

이광훈

오송첨단의료산업진흥재단 신약개발지원센터

Legionella pneumophila is a pathogen bacterium that causes Legionnaires' disease accompanied by severe pneumonia. Surprisingly, this pathogen invades and replicates inside macrophages, whose major function is to detect and destroy invading microorganisms. How L. pneumophila can be "immune" to this primary immune cell has been a focus of intensive research. Upon being engulfed by a macrophage cell, L. pneumophila translocates hundreds of bacterial proteins into this host cell. These proteins, called bacterial effectors, are thought to manipulate normal host cellular processes. However, which host molecules and how they are targeted by the bacterial effectors are largely unknown. In this study, we determined the three-dimensional structure of L. pneumophila effector protein VipD, whose function in macrophage was unknown. Ensuing analyses revealed that VipD selectively and tightly binds two host signaling proteins Rab5 and Rab22, which are key regulators of early endosomal vesicle trafficking. These interactions prevent the activated form of Rab5 and Rab22 from binding their downstream signaling proteins, resulting in the blockade of endosomal trafficking in macrophages. This work shows that L. pneumophila targets endosomal Rab proteins and delineates the underlying molecular mechanism, providing a new insight into the pathogen's strategies to dysregulate normal intracellular processes.

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Identification of ligands for RNA target by in silico virtual screening

박소정

성균관대학교 약학연구소

Computational virtual screening is well known tool as a rapid discovery of small molecules in the early stage of drug discovery pipeline. Recently, increased information of biological role of RNA caused more attention of RNA as an attractive new drug target. In spite of limitation of features of RNA structures such as conformational flexibility, high negative charge and salvation, number of successful studies targeting RNA using protein based computer program and newly modified algorithms have been increased. In this talk, some successful cases of virtual screening targeting RNA will be introduced. We identified ligands for RNA pseudoknot of SARS-CoV(severe acute respiratory syndrome coronavirus) and stem-loop RNA of HIV (Human immunodeficiency virus type 1). Many RNA viruses that have small compact genome utilize programmed -1 ribosomal frameshifting (-1 FS) to regulate protein synthesis using a stimulatory RNA pseudoknot or RNA Stem-Loop structures. The integrity of RNA structure and stability is the important for maintaining the efficiency of ?1 FS, which is highly conserved in each virus. Thus, small molecule anti-frameshift agents interacting with viral RNA would be potential antiviral agents targeting ?1 FS system specifically. To identify novel anti-frameshift agent targeting RNAs, virtual screening of chemical database was conducted. After screening, candidate compounds were selected based on the docking score and visual inspection. Their biological activities were test by in vitro cell based assays. Both cases, we identified novel ligands that inhibited -1 RF efficiencies. They are interesting lead for the design of anti-frameshift agents which may control the protein synthesis in target RNA virus.

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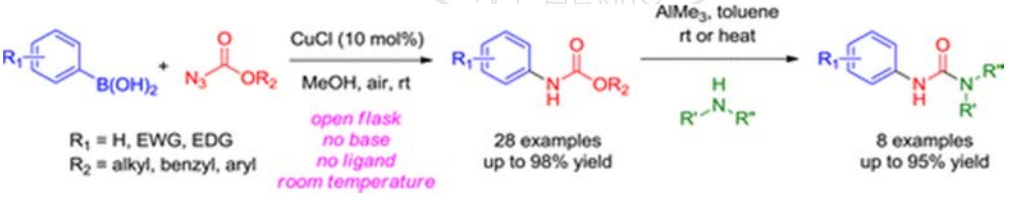
A Synthetic Approach to *N*-Aryl Carbamates via Copper-Catalyzed Chan-Lam Coupling at Room Temperature

KIMUBIN 김원석*

이화여자대학교 화학 나노과학과

A mild and efficient synthesis of *N*-arylcarbamates was achieved by reacting azidoformates with boronic acids in the presence of 10 mol % of copper chloride catalyst. The reaction proceeds readily in an open flask at room temperature without additional base, ligand, or additive. Rapid access to urea analogues via a two-step one-pot procedure is enabled by reacting *N*-arylcarbamates with aluminum?amine complexes. In addition, among several boronic acid derivatives prepared, dimethylphenyl boronate was found to react rapidly in its reaction with benzyl azidoformate, invoking *in situ* generation of this species in the catalytic cycle.



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발표코드: **ORGN.O-2**
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Synthesis of Pyrazines from Rhodium-Catalyzed Reaction of 2*H*-Azirines with *N*-Sulfonyl 1,2,3-Triazoles

류태규 이필호*

강원대학교 화학과

Development of a new synthetic method for azaheterocyclic compounds is highly significant in the investigation for new medicines, active pharmaceutical ingredients (API), and fine chemicals. In particular, pyrazine is one of the most representative privileged azaheterocyclic scaffolds, which show cytostatic, antifungal, and antitumor properties and are broadly present in flavorings and alarm pheromones. Accordingly, access to pyrazines from easily available starting materials is highly required. we report herein an efficient synthetic route to a wide range of trisubstituted pyrazines is developed from Rh-catalyzed reaction of 2*H*-azirines with *N*-sulfonyl-1,2,3-triazoles through the elimination of nitrogen molecule and arylsulfinic acid. The present reaction proceeds through formation of in situ generated dihydropyrazines.

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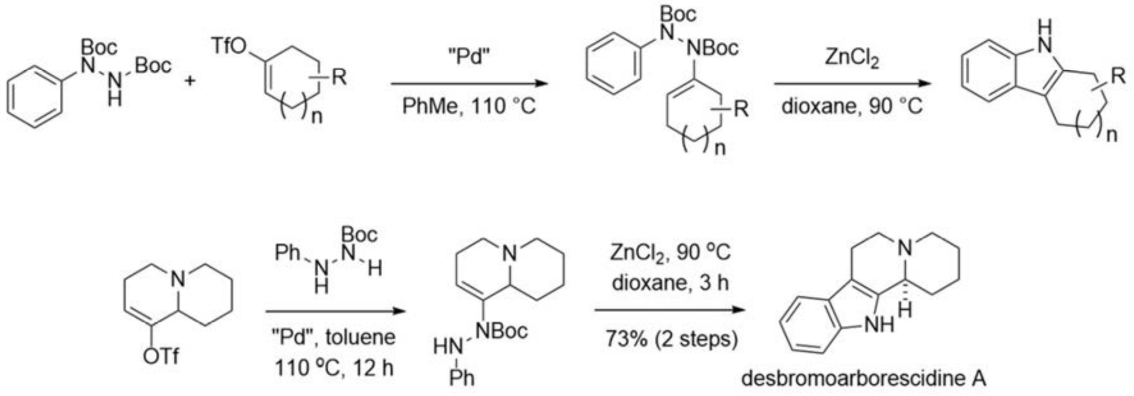
Ene-hydrazide from Enol Triflate for the Regioselective Fischer Indole Synthesis

임병윤 조천규*

한양대학교 화학과

Indole alkaloids are important class of natural products possessing intriguing molecular structures and biological activities. Over the years, many synthetic elaborations have been directed toward the indole-based natural products. The advance of the transition metal catalyzed C-N coupling reaction has particularly enriched the repertoire in indole synthesis. Despite the recent developments, the historic Fischer indole synthesis, reported in 1883, is still and often practiced because of its simplicity and reliability. However, it also suffers from two major drawbacks: the poor availability of the starting aryl hydrazine and the lack of regioselectivity. Ene-hydrazide prepared from enol triflate undergoes Fischer indolization reaction to give the indole with complete regioselectivity. The starting enol triflate is readily accessed in regiochemically defined form from the corresponding ketone via well-established thermodynamic/kinetic control in the enolate formation. This new protocol was successfully applied to the synthesis of desbromoarborescidine A, a natural *β*-carboline alkaloid, difficult to prepare with conventional Fischer indole synthesis.



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발표코드: **ORGN.O-4**
발표분야: Oral Presentation of Graduate Scholars in Organic Division
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A Facile Method for Sequence Determination of Cyclic Peptides/Peptoids via CNBr-Mediated One-Pot Ring-Opening/Cleavage Reaction

이강주 임현석*

포항공과대학교(POSTECH) 화학과

Macrocyclic peptides and peptidomimetics are of enormous interest as a promising class of protein binding ligands. Compared to their linear counterparts, cyclic peptides and peptidomimetics have increased conformational rigidity and relatively pre-organized structures, thus could bind more tightly to the target proteins without a major entropy loss. Moreover, they often have improved cell permeability and proteolytic stability. Despite many favorable features, the utility of macrocyclic peptides and peptidomimetics is limited by challenges in their sequence determination when using them in high-throughput screening (i.e. on-bead screening). Cyclic peptides and peptidomimetics from one-bead one-compound (OBOC) combinatorial libraries are not generally sequenced by Edman sequencing and tandem mass spectrometry. Here, we designed a cyclic system for sequencing cyclic peptides and peptoids, which has a thioether moiety embedded in the backbone of them. The thioether linkage is cleaved via a five-membered ring intermediate by treating with CNBr through the similar mechanism by which CNBr hydrolyzes methione-containing peptide sequences. Subsequent hydrolysis of the intermediate imminium salt results in cleavage of the linearized peptides/peptoids from the bead. The sequence of the resultant linear peptides/peptoids can be analyzed by tandem mass spectrometry.

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Constructing Dynamic Poly(disulfide)s as Activators of Biomolecules

방은경

한국과학기술연구원(KIST) 뇌의약연구단

The activities of dynamic polyion-counterion complexes in lipid bilayer membranes have been studied for their scientific utilities as transmembrane transporters / carriers, voltage gates, and sensors. Our Dynamic amphiphiles, having dynamic bonds between their charged head and their hydrophobic tails, can activate biomolecules (DNAs, siRNAs, CPPs) as counterion transporters. We have expanded this concept to poly(disulfide)s, dynamic polymers with disulfide repeats in their main chain, to deliver biomolecules through the cellular membrane. The disulfide bond is a dynamic covalent bond, which can be easily cleaved and reformed, but stronger than the non-covalent interactions present in supramolecular polymers. The most powerful advantage of poly(disulfide)s as carriers is that they are degradable by reductive depolymerization in the presence of glutathione in cells. Upon this step, the biomolecules, conjugated with poly(disulfide)s, can be easily realeased and the cytotoxicity can be minimized. Here, we report the synthesis of the counterion propagator units and subsequent polymerization by ring-opening disulfide exchange. The polymerization process was monitored by measuring fluorescence, the activities on the vesicles, and GPC. We also show that the most active fluorescent poly(disulfide)s reach the cytosol of HeLa cells within 5 min and depolymerize in less than 1 min to release the native substrate.

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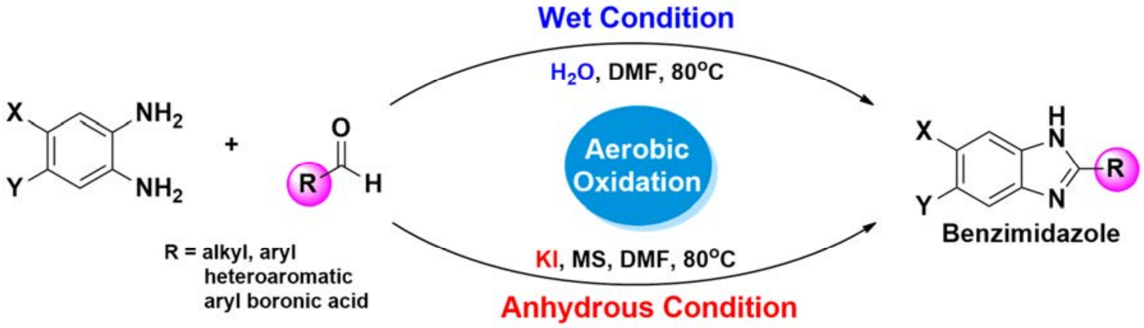
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 한순규

Green Synthetic Protocol to Benzimidazoles via Metal-Free Aerobic Oxidation

이예솔 천철홍*

고려대학교 화학과

Benzimidazoles are common building blocks found in biologically and therapeutically active compounds, natural products and material science. Thus, the development of efficient synthetic methods to access these important compounds has been extensively investigated. One of the conventional methods for the synthesis of benzimidazoles is oxidative cyclization which is starting from o-phenylenediamine and aldehyde through imine intermediates in presence of strong oxidants. Recently we have developed the novel one-pot protocol via metal-free aerobic oxidation using water or KI as a nucleophilic catalyst. In this regard, instead of the late-stage installation of the oxidative labile group like boronic acid, this mild synthetic methodology can be applied to direct formation of the benzimidazole scaffold bearing boronic acid derivatives, especially MIDA boronate using as a protecting group. Furthermore, this protocol can be applied to one-pot Suzuki-Miyaura coupling in moderate yield.



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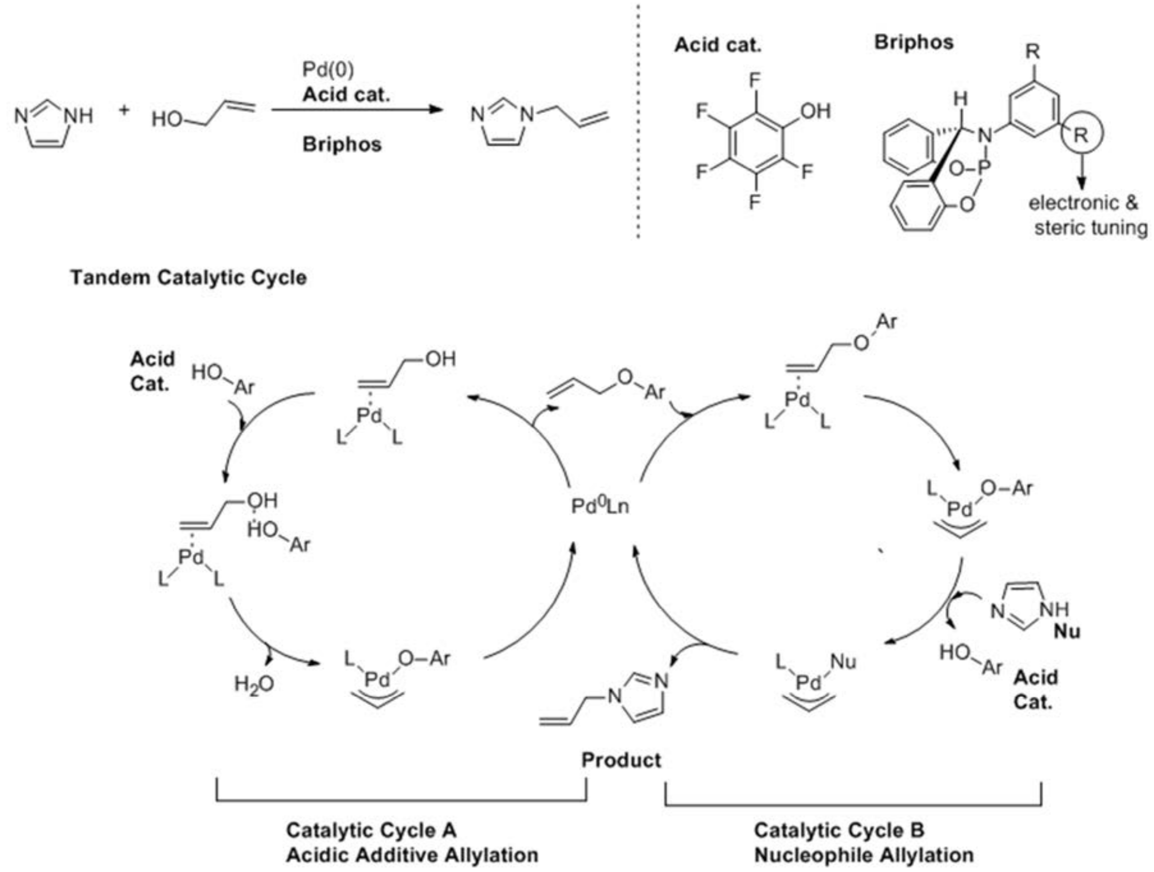
Pd-Catalyzed Allylation of N-Heterocycles with Allyl Alcohols via Tandem Catalysis Promoted by Briphos

강경준 김현우[*]

한국과학기술원(KAIST) 화학과

It has been reported that the reactivity and selectivity of transition-metal catalysts can be modulated by the choice of ligands such as phosphorus and N-heterocyclic carbene ligands. Thus, the ligand design is one of major topics in transition metal catalysis. For that purpose, we recently reported bicyclic bridgehead phosphoramidites (briphos) as a new type of π-acceptor ligand.1 Compared with their linear analogues such as monophos, briphos ligands show enhanced π-acceptor ability induced by geometrical constraints. In addition, briphos allows for facile steric and electronic tuning because of their simple and practical synthetic procedures. Here, we explored Pd-catalyzed allylations by using briphos ligands. Pd-catalyzed allylic substitution with allyl alcohols is attractive because only a stoichiometric amount of water can be produced as a by-product. However, the utilization of allyl alcohols is only limited to good nucleophiles such as malonates, alkyl amines, and anilines.2 Moreover, Pd-catalyzed substitution reactions of allylic alcohols with poor nucleophiles such as imidazoles and benzimidazoles are rarely reported.3 Herein, we report an efficient Pd-catalyzed allylation of allyl alcohols with a variety of N-heterocycles facilitated by a π-acceptor ligand, briphos, in a tandem catalytic cycle. References1. H. Kim, W. Y. Kim, A. Lee, S. Ahn and K. Kang, Org. Lett. 2014, 16, 5490.2. T. Ikariya, Y. Kayaki and T. Koda, J. Org. Chem. 2004, 69, 2595.3. M. Beller, D. Banerjee, R. V. Jagadeesh, K. Junge and H. Junge, Angew. Chem. Int. Ed. 2012, 51, 11556.


Pd(0)
Acid cat.
Briphos
Acid cat.
Briphos
R
electronic & steric tuning
Tandem Catalytic Cycle
Acid Cat.
Pd⁰Ln
Nu
Acid Cat.
Product
Catalytic Cycle A
Acidic Additive Allylation
Catalytic Cycle B
Nucleophile Allylation

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발표분야: Oral Presentation of Graduate Scholars in Organic Division

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Catalytic Asymmetric Insertion of Diazocompounds into Aldehydes

강병철 남동국 **JINMINGYU** 강기태 신성호 심수용 김태형 정현실 백은희 류도현*

성균관대학교 화학과

Mild and selective C-H bond insertion reactions provide potential advantages for synthetic strategies to make useful molecules. Among developments in this area, the formal diazo carbon insertion into C-H bonds is a powerful tool for the homologation of aldehydes and ketones. In this type of reaction, the formal C-H bond insertion reaction of aldehydes via a 1,2-hydride shift, namely the Roskamp reaction, has been well established, and asymmetric methods providing chiral beta-keto esters and alpha-aryl carbonyl compounds have recently been achieved. Synthetic utility of C-H bond insertion was demonstrated by the synthesis of aggregation pheromone sitophilate. References 1. Gao, L.; Kang, B. C.; Hwang, G.-S.; Ryu, D. H. Angew. Chem., Int. Ed. 2012, 51, 8322. 2. Gao, L.; Kang, B. C.; Ryu, D. H. J. Am. Chem. Soc. 2013, 135, 14556.3. Lundin, P. M.; Esquivias, J.; Fu, G. C. Angew. Chem., Int. Ed. 2009, 48, 154.4. Lou, S.; Fu, G. C. J. Am. Chem. Soc. 2010, 132, 1264.

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발표분야: Oral Presentation for Young Medicinal Chemists
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Synthesis of deuterium substituted [^{18}F]fluoromethyl-PBR28 and its preclinical comparison with [^{18}F]fluoromethyl-PBR28

문병석 이병철*

분당서울대학교병원 핵의학과

N-(2-[^{18}F]Fluoromethoxybenzyl)-N-(4-phenoxypyridin-3-yl)acetamide, ([^{18}F]fluoromethyl-PBR28, [^{18}F]1), sterically almost identical to [^{11}C]PBR28 which was well known for TSPO specific radiotracer, was developed by our group for TSPO PET (positron emission tomography) imaging but [^{18}F]1 had a little unstable in vivo due to probably defluorination. In this study, deuterium substituted [^{18}F]fluoromethyl-PBR28-d_2 ([^{18}F]1-D) was synthesized to develop a PET radiotracer for enhanced in vivo stability and compared with [^{18}F]1 in neuroinflammation rat models. [^{18}F]1-D was synthesized by two-step reaction from CD_2Br_2, followed by the alkyation of desmethyl-PBR28. Comparison between [^{18}F]1-D and [^{18}F]1 was performed in in vitro and in vivo experiments. The radiochemical yield for [^{18}F]1-D and [^{18}F]1 were 12.4 and 35.8% with >185 GBq/umol of specific activity, respectively. In vitro binding affinity and log P showed similar values. In biodistribution, the uptakes of [^{18}F]1-D and [^{18}F]1 in femur had different pattern as time elapsed (2.1 vs 2.9 %ID/g at 5 min postinjection; 1.5 vs 4.1 %ID/g at 120 min postinjection, respectively), indicating that [^{18}F]1-D was relatively stable in in vivo environment. In PET imaging studies, [^{18}F]1-D was selectively accumulated in the ipsilateral striatum with high target-to-background ratio. BPND of [^{18}F]1-D was about 1.4 times higher than that of [^{18}F]1. The results presented here suggest that [^{18}F]1-D hold promise as a neuroinflammation PET imaging agent in the field of brain disorders.

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발표분야: Oral Presentation for Young Medicinal Chemists

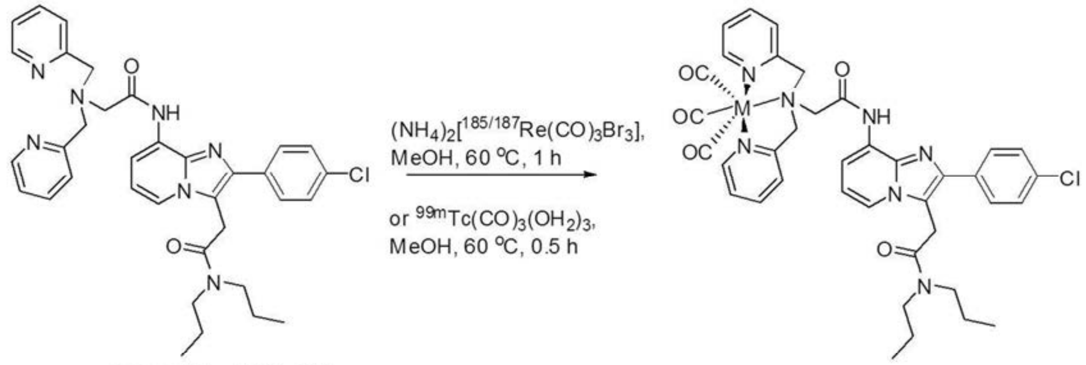
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 한수봉

Synthesis of $^{99m}Tc(CO)_3$ labeled 2-(4-chloro)phenyl-imidazo[1,2-a]pyridine analog (^{99m}Tc-CB256)

최지영 이병철[1,*]

서울대학교 융합과학기술대학원 방사선융합의생명전공 [1]분당서울대학교병원 핵의학과

The 18 kDa translocator protein (TSPO) is a mitochondrial protein associated with a wide number of biological processes including cell proliferation, apoptosis, steroidogenesis, and immunomodulation. In this work, we synthesized ^{99m}Tc-CB256 as a new TSPO-selective SPECT imaging agent and performed TSPO-positive tumor cell binding assay. Re-CB256 and ^{99m}Tc-CB256 were synthesized as described in Fig 1. ^{99m}Tc-CB256 was synthesized in 75~85% of radiochemical yield (d.c.) with over 98% of radiochemical purity. The chemical identity of ^{99m}Tc-CB256 was confirmed by comparing retention time of ^{99m}Tc-CB256 (22.5 min) with that of Re-CB256 (22 min), including NMR and HRMS. The obtained ^{99m}Tc-CB256 was shown to be highly stable (>99%) in human serum for 4 h and had a relatively low lipophilicity (log D = 2.15 ± 0.02). In vitro time dependent tumor cell binding uptake of ^{99m}Tc-CB256 was shown 10.26 ± 0.23 and 7.88 ± 0.23 %ID in C6 and U87-MG cells at 60 min, respectively. Our in vitro data indicated that ^{99m}Tc-CB256 can be considered as a new TSPO-positive cancer imaging agent and provides the foundation for further in vivo biological evaluation in tumor xenograft.



CB256 (IC_{50}=239 nM)

M = $^{185/187}$Re for **Re-CB256**
^{99m}Tc for **^{99m}Tc-CB256**(IC_{50}=364 nM)

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Novel dianilinopyrimidine derivatives as ALK inhibitors

윤정인 김형래[1,*] 윤창수[2]

충남대학교 약학대학 [1]한국화학연구원 난치성질환치료제연구센터 [2]한국화학연구원 신약연구본부 의약화학연구센터

Anaplastic lymphoma kinase (ALK) is a receptor tyrosine kinase (RTK) belongs to the insulin receptor superfamily. Recently, ALK has been elucidated as an interesting target for various cancers due to its implications of tumorigenesis by ALK fusion gene mutations and point mutations. ALK with chromosomal rearrangements have been detected in anaplastic large cell lymphoma (ALCL, 50-60%), inflammatory myofibroblastic tumors (IMT, 27%), and non-small-cell lung cancer (NSCLC, 4-7%). The representative of ALK fusion gene NPM-ALK (ALCL, IMT) and EML4-ALK (NSCLC) is known. Activating EML4-ALK mutations are key driven of NSCLC malignancy in approximately in of 4-7% patients. In 2011, Crizotinib (Xalkori) is the first EML4-ALK inhibitor in clinical use for NSCLC treatment. However, despite dramatic responses to Crizotinib, its efficacy is ultimately limited by the development of acquired drug resistance that occurred within a year. We already reported bis-ortho-alkoxy-para-piperazinesubstituted-2,4-dianilinopyrimidines (KRCA-0008) derivatives as a potent ALK inhibitor, however they were lack of metabolic stability due to 1,4-diaminobenzene moiety. In this report, we designed and synthesized new series of bis-*ortho*-alkoxy-*para*-piperidinesubstituted-2,4-dianilinopyrimidines derivatives in order to improve metabolic stability as well as its potency. Most pyrimidine derivatives showed good inhibitory activities and also showed good anti-proliferative activity against a panel of H3122 cell line. (H3122 cell line was contained with ALK fusion gene of EML4-ALK.)

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발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 한수봉

Novel 2,5-disubstituted quinolines: Design, synthesis, in-vitro antiproliferative activity and kinase profile

ELDAMASY ASHRAF KAREEM AWAD MOHAMMED 강순방[1] 금교창[2,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 뇌의약연구단 [2]한국과학기술연구원(KIST) 케모인포메틱스연구센터

Four novel series of 2,5-disubstituted quinolines (53 final compounds) have been designed and synthesized as anticancer sorafenib analogues. Two series (amides & ureas) were designed to possess a spacer between the terminal aryl and 2-aminoquinoline scaffold, whereas the other series (C & D) lack the spacer while conserving the oxypicolinamide or propoxy moiety at 5-position, respectively. All the target compounds were preliminary evaluated for their antiproliferative effect against three cancer cell lines (MCF7, HCT116 and SKBR3) by MTT assay and exhibited promising antitumor activity. Therefore, 35 compounds were selected to be tested over a panel of 60 cancer cell lines at a single dose concentration of 10 ?M at NCI to broadly screen their antiproliferative activity. Fifteen compounds have showed promising mean growth inhibitions and thus were further tested at five-dose testing mode to determine their GI50, TGI and LC50 over the 60 cell lines. The data obtained revealed that KK9087 is the most potent and efficacious derivatives with submicromolar GI50 value against some cell lines. Furthermore, it was screened against a panel of 46 oncogenic kinases at single dose of 10 ?M and showed selective high inhibition (96%) against TrKA with IC50 value of 2.5 ?M, so it can be an attractive candidate for further investigation.

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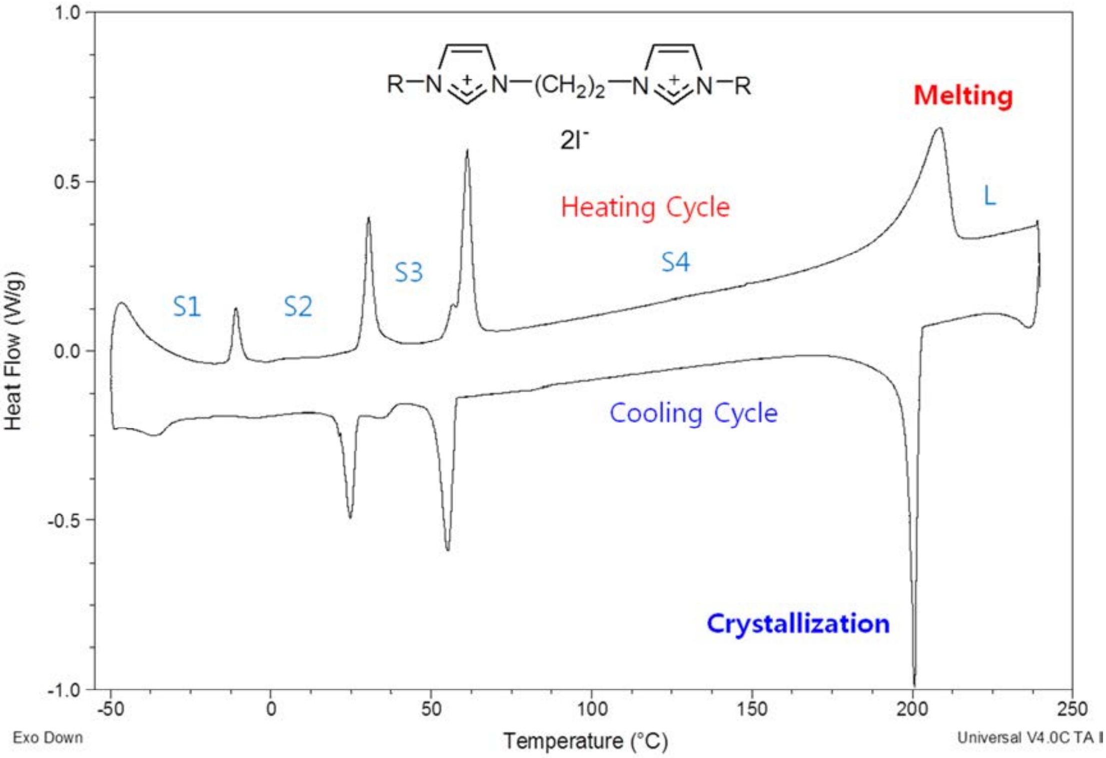
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 정 현

Imidazolium Salts as a New Class of Organic Ionic Plastic Crystals (OIPCs)

이민재

군산대학교 화학과

A new class of organic ionic plastic crystals (OIPCs) have been found during imidazolium salts, which are well known as a ionic liquid and a ligand for inorganic complexes. 1,2-Bis(N-alkylimidazolium)ethane salts show multiple solid-solid phase transitions below melting temperature. The structure of both imidazolium cations and counter-anions play an important role to have the unique phase behaviors of plastic crystals. Due to the big heat absorptions of the solid-solid phase transitions, some imidazolium salts have small ΔS_f values (< 20 J K^{-1}), which follows the definition of plastic crystals by Timmermans. This new class of imidazolium OIPCs can potentially be applicable to the solid-electrolytes in organic solar cells, fuel cells, or lithium batteries.


R–N N–(CH2)2–N N–R
2I⁻
Melting
Heating Cycle
L
S1
S2
S3
S4
Cooling Cycle
Crystallization
Heat Flow (W/g)
1.0
0.5
0.0
-0.5
-1.0
-50
0
50
100
150
200
250
Temperature (°C)
Exo Down
Universal V4.0C TA I

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발표코드: **MAT.O-2**
발표분야: Current Trends in Materials Chemistry
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Theoretical investigation of organic-inorganic hybrid perovskites ABI3 (A = CH3NH3, NH2CHNH2; B = Sn, Pb) as potential thermoelectric materials

이창훈* 심지훈 **Myung-Hwan Whangbo[1] Alessandro Stroppa[2]**

포항공과대학교(POSTECH) 화학과 [1]North Carolina State University [2]Consiglio Nazionale delle Ricerche - CNR-SPIN

To assess the feasibility of the organic-inorganic perovskite iodides ABI3 (A = CH3NH3, NH2CHNH2; B = Sn, Pb; X = I) for thermoelectric applications, we estimated their figures of merit (ZTs) as well as that of Bi2Te3, which is optimized for temperatures around 300 K, as a function of chemical potential on the basis of density functional theory calculations. Our analysis employed the tetragonal structures (P4mm) of (CH3NH3)PbI3 and (CH3NH3)SnI3, the trigonal (P3m1) structure of (NH2CHNH2)PbI3, and the orthorhombic (Amm2) structure of (NH2CHNH2)SnI3 to examine their thermoelectric properties around room temperature. Our work reveals that the ZTs of electron-doped ABI3 perovskites can be as large as that of hole-doped Bi2Te3 whereas those of hole-doped ABI3 are rather smaller so that, in thermoelectric performance, electron-doped perovskites ABI3 can be as good as hole-doped Bi2Te3.

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발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 정 현

Efficient Visible Light-Induced H_2 Generation by Self-Assembled CdS-$Ti_{(5.2-x)/6}Rh_{x/2}O_2$ Nanohybrid

이장미 황성주[1,*]

이화여자대학교 화학 나노과학과 [1]이화여자대학교 화학·나노과학과

Positively charged CdS quantum dot (CdS-QD) and negatively charged Rh-substituted titanate nanosheet ($Ti_{(5.2-x)/6}Rh_{x/2}O_2$) are hybridized by electrostatically-derived self-assembly. The partial substitution of mixed-valent Rh^{3+}/Rh^{4+} ions for Ti^{4+} ions is quite effective not only in improving visible light harvesting ability but also in depressing the recombination of charge carriers. According to diffuse reflectance UV-vis and photoluminescence (PL) spectroscopy, the obtained CdS-$Ti_{(5.2-x)/6}Rh_{x/2}O_2$ nanohybrids show the decrease of bandgap energy and the depression of PL signal upon Rh substitution. The resulting nanohybrid shows much higher photocatalytic activity for H_2 production without the deposition of Pt cocatalyst, which is superior to those of the unsubstituted CdS-TiO_2 nanohybrid and the precursor CdS QD. This is attributable to the enhancement of visible light absorption and the increase of the lifetime of electron and hole. The present study clearly demonstrates the effectiveness of Rh substitution in improving the photocatalytic activity of the titanate-based nanohybrids.

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Development of Highly Stable, Water-Dispersible Metal Nanoparticle-Decorated Polymer Nanocapsules and Their Catalytic Applications

윤경원 김기문[1,*]

기초과학연구원 복잡계자기조립연구단 [1]포항공과대학교(POSTECH) 화학과

The last decade has witnessed a rapid progress in new methods for synthesizing metal nanoparticles with controlled sizes and surface area. However, to date, long-term stability, high dispersibility, catalytic activity with recycling, and reusability in water remains a challenge. Here, we demonstrate a facile synthesis of highly stable, water-dispersible metal nanoparticle-decorated polymer nanocapsules (M@CB-PNs: M = Pd, Au, and Pt) was achieved in a simple two-step process employing a polymer nanocapsule (CB-PN) made of cucurbit[6]uril (CB[6]) and metal salts. The CB-PN serves as a versatile platform where various metal nanoparticles with a controlled size can be introduced on the surface and stabilized to prepare new water-dispersible nanostructures useful for many applications. As a representative material, the Pd nanoparticles on CB-PN exhibit high stability and dispersibility in water, as well as excellent catalytic activity and recyclability in carbon-carbon and carbon-nitrogen bond formation reactions in aqueous media suggesting potential applications as an eco-friendly catalyst. Details of this work will be presented.

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Hollow Vesicles of Ligand-Stabilized Gold Nanoparticles Formed through Dynamic Ligand Rearrangement

서명주 박소정[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학

We have recently reported a novel approach to fabricate all-nanoparticle-vesicles using ligand-stabilized gold particles as building blocks. Hollow vesicle-like assemblies were spontaneously formed from hydroxyalkyl-terminated gold nanoparticles in water without any template. Here, we show that this approach is applicable for nanoparticles modified with mixed ligands of mercaptoundecanol (MUL) and dodecnanethiol (DT). The unusual vesicle formation was attributed to the segregation of the two different ligands upon the addition of water. The overall shape of the assemblies and the wall thickness of vesicles varied depending on the DT percentage. Well-defined hollow vesicles were formed with nanoparticles modified with 80% MUL and 20% of DT. With increasing the DT content, the membrane thickness gradually increased. At 50% MUL, solid assemblies were formed instead of hollow vesicles. The assembly structure was also controllable by changing the solvent composition; a string to vesicle morphology change was observed with increasing the water content. Furthermore, we show that MUL-stabilized nanoparticles can act as efficient surfactants for hydrophobic nanoparticles. In the presentation, we will discuss what controls the assembly of nanoparticles stabilized with the mixed ligands and how their self-assembly behavior compares with that of molecular surfactants.

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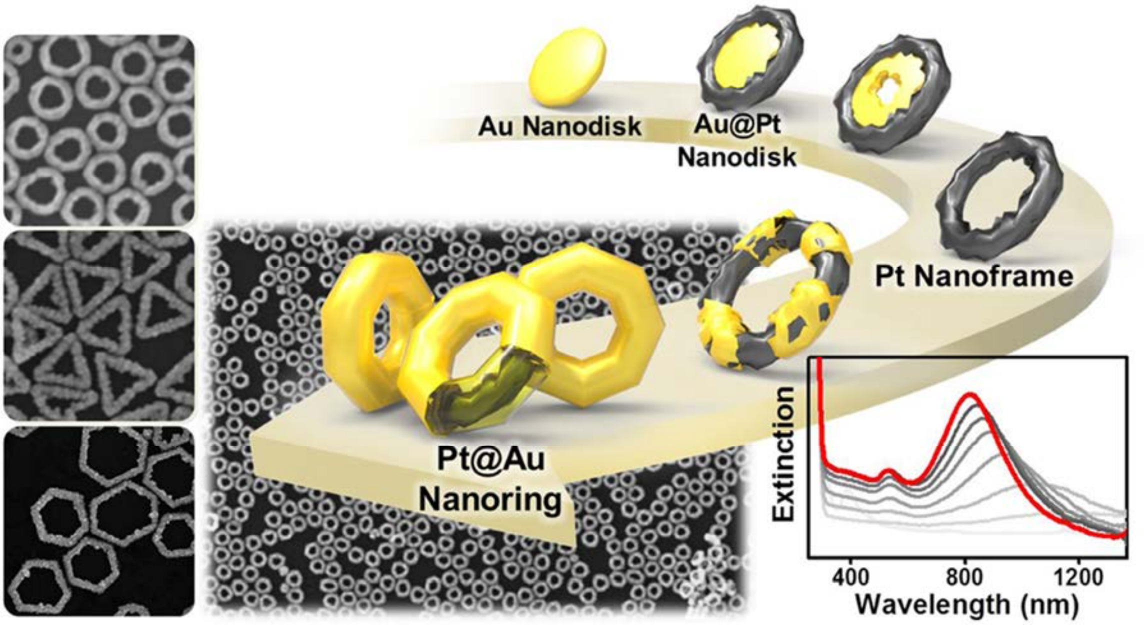
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 백승민

Synthesis of Plasmonic Nanorings with Pt Framework via Wet Chemistry

장희정 송유경 이상지 박성호*

성균관대학교 화학과

Controlling the shape of optically active nanostructures has attracted interests due to their unique optical properties. Nanostructures composed of Au and Ag effectively interact with the light at the specific wavelength depending on their shapes. For the purpose of synthesizing Au nanoframes, most researchers have selected the galvanic replacement reaction on Ag templates as a strategy, but the structural weakness of thin Au ring easily induces aggregates. In my presentation, I will exhibit an effective synthetic strategy to fabricate Au-coated Pt (Pt@Au) nanorings. The Pt nanoframe at the core acts as a framework, and Au coated on the Pt nanoframes allows the nanostructure to behave optically active as pure Au nanorings due to surface plasmon coupling between Au and Pt. This research provides fundamental understanding regarding the optical property of Au nanorings. We adopted the experimental procedure involving site-selective growth of Pt, etching of Au, and regrowth of Au. The resultant product is in the form of Au nanorings with Pt framework, providing relatively high permeability toward light and chemicals.


Au Nanodisk
Au@Pt Nanodisk
Pt Nanoframe
Pt@Au Nanoring
Extinction
400
800
1200
Wavelength (nm)

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발표코드: **MAT.O-7**

발표분야: Current Trends in Materials Chemistry

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Fabrication of Reduced Graphene Oxide Nano-ring Arrays by Au@Pt Nanoplate Lithography

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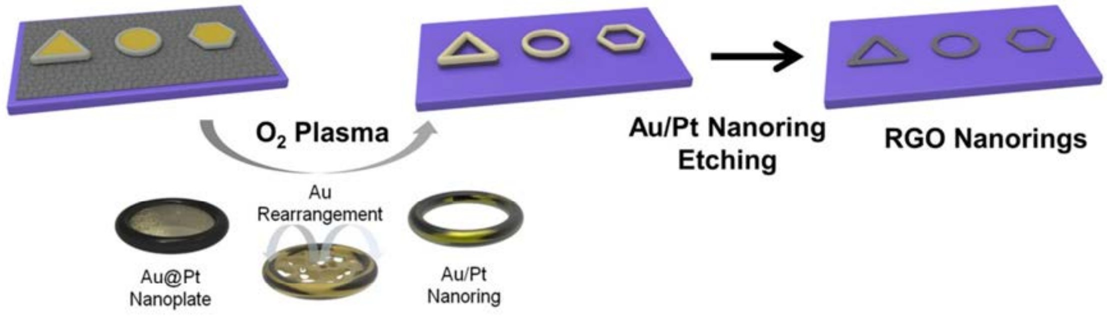
성균관대학교 에너지과학과 [1]성균관대학교 화학과

Distinctive graphene shape such as nanomesh and nanoribbon has gained a great deal of attention for electronic device applications. Here, we fabricated the graphene nano-ring arrays using Au@Pt nanodisks as a pattern mask. The homogeneous and monolayer arrangement of Au@Pt nanodisks and reduced graphene oxide were fabricated using water/oil interface with MPTMS. Fabricated graphene nano-rings were analyzed using SEM, Raman spectroscopy and I-V measurement. We also controlled the shape of graphene frames by applying various shapes of Au@Pt nanoplates. This fabrication method for graphene nano-rings will suggest the future graphene electronics.



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발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
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Effect of π-Conjugated Bridges of TPD-based Medium Bandgap Conjugated Copolymers for Efficient Tandem Organic Photovoltaic Cells

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부산대학교 화학과 [1]경기대학교 화학과 [2]동아대학교 전자공학과 [3]School of Materials Science and Engineering, Nanyang Technological University

Conjugated donor (D)-π-acceptor (A) copolymers, PBDT-TPD, PBDT-ttTPD, PBDTT-TPD, and PBDTT-ttTPD, based on a benzodithiophene (BDT) donor unit and thieno[3,4-c]pyrrole-4,6(5H)-dione (TPD) acceptor unit were designed and synthesized with different π bridges via Pd-catalyzed Stille-coupling. The π bridges between BDT and TPD were thiophene in PBDT-TPD and PBDTT-TPD, and 6-alkylthieno[3,2-b]thiophene in PBDT-ttTPD and PBDTT-ttTPD. The effects of the π bridges on the optical, electrochemical, and photovoltaic properties of the polymers were investigated, in addition to the film crystallinities and carrier mobilities. Copolymers with the 6-alkylthieno[3,2-b]thiophene π-bridge exhibited high crystallinity and hole mobility. Improved Jsc and FF were obtained to increase the overall power conversion efficiencies (PCE) in inverted single organic photovoltaic cells. A PCE of 6.81% was achieved from the inverted single device fabricated using the PBDTT-ttTPD:$PC_{71}BM$ blend film with 3 vol% 1,8-diiodooctane. A tandem photovoltaic device comprising the inverted PBDTT-ttTPD cell and a PTB7-based cell as the bottom and top cell components, respectively, showed a maximum PCE of 9.35% with a Voc of 1.58 V, Jsc of 8.00 mA/cm^2, and FF of 74% under AM 1.5 G illumination at 100 mW/cm^2. The obtained PCE of the bottom cell and FF of the tandem cell are, to the best of our knowledge, the highest reported to date for a tandem OPV device. This work demonstrates that PBDTT-ttTPD may be very promising in applications in tandem solar cells. Furthermore, 6-alkylthieno[3,2-b]thiophene π-bridge systems in medium bandgap polymers can improve the performance of tandem organic photovoltaic cells.

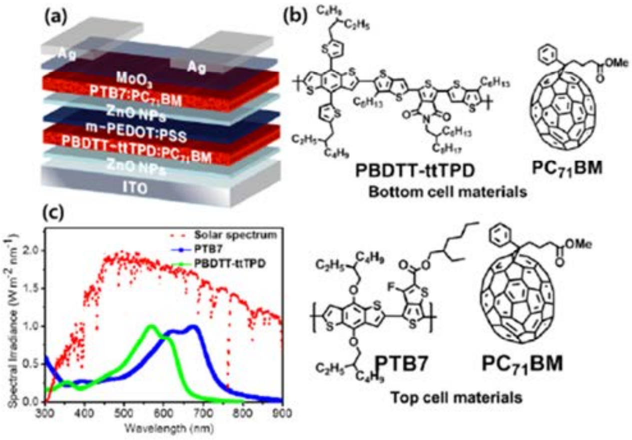

Fig. 1. Inverted tandem photovoltaic device. (a) Device structure of the inverted tandem photovoltaic device. (b) Chemical structures of bottom cell materials (PBDTT-ttTPD and $PC_{71}BM$) and top cell materials (PTB7 and $PC_{71}BM$). (c) UV−visible spectra of the PBDTT-ttTPD of bottom cell, the PTB7 of top cell, and the solar spectrum.

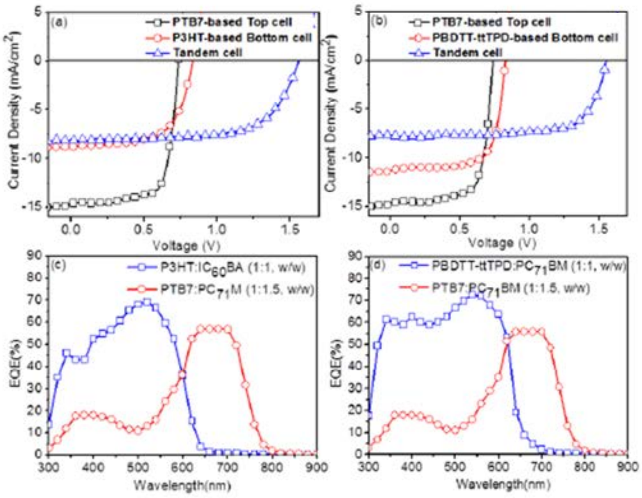

Fig 2. Current density-voltage characteristics of the inverted tandem OPVs under AM1.5 G illumination (100 mW/cm^2). (a) P3HT-based bottom cell in the tandem OPVs and (b) PBDTT-ttTPD-based bottom cell in the tandem OPVs. EQEs of the (c) P3HT:$IC_{60}BA$-based and (d) PBDTT-ttTPD-based bottom cell, and PTB7:$PC_{71}BM$-based top cell in a typical tandem device.

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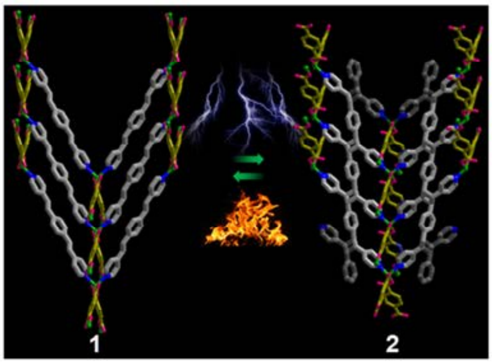
MOFs Based on Olefinic Dipyridine and Photo-Cycloaddition Reaction

박인혁 Raghavender Medishetty[1] 이형환 Anjana Chanthapally[1] 김자연 이심성[*]
Jagadese J. Vittal[1,*]

경상대학교 화학과 [1]Department of Chemistry, National University of Singapore

Since the pioneering work by G. M. J. Schmidt, the photo-induced [2+2] cycloaddition of olefin compound in solid state has become a fascinating field in crystal engineering due to its high efficiency and distinguished selectivity. In this presentation, our results for the photo-driven fabrications of novel materials including the organic polymers as a first case together with the metal-organic frameworks (MOFs) incorporating polyrotaxanes are introduced. For instance, the polymerization of 1,4-bis[2-(4’-pyirdyl)ethenyl]benzene (bpeb) occurs inside an interpenetrated MOF 1 by the [2+2] cycloaddition of a herringbone-type packing. This single-crystal to single-crystal (SCSC) transformation resulted in a metal-oragano-polymeric framework (MOPF 2), due to the formation of cyclobutane rings. Interestingly, depolymerization occurs by the cleavage of cyclobutanes in 2 to 1 in an SCSC manner when 2 was heated. While, assemblies of 2D Zn(II) MOFs incorporating 4,4'-sulfonyldibenzoate (sdb) and bpeb in different solvents gave four supramolecular isomers (MOF 3-6), of which two have polyrotaxane structures. One pair of bpep in one isomer (6) undergoes photo-cycloaddition to form dimerized product (7). Structurally similar supramolecular isomers to exhibit different photochemical reactivity and sensing abilities for nitro compounds appear to be unprecedented.


1
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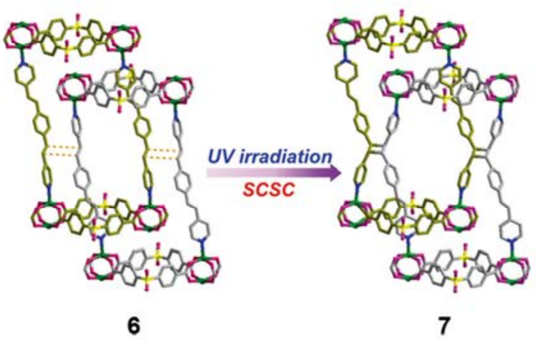
UV irradiation
SCSC
6
7

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발표코드: **KCS1.O-3**

발표분야: 한국다우케미칼 우수논문상 수상자 구두발표

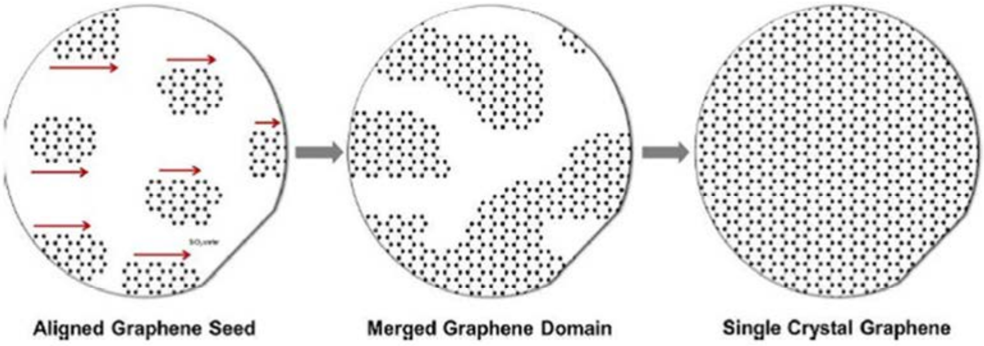
발표종류: 구두발표, 발표일시: 금 10:40, 좌장:

Growth of single crystalline graphene on germanium surface

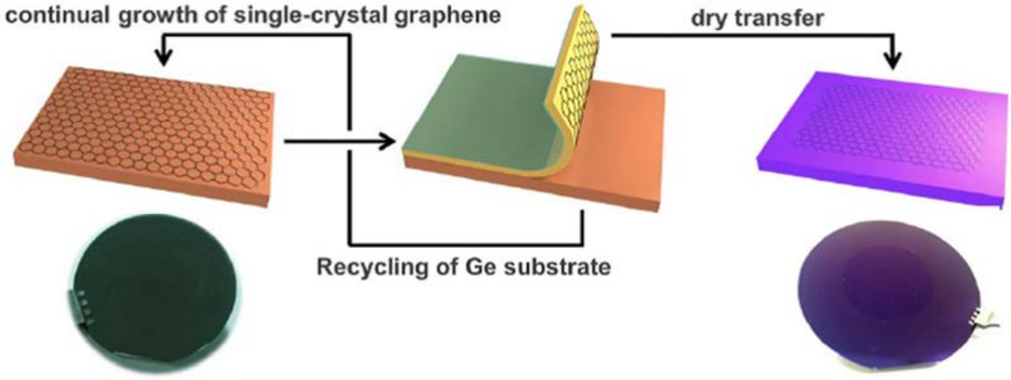
이재현 황동목[1,*]

성균관대학교 성균나노과학기술원 [1]성균관대학교 신소재공학부

The uniform growth of single-crystal graphene over wafer-scale size remains a challenge toward for realization of various applications. In this presentation, I will talk about our current progress of the growth of single-crystal monolayer graphene on Ge (110) surface. A single-crystal Ge surface is a promising candidate for the growth of single crystal graphene, because of (i) its catalytic activity for the formation of graphitic carbon on the surface; (ii) the extremely low solubility of carbon in Ge even at its melting temperature, enabling growth of complete monolayer graphene; (iii) the anisotropic atomic arrangement of single crystal Ge surface, enabling aligned growth of multiple seeds. We observed that well-defined atomic arrangement on the single crystal Ge surface enabled seamless stitching of multiple graphene domains without grain boundaries. Furthermore, a weak van der Waals interaction between graphene and underlying Ge surface enabled facile dry transfer of graphene and recycling the Ge wafer for continuing growth.



< Fig. 1 Schematic illustration of "Seed Orientation Control Growth" >



< Fig. 2 Schematic illustration of the etch-free dry transfer and re-growth process >

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발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 금 10:55, 좌장:

Dual Changes in Conformation and Optical Properties of Fluorophores within a Metal-Organic Framework during Framework Construction and Associated Sensing Event

조원 이희정 최고은 최소라 오문현*

연세대학교 화학과

The heavy metal ions such as Pb, Hg, and Cu were known as toxic materials. Among them, Cu^{2+} is closely related to Wilson's disease and Alzheimer's disease. Therefore, it is important to develop the sensor materials for the selective and sensitive detection of Cu^{2+}. Over the past few decades, several research groups have developed many chemosensors including homogeneous chemosensors based upon organic molecules and heterogeneous chemosensors based upon solid materials for the detection of Cu^{2+}. Heterogeneous chemosensors are especially interesting sensing materials because they might be useful in removing analytes from solutions not only as sensors. By the way, metal-organic frameworks (MOFs) are fascinating candidates for the heterogeneous chemosensors because their properties can be easily tuned through changes in metal ions and functionality of organic building blocks. Herein, we report a micro-sized heterogeneous chemosensors based on a pyrene functionalized MOF for Cu^{2+} sensing. In addition, we report dual changes in conformational and optical properties of fluorophore within a MOF structure during MOF construction and associated sensing event.

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Superprotonic Conductivity of a UiO-66 Framework Functionalized with Sulfonic Acid Groups by Facile Postsynthetic Oxidation

방원주 조현아 이우람 송정화 유기천[1] 김봉수[1] 홍창섭[*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 광전하이브리드 연구센터

Efforts to utilize a metal-organic framework for a proton conducting material will be presented. Facile postsynthetic oxidation of the thiol-laced UiO-66-type framework UiO-66$(SH)_2$ enabled the generation of UiO-66$(SO_3H)_2$ with sulfonic acid groups covalently linked to the backbone of the system. The oxidized material exhibited a superprotonic conductivity of 8.4 x 10^{-2} Scm^{-1} at 80 ℃ and 90% relative humidity, and long-term stability of the conductivity was observed. This level of conductivity exceeds that of any proton-conducting MOF reported to date and is equivalent to the conductivity of the most effective known electrolyte, Nafion.

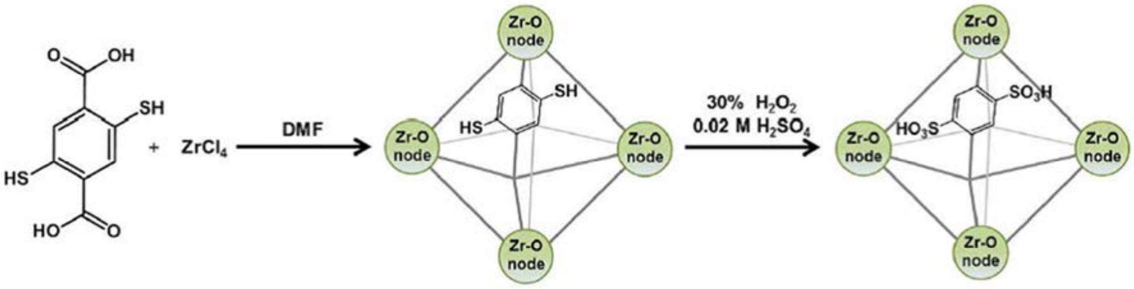

Figure 1. Synthesis of UiO-66$(SH)_2$ and postsynthetic oxidative modification of UiO-66$(SH)_2$ to UiO-66$(SO_3H)_2$. DMF=*N,N*-dimethylformamide.

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발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 금 11:25, 좌장:

Cross-Stacked Single-Crystal Organic Nanowire p-n Nanojunction Arrays by Nanotransfer Printing

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한양대학교 화학과 [1]서울대학교 전기정보공학부

We fabricated cross-stacked organic p-n nanojunction arrays made of single-crystal 6,13-bis (triisopropylsilylethynyl) pentacene (TIPS-PEN) and fullerene (C_{60}) nanowires as p-type and n-type semiconductors, respectively, by using a nanotransfer printing technique. Single-crystal C_{60} nanowires were synthesized inside nanoscale channels of a mold and directly transferred onto a desired position of a flexible substrate by a lubricant liquid layer. In the consecutive printing process, single-crystal TIPS-PEN nanowires were grown in the same way and then perpendicularly aligned and placed onto the C_{60} nanowire arrays, resulting in a cross-stacked single-crystal organic p-n nanojunction array. The cross-stacked single-crystal TIPS-PEN/C_{60} nanowire p-n nanojunction devices show rectifying behavior with on/off ratio of ~ 13 as well as photodiode characteristic with photo gain of ~ 2 under a light intensity of 12.2 mW/cm^2. Our study provides a facile, solution-processed approach to fabricate a large-area array of organic crystal nanojunction devices in a desired arrangement for future nanoscale electronics.

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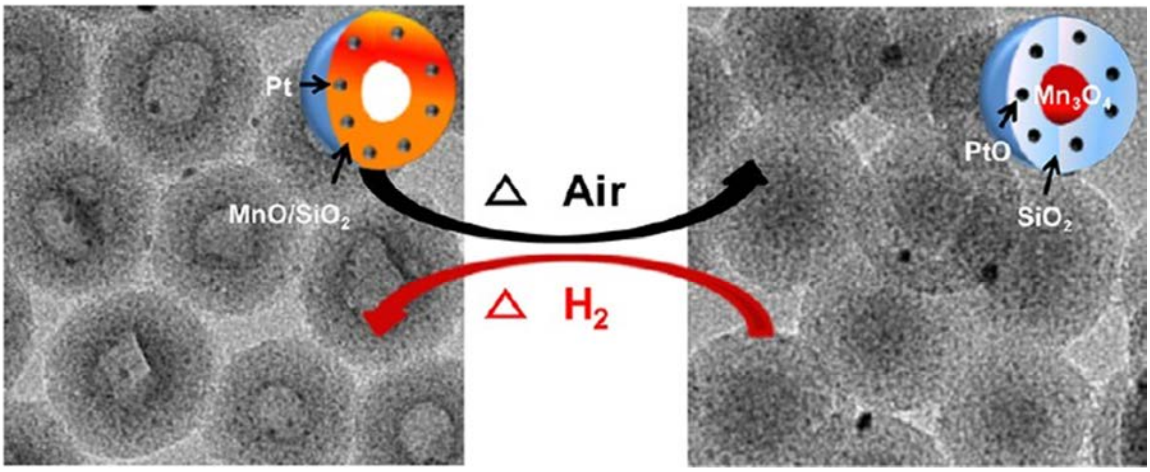
Reversible and Cyclical Transformations between Solid and Hollow Nanostructures in Confined Reactions of Manganese Oxide and Silica within Nanosized Spheres

김진구 하태린 김수민 이인수*

포항공과대학교(POSTECH) 화학과

Annealing of MnO@SiO_2 nanospheres in a reducing gas environment resulted in the transformation of the core-shell structure into a hollow structure as a result of outward diffusion of MnO species into the thermodynamically more stable silicate phase. When the hollow silicate nanospheres were oxidized, the interior cavities were refilled with a Mn_3O_4 phase segregated from the silicate phase, and the hollow structure reverted to the initial core-shell structure. More interestingly, when catalytically active Pt nanocrystals were introduced into the manganese oxide/silica system, the Mn_3O_4 was readily reduced to the chemically reactive MnO, even at low temperature, which enabled reconversion of the solid nanospheres with a Mn_3O_4 core to hollow nanostructures during reductive annealing. Therefore, when MnO@SiO_2/Pt(II) nanospheres were subjected to an oxidation/reduction cycle by repeatedly switching the flowing gas between air and hydrogen, the nanospheres underwent a reversible change between solid and hollow structures, depending on the gas environment. The solid-to-hollow-to-solid transformation was successfully cycled many times simply by repeatedly switching the flowing gas during annealing.


Pt
MnO/SiO$_2$
△ Air
△ H$_2$
Mn$_3$O$_4$
PtO
SiO$_2$

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발표종류: 구두발표, 발표일시: 금 11:55, 좌장:

Foldecture as a Core Material with Anisotropic Surface Characteristics

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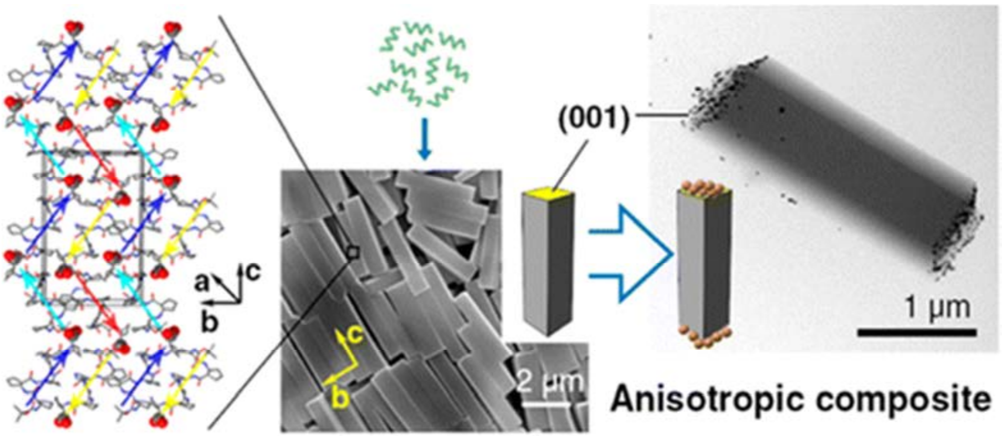
한국과학기술원(KAIST) 화학과, 인터페이스 분자제어 연구센터 [1]한국과학기술원(KAIST) EEWS 대학원 [2]한국과학기술원(KAIST) 인터페이스 분자제어 연구센터 [3]한국과학기술원(KAIST) 화학과 [4]전남대학교 응용화학공학부

The synthesis of microscale, polyhedrally shaped, soft materials with anisotropic surface functionality by a bottom-up approach remains a significant challenge. Herein we report a microscale molecular architecture (foldecture) with facet-dependent surface characteristics that can potentially serve as a well-defined catalytic template. Rhombic rod shaped foldectures with six facets were obtained by the aqueous self-assembly of helical β-peptide foldamers with a C-terminal carboxylic acid. An analysis of the molecular packing by X-ray diffraction revealed that carboxylic acid groups were exposed exclusively on the two (001) rhombic facets due to antiparallel packing of the helical peptides. A surface energy calculation by molecular dynamics simulation was performed to provide a plausible explanation for the development of anisotropy during foldecture formation. The expected facet-selective surface properties of the foldecture were experimentally confirmed by selective deposition of metal nanoparticles on the (001) facets, leading to a new class of sequentially constructed, heterogeneous “foldecture core” materials.


a
c
b
c
b
2 μm
(001)
1 μm
Anisotropic composite

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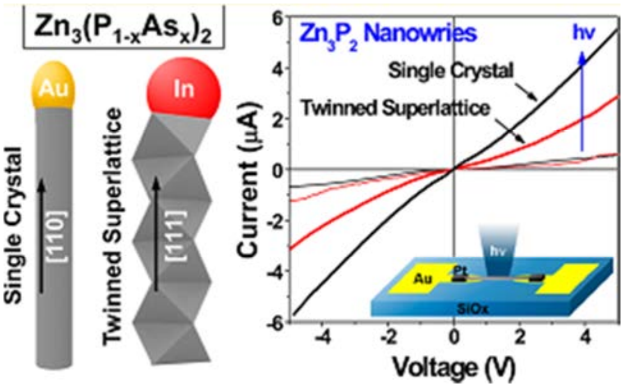
Zn_3P_2-Zn_3As_2 Solid Solution Nanowires

임형순 박기동 장동명[1] 정찬수[1] 박정희[1,*] 유승조[2] 김진규[2]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과 [2]한국기초과학지원연구원 전자현미경부

Semiconductor alloy nanowires (NWs) have recently attracted considerable attention for applications in optoelectronic nanodevices because of many notable properties, including band gap tunability. Zinc phosphide (Zn_3P_2) and zinc arsenide (Zn_3As_2) belong to a unique pseudocubic tetragonal system, but their solid solution has rarely been studied. Here In this study, we synthesized composition-tuned $Zn_3(P_{1-x}As_x)_2$ NWs with different crystal structures by controlling the growth conditions during chemical vapor deposition. A first type of synthesized NWs were single-crystalline and grew uniformly along the [110] direction (in a cubic unit cell) over the entire compositional range ($0 \leq x \leq 1$) explored. The use of an indium source enabled the growth of a second type of NWs, with remarkable cubic-hexagonal polytypic twinned superlattice and bicrystalline structures. The growth direction of the Zn_3P_2 and Zn_3As_2 NWs was also switched to [111] and [112], respectively. These structural changes are attributable to the Zn-depleted indium catalytic nanoparticles which favor the growth of hexagonal phases. The formation of a solid solution at all compositions allowed the continuous tuning of the band gap (1.0 - 1.5 eV). Photocurrent measurements were performed on individual NWs by fabricating photodetector devices; the single-crystalline NWs with [110] growth direction exhibit a higher photoconversion efficiency compared to the twinned crystalline NWs with [111] or [112] growth direction.


$Zn_3(P_{1-x}As_x)_2$
Au
In
Single Crystal
[110]
Twinned Superlattice
[111]
Zn_3P_2 Nanowries
hv
Single Crystal
Twinned Superlattice
Current (μA)
6
4
2
0
-2
-4
-6
hv
Au
Pt
SiOx
-4
-2
0
2
4
Voltage (V)

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발표분야: Oral Presentation for Young International Chemists
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: Jean Bouffard

Photocatalytic Water Splitting with Different Facet Oriented ZnO Electrode

Amol Uttam Pawar 강영수*

서강대학교 화학과

Artificial photosynthesis would be the best prominent way to produce clean and renewable energy. Since last several years many photocatalytic materials have been introduced in artificial photosynthesis [1-3]. The photocatalytic property of those materials depends upon several parameters such as shape, size, photo-active facet etc. ZnO is one of the most appropriate materials in this field (photocatalyst) because of its direct band gap (3.27eV), large excitation binding energy (60 meV) and high electron mobility. It is well known that the properties of ZnO nanostructures strongly depend upon their crystalline structure, morphology, impurity or dopant and defects. The surface energy of ZnO different facets depends upon the atomic arrangement of basic elements such as Zinc and Oxygen, this surface energy can be affect the electron-hole separation. In this sense, the improvement of the photocatalytic activity of ZnO prepared electrode might be achieved by controlling the charge carrier dynamics or the surface catalytic process. Hence, here we describe the hexagonal, pyramidal and rod type ZnO using solvothermal synthesis, which would provide the acceptable structural and surface properties for photocatalytic applications.

References

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Novel 2,5-disubstituted quinolines: Design, synthesis, in-vitro antiproliferative activity and kinase profile

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Four novel series of 2,5-disubstituted quinolines (53 final compounds) have been designed and synthesized as anticancer sorafenib analogues. Two series (amides & ureas) were designed to possess a spacer between the terminal aryl and 2-aminoquinoline scaffold, whereas the other series (C & D) lack the spacer while conserving the oxypicolinamide or propoxy moiety at 5-position, respectively. All the target compounds were preliminary evaluated for their antiproliferative effect against three cancer cell lines (MCF7, HCT116 and SKBR3) by MTT assay and exhibited promising antitumor activity. Therefore, 35 compounds were selected to be tested over a panel of 60 cancer cell lines at a single dose concentration of 10 μM at NCI to broadly screen their antiproliferative activity. Fifteen compounds have showed promising mean growth inhibitions and thus were further tested at five-dose testing mode to determine their GI_{50}, TGI and LC_{50} over the 60 cell lines. The data obtained revealed that KK9087 is the most potent and efficacious derivatives with submicromolar GI_{50} value against some cell lines. Furthermore, it was screened against a panel of 46 oncogenic kinases at single dose of 10 μM and showed selective high inhibition (96%) against TrKA with IC_{50} value of 2.5 μM, so it can be an attractive candidate for further investigatio

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Real-time Dynamic Super-Resolution Imaging of Mg^{2+} Signaling and Wave Propagation by Direct Stochastic Optical Reconstruction Microscopy

Chakkarapani Suresh Kumar 강성호[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Magnesium ion (Mg^{2+}) signaling and dynamics in wave propagation were monitored and imaged by direct stochastic optical reconstruction microscopy (dSTORM). dSTORM, a super-resolution technique with an increased spatial resolution have the potential to monitor and image the intracellular organization of the cell with sub-nanometer resolution. In dSTORM, fluorophores were photoswitched between fluorescent on state and fluorescent off state by simultaneous irradiation of an activation laser and an excitation laser in the presence of a photoswitching buffer. Mag-fluo-4-AM, an intracellular fluorescent indicator dye was incubated in human embryonic kidney 293 (HEK-293) and photoswitched to super-localize the position of Mg^{2+} with subdiffraction-limit resolution. The resulting point spread function measured from activated fluorophores was analyzed by applying Guassian fitting. Further, Na^+ATP was added along with mag-fluo-4-AM to monitor and image the wave propagation of Mg^{2+} in the membrane sites of HEK-293 cell. The real-time dynamics in wave propagation was observed at 0.2 s time interval with spatial resolution of around 20 nm. The results suggest that the intracellular Mg^{2+} signaling and wave propagation was imaged with sub-nanometer spatial resolution and lower temporal resolution of 0.2 s

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Two-Photon Fluorescent Probes for Monitoring Intracellular Zinc Ions

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Among the various transition metals ions, zinc is the most abundant ion in the human body[1]. It is widely found in proteins where it plays important role in various biological processes. The biological imbalance in its concentration has been linked to many neurological disorders such as Alzheimer's and Parkinson's diseases[2]. Recently, the zinc ions have been regarded as quantitative imaging biomarker for the early detection of prostate cancer[3]. Out of the total Zn^{2+} ion (approximately 0.2 mM) content in mammalian cells, fee Zn^{2+} concentration is as low as picomolar to nanomolar levels. A number of one photon fluorescent probes for the detection of zinc ions have been developed and investigated[4]. However these probes have certain limitations as they requires a rather short excitation wavelength that limits their use in tissue imaging up to deep penetration depth ($^{2+}$ chelator. Both derivatives show the dramatic increase in their fluorescence intensities upon the addition of Zn^{2+} ions. Further the good water solubility, high selectivity, K_d values in nanomolar range and insensitivity to biological relevant pH range make them suitable candidate for monitoring the zinc ions in live cells and tissues. In the oral presentation, the synthesis, photo-physical behaviour and bio-imaging applications of these probes will be discussed.

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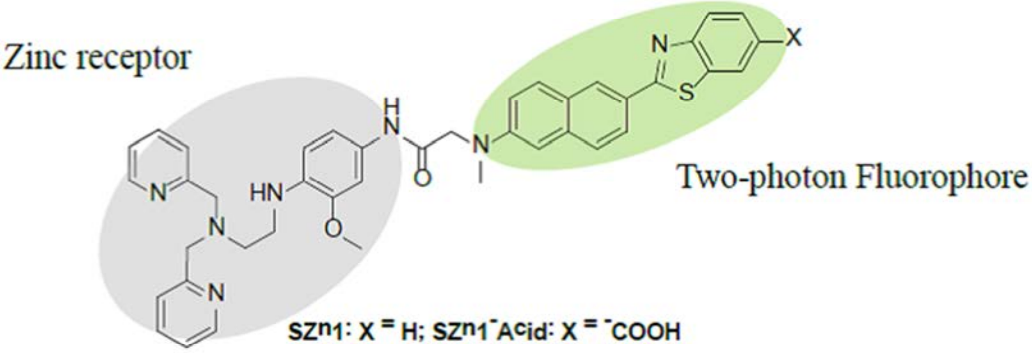
Zinc receptor
Two-photon Fluorophore
H
N
O
N
HN
N
N
N
O
N
S
X
SZn1: X = H; SZn1-Acid: X = -COOH

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Synthesis and Structural Properties of Multicomponent Nanodots Assemblies Core - Silica Shell Nanosystem

KOSTYUKOVADIANA 유효종*

한림대학교 화학과

Highly spherical nanoparticles with a core comprising multiple gold (Au) or platinum (Pt) nanodots assembly and a silica shell (multi-Au@SiO2 NPs, multi-Pt@SiO2 NPs, multi-Au/Pt@SiO2 NPs, and multi-Pt@SiO2 NCs (NCs; nanochains) were successfully synthesized through a reverse (water-in-oil) microemulsion-based method. The microemulsion was prepared by mixing a surfactant (Brij35), cyclohexane, n-hexanol, and aqueous HAuCl4 and K2PtCl4 solutions. Multiple Au-nanodots with a maximum diameter of ~5 nm could be assembled and encapsulated within a silica matrix during the growth process. For investigation the availability of multi-Au@SiO2 NPs, we generated multiple gold (Au) nanodots core-mesoporous silica shell nanoparticles (multi-Au@mesoporous-SiO2 NPs) without using any surface-protective or etching agents. Thermal treatment of multi-Au@SiO2 NPs in an aqueous media lead to generation of mesopores silica shell without any other morphology changes. The multi-Au@mesoporous-SiO2 NPs showed much higher catalytic activity in the reduction of 4-aminophenol than multi-Au@SiO2 NPs and other single Au nanodot core-silica shell nanoparticles with yolk-shell morphologies, which were also effectively fabricated. Multi-Pt@SiO2 NPs and multi-Pt@mesoporous-SiO2 NPs were also prepared through the similar synthetic strategies to the Au counterparts. As for the multi-Pt@SiO2 NCs - they were also synthesized through a reverse (water-in-oil) microemulsion-based method in the presence of HCl (aq.). By changing pH of the reaction media we could successfully synthesize the Pt nanoparticle-embedded silica nanochains with the average width of was 20 nm. The kinetically controlled reduction of K2PtCl4 and HAuCl4 by Brij35 surfactant within reverse micelles, followed by condensation of TEOS, led to the formation of hybrid multi-Au/Pt@SiO2 NPs multiple metal core-silica shell systems. The average diameter of Pt nanodots were ~2 nm and of Au nanodots were ~5 nm. Pt-nanoparticles were much more dominant comparatively. Further increasing of the temperature is hopefully going to generate the yolk-shell and mesoporous multi-Pt@SiO2 assemblies systems that could be in future applied in particular as part of promising functional nanomaterials for a variety of applications such as catalysis.

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Direct C-H arylation synthesis of (DAD`A`) constituted alternating polymers with low bandgaps and their photovoltaic performance

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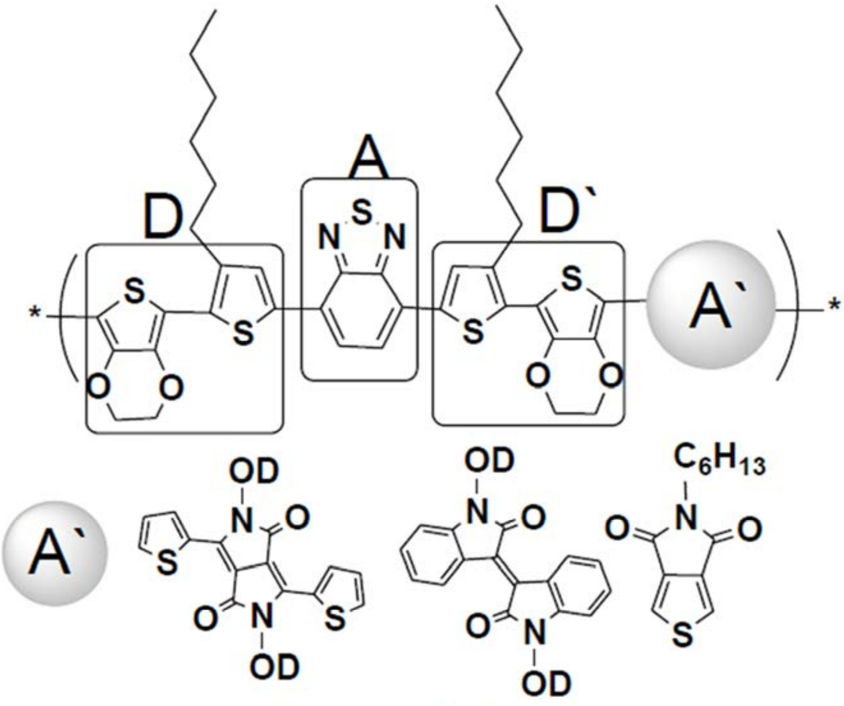
광주과학기술원(GIST) 나노바이오재료전자공학과 [1]광주과학기술원(GIST) 신소재공학과

A series of new constituted (DAD`A`)-conjugated polymers were synthesized via C-H arylation with the aid of a Pd(OAc)2/Bu4NBr catalytic system and were based on 4,7-bis(4-hexylthiophen-2-yl)-2,1,3-benzothiadiazole (HT.BT.HT), which alternated with 3,4-ethylenedioxythiophene (EDOT) as a second donor and a lactam- and/or imide-containing material as a second acceptor. The synthesis methodology avoided the drawbacks of Stille and Suzuki coupling and obtained high yields. All of the new polymers possessed broader absorption windows with low energy bandgaps (1.34-1.64 eV), as well as low-lying HOMO energy levels. The prescreening of these polymers as an active material in bulk heterojunction solar cells was investigated and power conversion efficiency of 2.36% was achieved.



* OD = octydodecyl-

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Purine scaffold Hsp90 inhibitors as mitochondria targeting anticancer and theranostics agents

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울산과학기술대학교(UNIST) 자연과학부/화학과 [1]울산과학기술대학교(UNIST) 자연과학부 화학과

Mitochondria, the powerhouse of cell are a potential target in cancer treatment. Heat shock proteins (Hsp) and their paralogs have major role in coordinating the various functions including cell proliferation, metabolism and even apoptosis. The mitochondrial pool of Hsp90 and its mitochondrial paralog, TRAP1, suppresses cell death and reprograms energy metabolism in cancer cells; therefore, Hsp90 and TRAP1 have been suggested as target proteins for anticancer drug development. On the other hand, theranostics refers to an appealing new approach to drug development wherein therapeutic modalities are combined with those associated with diagnostic imaging. The field has emerged as an interdisciplinary research area involving chemistry, material science, biology, and medicine that combine diagnostics and therapeutics, enabling early detection, targeted drug delivery and release, and monitoring of therapeutic response with the aid of imaging modalities in a single procedure. In this context, purine-scaffold Hsp90 inhibitor series has been reported to be potent and selective against Hsp90 both in vitro and in vivo models of cancer. In this work we describe the design and synthesis of a few purine based molecules for mitochondrial TRAP1 targeting and theranostics application.

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Enhanced Photophysical Properties of Semiconductor Nanostructures by Surface Plasmons

Saji Thomas 김동하*

이화여자대학교 화학나노과학과

Since plasmonic metal nanostructures possess the unique characteristic to interact with visible light through excitation of surface plasmons (SPs), inclusion of plasmonic metal onto semiconductors is a facile strategy to improve the photophysical properties of semiconductor by the transfer of energy or charge from the metal to the semiconductor. The luminescence of semiconductors can be significantly enhanced by incorporating plasmonic metal nanoparticles (NPs) appropriately. Reduction of defect emission (DE) and enhancement of band emission of ZnO can be achieved by incorporating Au NPs on ZnO. Since energy of defect emission (DE) and surface plasmon absorption energy of Au are overlapped, SPs of Au can be excited using the energy of DE, and thus formed energetic electrons in Au are transferred to the conduction band of ZnO leading to the enhancement in the recombination of excitons (Figure 1a-b). Similarly, Förster resonance energy transfer (FRET) efficiency can be enhanced by placing Au at an appropriate distance from the donor, and the enhanced emission energy of donor can be transferred to the acceptor, resulting in an overall enhancement in the FRET efficiency (Figure 2a-b).

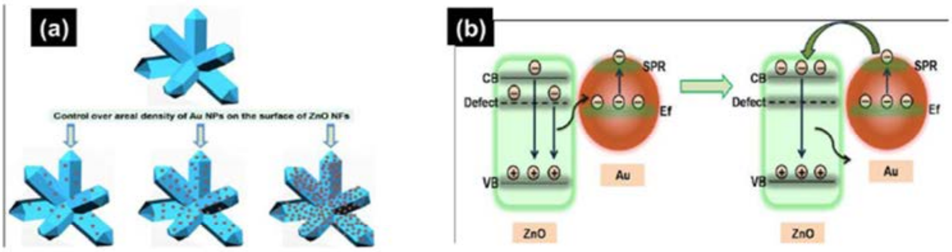

Figure 1a: Hexagonally shaped ZnO nanorods attached together at one end to give a flower-like nanostructured morphology. The density of citrate-capped Au NPs on the surface of the ZnO NFs was adjusted to afford optimum photoluminescence efficiency. The spheres on the surface of the ZnO NFs represent citrate-capped Au NPs. **b:** Surface-plasmon-mediated quenching of defect emission and the enhancement of band emission; the defect emission of the ZnO NFs was in resonance with the surface plasmon excitation of the Au NPs, which led to the conversion of defect loss into band-gap emission.

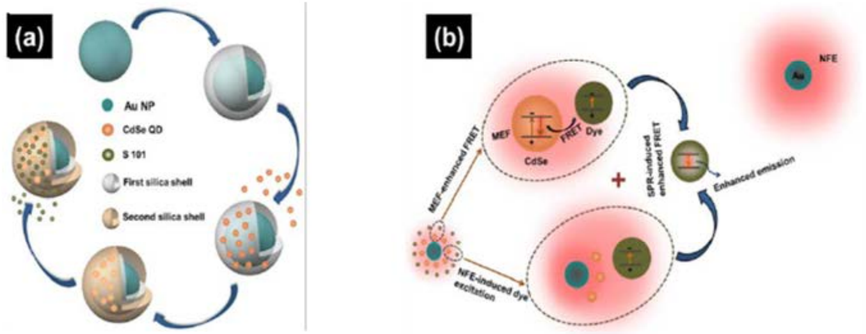

Figure 2a: Schematic representation of the entire fabrication process of multilayer core-shell nanostructures, where 30-nm Au NPs are is used as the inner core. Additional shells are developed subsequently on the Au NPs. **b:** Schematic representation of mechanisms playing role in the SPR induced enhanced FRET.

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A Crystal Facet Engineering of the Morphology and Structure of Nanomaterial for Enhancing Photo-Catalytic Activity

van thanh khue 강영수*

서강대학교 화학과

Taking advantages of selective adsorption of surfacatnts or forein chemical species, the morphology-controlled synthesis of various shapes of photocatalytic materials was done to obtain the highest photoactivity. As the results, by using cetyltrimethylammonium bromide (CTAB) which acts as surfactant, dispersed CdS single crystals were obtained via a hydrothermal condition. Strong interaction between the cationic head groups of CTAB and the {001} planes of CdS hexagonal crystals result in a single-crystalline growth along [100] direction. On the other hand, uniform and single-crystalline α-Fe_2O_3 polyhedral nanoparticles in hexagonal crystal system named truncated hexagonal bipyramid (THB) were fabricated. Under hydrothermal condition, carboxymethyl cellulose (CMC) and hydrazine molecules play roles such as dispersant and capping agents, respectively, during the crystallographical growth. The optical and magnetic properties of the hematite particles were investigated as well.

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Fluroescent and high conductive iron-based nanoparticles via wet chemistry method

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부산대학교 나노과학기술학과 [1]부산대학교 나노메디컬공학과

Iron based chalcogenides nanocrystrals (NCs) hold considerable promise for both solar energy conversion and electrical storage. Their utilization is hampered by lack of control over crystallinity and nanoscale organization of the homogeneous fabrications, the availability of high quality NCs of these materials will help us understand better both the photophysical processes in them and acquire building blocks to make better mesoscale materials from them. Therefore, two kinds of ~30nm diameter NCs $FeSe_x$ (X=1, 2) have been synthesized and which display strong photoluminescence indicative of minimal defect density which are previously unavailable. $FeSe_x$ (X=1, 2) displays photoluminescence (PL) peaks at 447nm and 462nm respectively while quantum yields are as high as 20%. Additionally, the synthetic route for iron based ternary chalcogenides NCs also have also been developed by doping Cr elements in the synthetic process, i.e., $FeCr_2Se_4$ and $FeCr_2S_4$ are synthesized through using a facile wet chemical method. $FeCr_2Se_4$ and $FeCr_2S_4$ NCs possessed narrow size distribution with high quality. $FeCr_2Se_4$ and $FeCr_2S_4$ NCs offer a promising conductivity for integration as electrical application. Importantly, these colloidal NCs can be considered be suitable for biomedical fluorescence marker and as the environmentally benign substitutes for optical, electronic and photovoltaic materials. Additionally, iron based bimetallic magnetic nanomaterials have been studied as advancement.

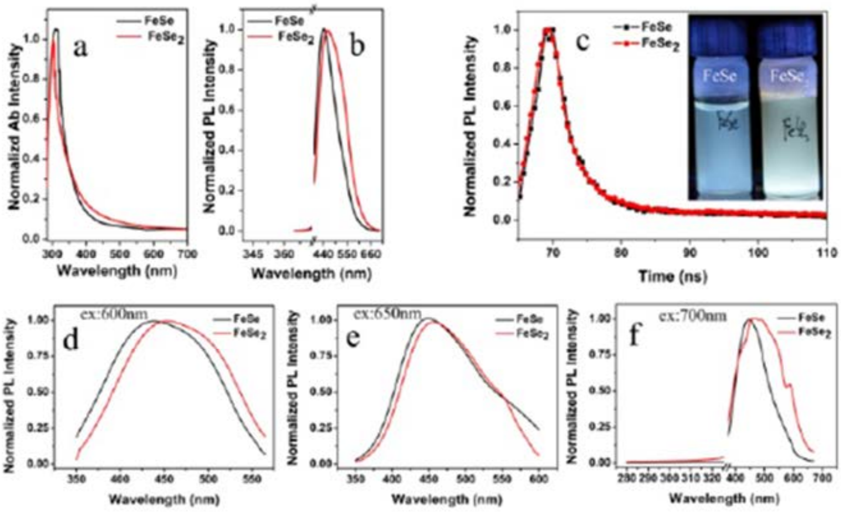

Figure 1: The optical property of FeSe$_x$ nanoparticles. a) the UV-vis absorption of FeSe and FeSe$_2$ NPs respectively; b) the photoluminescent property of FeSe and FeSe$_2$ nanoparticles; c) the life-time measurement of two kinds NPs; d)-e) two-photo photoluminescent property by using the different excited wavelength (600nm, 650nm. 700nm).

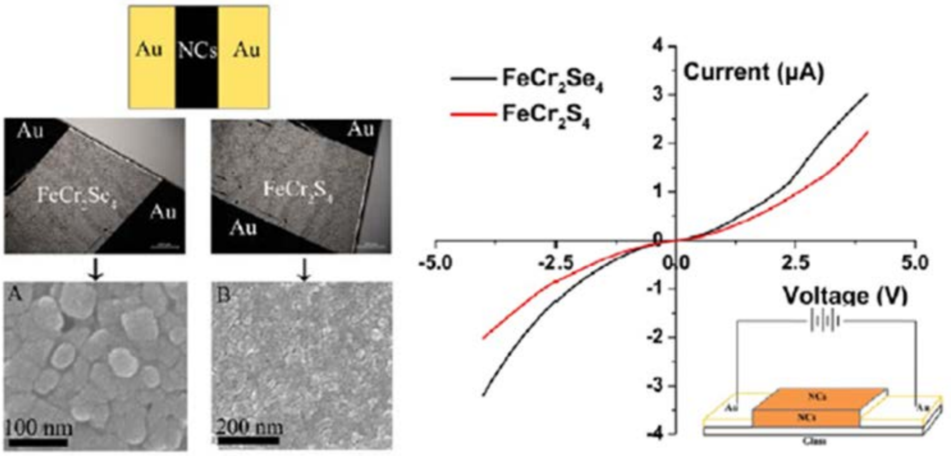

Figure 2: Left-The device fabrication for the measurement of conductivity in two kinds of forms by using the FeCr$_2$Se$_4$ and FeCr$_2$S$_4$ NCs respectively; Right-The current value of conductivity whole measuring at the room temperatures. The inset image is the simple device mechanism.

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Oxidation-reduction of dopamine modified hyaluronic acid shell on silica particle induced by pH control

이정욱 고재형[1] 유정주 손대원*

한양대학교 화학과 [1]한양대학교 고분자 물리화학 연구실

Hyaluronic acid (HA) has currently several therapeutic applications due to relevant advantages of biocompatible, biodegradability, and specific targeting on cancer cell. This research focused on core-shell formation with silica particle and dopamine modified HA. The process was performed on different pH conditions in order to investigate core-shell formation. It was found that the redox state of dopamine is a key factor to form core-shell particles. Substituted ratio of dopamine modified HA was determined by using 1H-NMR. The particles` size and morphology were measured by DLS, AFM. The chemical composition of hyaluronic acid shell formed in different pH was analyzed by FT-IR, XPS. To suggest definite image of structure, the core-shell particles were observed by SEM, Bio-TEM.

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Fabrication and Evaluation of Cholesterol Chitosan Nanoparticle for Gene Transfection

김희권

전북대학교 의학전문대학원/핵의학교실

Cholesterol-Chitosan was synthesized from chitosan oligosaccharide lactate and cholesteryl chloroformate. And a series of modified chitosans which blends with poly(L-lysine) (PLL), polyethyleneimine (PEI), and poly(ethylene glycol) (PEG) were prepared by a one-step aerosol method. Agarose gel retardation assays indicated that plasmid DNA was associated with new chitosans. From the transfection experiments with HEK 293 cells, cholesterol-chitosan showed more effective transfection than unmodified chitosan. Also, the polymeric complexes of PEI with chitosan enhanced the transfection efficiency. Our study suggests that cationic property and cholesterol structure of chitosan can increase gene transfection efficiency.

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One-Step Functionalization of Zwitterionic Sulfobetaine Polymer Surfaces by Metal-Polyphenol Coating

김수엽 조우경[1] 강성민*

부경대학교 해양바이오신소재학과 [1]충남대학교 화학과

Zwitterionic sulfobetaine polymer surface has been of interest because of its excellent non-biofouling property, long-term stability, and easy availability of the monomer. However, lack of surface functionalizability has hampered further applications. In the present study, we report that metal-polyphenol coating provides an important platform for functionalizing zwitterionic poly[(3-(methacryloylamino)propyl)dimethyl(3-sulfopropyl)ammonium hydroxide] (poly(MPDSAH)) surfaces. In addition, the coating is easily combined with conventional soft lithography, microcontact printing, enabling selective functionalization of poly(MPDSAH) surfaces. We believe that our findings can be a general route for post-functionalization of non-biofouling surfaces including zwitterionic polymer surfaces.

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Enhancing Performance of Polymer Solar Cells using Down-conversion with Customized Energy Donor Materials

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One of the major challenges in polymer solar cells (PCS) is to fabricate devices that efficiently absorb sunlight from UV-vis to near infra-red region. For this aim, the most of research has been focused on the increase of absorption range of active materials into near IR-region. However, it is not easy to satisfy the wide absorption range with single materials. Furthermore, the PCS can't efficiently absorb high photon energy between 350- 450 nm due to thermolization loss compared with low energy photon. To efficiently use the high energy photon without theromolization loss, we introduce the down-conversion process using an addition of iridium complexes as an energy donor into active layers comprised of PTB7 and PC$_{70}$BM. The iridium complexes efficiently convert high energy photon into lower energy photon (energy acceptor, in this study PTB7) through triplet-singlet energy transfer, resulting in the increase of current density. To find out customized energy donor materials for PTB7, we developed four energy donor materials (1pq-OH, 2pq-OH, ppy-OH, and F$_2$ppy-OH), that have different absorption, emissions, and quantum yields, which are critical factors for energy transfer, and investigated energy transfer efficiency by transient photoluminance method, followed by the fabrication of the inverted devices (ITO/ZnO/PTB7:PC$_{70}$BM: 10 wt% Ir complex/MoO$_3$Ag). As a result, the best device performance can be reached with 2pq-OH, followed by, 1pq-OH, F$_2$ppy-OH, ppy-OH, and reference. There results are related with quantum yield of energy donor and overlap between the emission of energy donor and the absorption of energy acceptor.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Bio-Inspired Multilayer Films by Layer-by-Layer Deposition of Dopamine-Modified Hyaluronic Acid and Polyethylenimine for Metal Sensitive Sensors

노시은 손대원 노재근*

한양대학교 화학과

Layer-by-layer (LbL) self-assembly is one of the simple methods for fabricating multilayer thin films on silicon wafer. In this study, dopamine modified hyaluronic acid (HA_Dopa) and polyethylenimine (PEI) multilayer is built on the surface of silicon wafer. LbL method is based on the consecutive adsorption of polyanions and polycations via electrostatic interactions that form multiple layers. Hyaluronic acid (HA) is a natural polyanions that plays important role in initiating of the biological reactions, such as early-and long-range engagement between cells with substrates. Dopamine contains the catechol functional group, which forms strong interaction with a variety of substrates via covalent or noncovalent bonds. With this advantage, it is possible to produce a biocompatible multilayer films using a layer by layer self assembled method using dopamine modified hyaluronic acid. Multilayer films consisting of PEI and HA_Dopa were utilized as bio-inspired heavy metal sensitive films. In this study, we hypothesize that the formation of multilayer films of conjugate HA_Dopa and PEI can produce surfaces with distinct properties, when compared with the conventional HA and PEI. To know a successful synthesis of the conjugate, the product of synthesis is analyzed by 1H-NMR. In addition, the formation of HA_Dopa and PEI multilayer films by the LbL technique was investigated using atomic force microscopy (AFM) and UV/Visible spectroscopy. Also, the various heavy metal ions are captured by multilayer films, it can be also confirmed through the UV/Visible spectroscopy.

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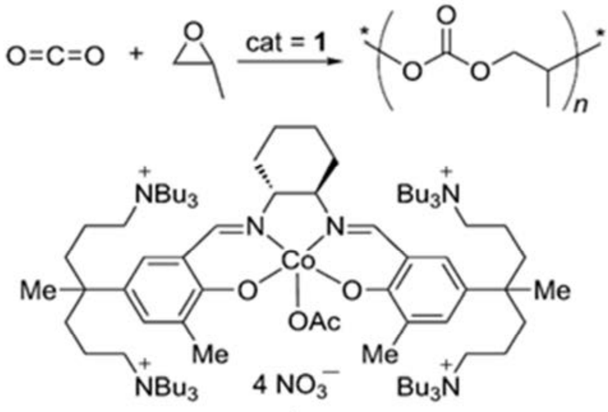
발표종류: 포스터, 발표일시: 수 16:00~19:00

(salen)Co(III) complex tethering four quaternary ammonium salts, an effective catalyst for the copolymerization and terpolymerization of carbon dioxide/propylene oxide/phthalic anhydride

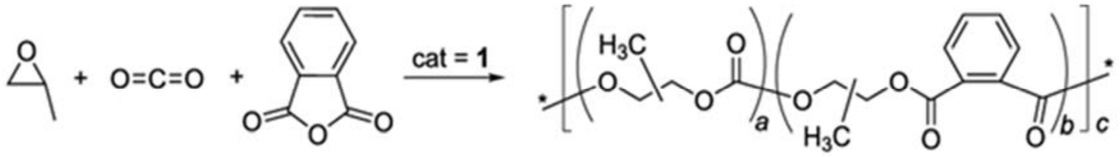
어성찬 이분열*

아주대학교 분자과학기술학과

The (salen)Co(III) complex 1 tethering four quaternary ammonium salts, which is a highly active catalyst in CO2/epoxide copolymerizations, shows high activity for propylene oxide/phthalic anhydride (PO/PA) copolymerizations and PO/CO2/PA terpolymerizations. In the PO/PA copolymerizations, full conversion of PA was achieved within 5 h, and strictly alternating copolymers of poly(1,2-propylene phthalate)s were afforded without any formation of ether linkages. In the PO/CO2/PA terpolymerizations, full conversion of PA was also achieved within 4 h. The resulting polymers were gradient poly(1,2-propylene carbonate-co-phthalate)s because of the drift in the PA concentration during the terpolymerization. Both polymerizations showed immortal polymerization character; therefore, the molecular weights were determined by the activity (g/mol-1) and the number of chain-growing sites per 1 [anions in 1 (5) + water (present as impurity) + ethanol (deliberately fed)], and the molecular weight distributions were narrow (Mw/Mn, 1.05?1.5). Because of the extremely high activity of 1, high-molecular-weight polymers were generated (Mn up to 170,000 and 350,000 for the PO/PA copolymerization and PO/CO2/PA terpolymerization, respectively). The terpolymers bearing a substantial number of PA units (fPA, 0.23) showed a higher glass-transition temperature (48 °C) than the CO2/PO alternating copolymer (40 °C).



1



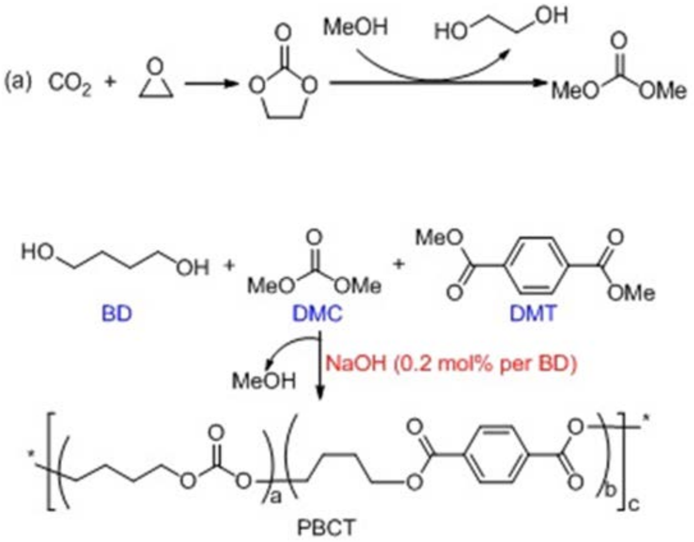
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-7**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Branched Poly(1,4-butylene carbonate-co-terephthalate)s : LDPE-like Biodegradable Semicrystalline Thermoplastics

박성연 이분열*

아주대학교 분자과학기술학과

Dimethyl carbonate (DMC) is an attractive candidate as a sustainable monomer, as it can be produced inexpensively on a large scale using CO2 [scheme (a)]. Previously, it was prepared expensively using hazardous phosgene and its utilization as a monomer in the step-growth polymerization had been limited. In addition, 1,4-butanediol (BD) can be also considered as a green monomer. BD has been produced on a large scale from petroleum or coal but, recently, its production using renewable resources via fermentation has been demonstrated. Branched poly[1,4-butylene carbonate-co-terephthalate]s (PBCTs) have been synthesized by the addition of a small amount of glycerol propoxylate (1) or pentaerythiritol (2) in the polycondensation of 1,4-butanediol, dimethyl carbonate, and dimethyl terephthalate. To avoid gel formation, the feed amount of 1 or 2 was carefully controlled at below 0.5 mol% for 1 and below 0.3 mol% for 2. When feed of 1 or 2 was used, a high-molecular-weight melt state (Mw ~180,000 g/mol) was reached in a total reaction time of 5.5 to 6.5 h with a yield higher than 90%. The generated PBCTs were a semicrystalline polymer (Tg ~5 °C and Tm ~120 °C) when the terephthalate content (F[TPA]) was 45?50 mol%. The crystallization rate increased with increasing F[TPA] and branch content (F[1 or 2]); PBCT composed of F[TPA] = 49 mol% and F[1] = 0.44 mol% was crystallized completely in a short time, ~3 min, at a crystallization temperature of 50 °C. The branched PBCT exhibited more pronounced toughness in tensile test while providing the advantage of processibility at high shear rates due to the pronounced shear thinning in melt. It was also found that the branched PBCTs were biodegradable by a buffer solution containing a lipase.


(a)
CO2
MeOH
HO OH
MeO OMe
BD
DMC
DMT
NaOH (0.2 mol% per BD)
MeOH
a
b
c
PBCT

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photophysical Properties of Hyperbranched Trimethylsilyl Substituted Poly(para-phenylene vinylene) Derivatives

김의찬 안택*

경성대학교 화학과

Conjugated polymers have emerged as viable electronic materials for numerous applications. So far, the majority of work on conjugated polymers has been focused on linear one-dimensional polymers. Although a few of two-dimensional conjugated polymers, such as hyperbranched conjugated polymer have been reported to exhibit comparable charge transferring and processing properties to their linear counterparts, two-dimensional conjugated polymeric light-emitting materials have been less discussed in the literature. Here, we report the synthesis and light-emitting properties of trimethylsilyl containing hyperbranched conjugated poly(para-phenylene vinylene) derivatives through A2 and B3 type monomer. A synthesized trimethylsilyl containing hyperbranched polymer showed pure blue emission as film state at 457 nm in photoluminescence (PL) measurement and was found to showing almost no excimer emission peak even the polymer film was annealed at 80 oC. Detailed synthetic routes and photophysical properties of trimethylsilyl containing hyperbranched conjugated poly(para-phenylene vinylene) derivatives will be discussed.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Growth of Polymeric Large Spherulites by using Organic Crystallite Templates and Fabrication of High-performing Electronic Devices

김재윤 박지은 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Conjugated polymers request to substantial interest for using in organic solar cells, field effect transistor and optoelectronic devices of our day. We synthesized π-extended conjugated donor-acceptor (D-A) polymer, PDPPBT. PDPPBT polymer indicated high crystallinity in a film state following thermal treatment, with the corresponding TFT device exhibiting a high carrier mobility. In this study, we have optimized the concentration of crystallizable additive, 1,3,5-trichlorobenzene (TCB), to form a macroscopic alignment in spin-coated thin film. Also, we could compare charge-transport properties of radial direction and perpendicular direction having lamella or amorphous region in epitaxial crystalline. Therefore, TCB additive is recognized as a very promising method to increase the performance of electronic devices requiring high anisotropy of the conjugated molecules and polymers.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Diketopyrrolopyrrole-based Alternating Conjugated Terpolymer

김상범 김형종 엄현아 조민주 최동훈*

고려대학교 화학과

Organic semiconductors have attracted great attentions owing to their potential advantages as low-cost, flexible, and feasible large-area devices. Recently, the alternating acceptor-donor-acceptor-donor’ (A-D-A-D’) terpolymer structure has been demonstrated as a highly efficient approach to improve the electronic device performance concerning their tunable energy level between highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). In this study, we synthesized new diketopyrrolopyrrole (DPP)-based alternating conjugated terpolymers bearing different donating units such as fluorene and bithienyl unit, and applied them to electronic and optoelectronical device. Moreover, we studied thermal, physical, and electronic properties. The efficient properties of A-D-A-D’ terpolymer were investigated and compared with the corresponding A-D and A-D’ copolymers.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Diketopyrrolopyrrole-based Polymers bearing π-extended (E)-1,2-di(thiophen-2-yl)ethane and (E)-1,2-di(selenophen-2-yl)ethane for High Performance Organic Solar Cells

엄현아 신지철 이태완 조민주 최동훈*

고려대학교 화학과

Diketopyrrolopyrrole (DPP)-based conjugated polymers have been intensely studied. The DPP moiety exhibits a planar conjugated bicyclic structure, which leads to strong π-π interactions that can allow for optimization of the performance of organic semiconductors. Among the various types of DPP-based polymers, DPP copolymer incorporating a vinyl group have reported high performance field-effect transistors (FETs). Although a number of studies have exhibited the outstanding characteristics of charge-transport properties of these polymers, not many precise studies have been conducted to investigate organic photovoltaics. In this work, we synthesized DPP-based conjugated polymers containing vinyl group as donor and successfully fabricated high efficiency organic solar cell devices by using solvent method.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Mechanical Properties from Molecular Covalent Bridge in Carbon Nanotube Fiber

김현주 이재관[1,*] 구본철[2,*]

조선대학교 탄소소재학과 [1]조선대학교 화학교육과/탄소소재학과 [2]한국과학기술연구원(KIST) 탄소융합소재연구센터

Traditional powder-based CNTs have significant problems in translation to real-world applications due to their tendency to strongly aggregate as well as the complications in synthesizing CNTs long enough to utilize their excellent electrical and mechanical properties. As a result, there has been considerable interest in the production of CNT fibers or yarns, which require less processing than traditional CNTs, but have the potential for a wide-range of applications. However, even the CNT fibers suffer from less-than desirable strengths and conductivities due to poor interfacial interactions between individual CNTs. In this study, we evaluated a simple and efficient post treatment method for improving the performance of carbon nanotube fibers (CNTF) from using molecular covalent bridge . The tensile strength and tensile modulus of cross-linked CNT fibers were increased by 180% and 210% compared to that of neat CNT fiber following thermochemical treatment.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Side-chain Engineering on Semiconducting Properties of Isoindigo-Based Polymers

박지은 신지철 조민주 최동훈*

고려대학교 화학과

Tuning the side-chain has a significant strategy to advance high performance semiconducting polymers for electronic and optoelectronic applications. The alkyl chains tethered in conjugated polymer backbone have impacts on the properties of polymers such as the molecular energy levels, internal morphology, and charge transport performance. In particular, systematically moving the alkyl-chain branching point position away from the polymer backbone revealed the advantages which are reducing the steric hindrance between bulky side chain and polymer backbone and the intermolecular π-π stacking distance. This study demonstrated the specific effect of the alkyl-chain branching position is thought to be critical according to related work on organic electronics.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Diktopyrrolopyrrole-Based Polymers Containing Benzo[1,2-b;4,5-b’]dithiophene and Anthracene and their Semiconducting Properties

이대희 김애선 박지은 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Diketopyrrolopyrrole (DPP)-based copolymers have been identified as highly promising materials for organic field-effect transistors (OFETs) and organic photovoltaics (OPVs) because they have significantly high carrier mobilities in thin film transistors and high power conversion efficiencies in OPVs. In the previous research, we synthesized the low bandgap alternating copolymers containing benzo[1,2-b;4,5-b’]dithiophene (BDT) and anthracene (ANT)-based monomer. It was newly made that BDT and ANT units were tethered to the polymer backbone in an orthogonal fashion, which might aid high crystallinity and strong polymer chain interaction. In this study, we investigated the OPV properties of the PCBM blend films with copolymers. Also, we also confirmed the effect of surface treatment on the device performances.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thiazolyl Diketopyrrolopyrrole-Based Conjugated Polymer Containing Electron-Accepting Moiety for Electronic Applications

홍한나 이대희 신지철 조민주 최동훈*

고려대학교 화학과

Major efforts for electronic devices research have been focused on developing new building blocks for constructing semiconducting, electron-accepting polymer. In the past few years, diketopyrrolopyrrole (DPP) was found to be an excellent electron accepting moiety for building a large number of polymer semiconductors. To further bring down highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels of DPP polymers, we replace thiophene flanked into DPP unit by thiazole which is bearing the electronegative nitrogen atom. We successfully synthesized the polymer containing DPP core flanked with two 2-thiazolyl substituents. Thermal analysis, cyclic voltammetry, X-ray diffraction (XRD) and absorption spectroscopy were carried out to investigate their physical and optoelectronic properties. Electronic devices were fabricated to study their semiconducting properties.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Monosubstituted Hybrid Giant Molecular Nanoparticles for Vertical Alignment of Liquid Crystals

윤원진 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

For the formation of vertical alignment (VA) of liquid crystal (LC), polyhedral oligomeric silsesquioxanes (POSS) can be used. However, the pristine POSS are highly aggregate themselves in the LC media and make the macroscopic particles due to their poor compatibility and weak interaction with LC hosts, resulting in severe light scatterings. To overcome this problem, we newly synthesized the cyanobiphenyl monosubstituted POSS giant molecule (CBM-POSS), which showed an excellent dispersion in nematic (N) LC media and formed the perfect VA of LC without using conventional polymer-based VA layers. On the basis of the systematic experiments and careful analysis, we realized that cyanobiphenyl part chemically attached to the pristine POSS with an alkyl chain can improve the initial solubility and interaction with LC media but CBM-POSS to gradually diffuse onto the substrate of LC cell for the formation of VA layer without forming the macroscopic aggregations. Therefore, the novel CMS-POSS VA layer can allow us to open the new doors for electro-optical applications and to cut the manufacturing cost. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806) and BK21Plus Program, Korea.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Alternating Conjugated Copolymers for Electronic Applications

최수나 신지철 박지은 조민주 최동훈*

고려대학교 화학과

Fused-thiophene ring systems lead to elevated structural rigidity in polymer backbones due to lack of structural distortion and promote highly ordered π ? π stacking between the polymer chains. Among fused-thiophene derivatives, Dithieno[3,2-b:2′,3′-d]thiophene (DTT) units containing three fused thiophenes have been developed for the application of organic semiconductors recently. In addition, incorporating alkyl chains into the DTT moiety alleviate poor solubility caused by rigidity of DTT unit. In this study, we successfully synthesized DTT-based conjugated polymers and conducted optical, physical and electrochemical characterization. Eventually, we demonstrated the performance of organic semiconductors resulting from the properties of the DTT-based new polymer.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regular Alternating Terpolymer Containing Diketopyrrolopyrrole for Efficient Organic Solar Cells

김애선 신지철 조민주 최동훈*

고려대학교 화학과

The use of the donor-acceptor (D-A) concept to create an alternating semiconducting copolymer structure has been recently demonstrated as a highly efficient approach to improve the device performance. From this perspective, terpolymer system which consists of three different units in the polymer backbone is considered to be promising candidates for designing conjugated polymers for highly efficient polymer solar cells. We could be recognized the advantages of the reported donor and acceptor moieties and add new combinations of them to satisfy the desired properties of conjugated polymers. The molecular energy levels, intermolecular interaction, light harvesting property, and charge transport property could be tuned with the kind of acceptor and donor monomer. In this study, alternating terpolymer ($-(A-D_1-A-D_2)_n-$) is have been synthesized by electron accepting DPP units (A) between two different electron donors such as pyrene (D_1) and thiophene (D_2) to enhance the π-π interaction while still retaining good solubility. We performed a systematic study of their structural, optical, electrical properties and fabricated thin-film transistors and photovoltaic cells.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Donor'-Acceptor-Donor'' Type Conjugated Terpolymer for Electronic Applications

고은이 박지은 신지철 조민주 최동훈*

고려대학교 화학과

Extensive investigations on design and synthesis of donor-acceptor (D-A) conjugated polymers have been the major attractive area due to their unique electronic and optoelectronic properties lately. Among the various polymers, it is demonstrated that diketopyrrolopyrrole (DPP)-based D-A conjugated copolymers showed high performance for electronic applications recently. These polymers can have a high degree of crystallinity by using different donor moieties owing to π ?π stacking intermolecular interaction. Also, D'-A-D'' terpolymer structure can easily tune the energy levels of HOMO and LUMO with the kind of donors. We designed D'-A-D'' conjugated terpolymer containing two kinds of donors as a new strategy of D-A type that can have both advantages of two different donors. In this study, we successfully synthesized DPP-based terpolymer with two kinds of donors. We demonstrated the physical, optical and electrochemical properties of the terpolymer. Furthermore, we investigated semiconducting properties of DPP-based terpolymer.

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Macroscopically oriented hierarchical structure of the programmed amphiphilic tetrathiafulvalene molecule

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In this aspect, we newly designed and synthesized an asymmetric amphiphilic TTF molecule (amph-7TTF14) by covalently connecting two tri(ethylene oxide) (TEO) tails at both sides of the TTF group and two alkyl tails with 14 carbon atoms at one end of the TTF group. Phase behavior of amph-7TTF14 was studied by combined techniques of Differential scanning calorimetry (DSC) and one-dimensional (1D) wide angle X-ray diffraction (WAXD) techniques revealed that a highly ordered crystalline phase emerged below the isotropic phase. The ordered molecular packing was identified from the 2D WAXD pattern, and its molecular arrangement was confirmed by selected area electron diffraction (SAED) and polarized ultraviolet-visible (UV-Vis) spectroscopy. The morphological observations using transmission electron microscopy (TEM), atomic force microscopy (AFM), and polarized optical microscopy (POM). Based on the experimental results and careful analyses, it was realized that the scrolls and helices were induced by the unbalanced surface stresses generated during the crystallization process. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), BK21Plus Program, Korea

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Characterization of a gold-graphene nanocomposite for electrochemical detector used for active microfluidic paper chip

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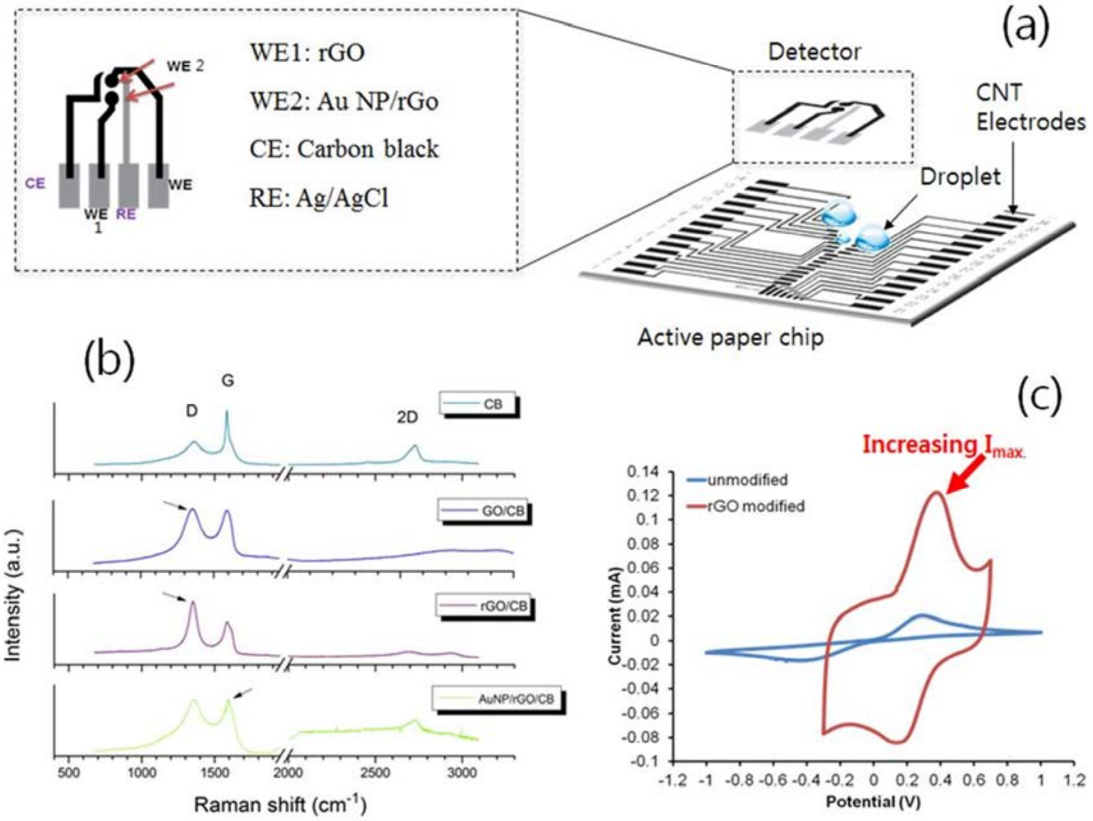
A gold-reduced graphene oxide (Au?rGO) nanocomposite was formulated on the surface of carbon black (CB) electrode of an electrochemical detector for an increasing of the sensitivity of detection (Fig. 1a). Graphene oxide and Au nanoparticles (Au NP) were deposited by using silk-printing subsequently, and then instead of the conventional methods, cyclic voltammetry and amperometry with adjusting a constant potential have been applied for the reduction of graphene oxide and formulation of Au-rGO nanocomposite, subsequently. As shown in Fig. 1b, Raman spectra clearly show the results of this two of treatments in such a way that the typical Raman shifts of D-, G- and 2D-bands were clearly observed enough to identify the footprints of graphite of CB, GO, rGO and Au NP, indicating that the two complementary electrochemical method exhibited both the good reduction of GO and the well formulation of Au-rGO nanocomposite. Because this formation of Au-rGO nanocomposite has increase the electroactive surface area of catalysts and the conductivity of the Au?rGO nanocomposite, it should provide an increasing sensitivity of detecting of glucose and we confirmed it clearly in Fig. 1c [1]. Morphology will be further investigated to analyze the uniformity, the dispersion and the particle size of Au particles on rGO by using a scanning electron microscope, atomic force microscopy and X-ray spectroscopy in future. And this detector will be mount on the active mictrofluidic paper chip that we have developed for point-of-care tester for detection of glucose in human blood [2].


(a)
WE 2
CE
WE 1
RE
WE
WE1: rGO
WE2: Au NP/rGo
CE: Carbon black
RE: Ag/AgCl
Detector
CNT Electrodes
Droplet
Active paper chip
(b)
D
G
2D
CB
GO/CB
rGO/CB
AuNP/rGO/CB
Intensity (a.u.)
500 1000 1500 2000 2500 3000
Raman shift (cm^{-1})
(c)
Increasing I$_{max.}$
unmodified
rGO modified
Current (mA)
0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02 -0.04 -0.06 -0.08 -0.1
-1.2 -1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.2
Potential (V)

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Cellulose-based Comb-like PLLA Copolymers

류미희

한국화학연구원 바이오융합화학연구센터

Nowadays, sustainable and degradable natural polymers have received enormous attention because of environmental concerns about oil-based products. Among eco-friendly materials, cellulose is one of the most abundant renewable polymers in nature. However, cellulose has a poor processability due to its extensive inter and intra molecular hydrogen bonds. To overcome this drawback, cellulose modification and functionalization such as grafting synthetic polymer have been studied.Based on this concept, we designed and synthesized new cellulosic PLLAs in which PLLA was grafted to the cellulose by the ring opening polymerization. First of all, short chain of PLLA (DP = 3.31) was grafted to the cellulose ring under mild conditions using ionic liquid. The resulting cellulosic polymer turned out to be soluble in organic solvents such as chloroform, and then we tried to increase the PLLA chain further by the solution polymerization in chloroform not using expensive ionic liquid with thin octoate as catalyst, and it was successful to obtain higher molecular weight (about 10,000 g/mol) of PLLA grafted chains. The short chain PLLA grafted cellulose showed only T_g at 50.9^{o}C without melting, but when the PLLA chain was increased as mentioned above, T_g and T_m were appeared from the DSC scan: T_g was about 70 ^{o}C and T_m 165 ^{o}C. From this data, we found that grafting PLLA short chain onto cellulose ring can make the cellulose processable by melt process and soluble in organic solvents and further increase in the PLLA chain length induces crystallinity in the PLLA grafted cellulose copolymers. The characteristics of the polymers prepared were studied further with ^{1}H NMR, ^{13}C NMR, FT-IR and TGA.

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친수화된 다공성 지지체 활용 PTFE-g-PAA/Nafion/ZrP 강화 나노 복합 멤브레인 제조 및 특성 평가

박병희 손준용 신준화*

한국원자력연구원 첨단방사선연구소 공업환경연구부

본 연구에서는 방사선 그라프팅 기술을 이용하여 친수화된 다공성 polytetrafluoroethylene(PTFE) 지지체에 고분자 전해질인 Nafion 을 함침하고, zirconium phosphate(ZrP) 나노입자 도입을 통해 연료전지용 PTFE-g-PAA/Nafion/ZrP 강화 나노 복합 멤브레인을 제조하고, 특성을 분석하였다. 제조된 멤브레인에 대해 이온교환용량, 함수율, 치수안정성, 수소이온전도도를 특정하여 ZrP 나노입자의 도입으로 인한 멤브레인의 물성이 향상되는 것을 확인하였고, SEM-EDS, XRD, SAXS 분석을 통하여 ZrP 나노입자가 멤브레인의 결정 구조에 미치는 영향을 평가하였다.

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Synthesis, characterization and comparison of properties between a newly synthesized conjugated polymer and another polymer containing benzobisthiazole unit

차주현 김인태*

광운대학교 화학과

A newly synthesized conjugated polymer was successfully synthesized using Microwave. Another polymer with benzobisthiazole derivatives was synthesized by Stille cross-coupling reaction. The structures of polymers were identified by ^{1}H-NMR and ^{13}C-NMR. The thermal stability of these polymers was investigated by Thermogravimetric Analysis(TGA) and molecular weights were measured using Gel Permeation Chromatography(GPC). A newly conjugated polymer was compared with the polymer containing benzobisthiazole unit by UV-Vis spectroscopy and photoluminescence.

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Synthesis, Characterization and Properties of a New Conjugated Conductive Polymer Containing Heteroatomic Unit in the Main Chain

김준헌 김인태*

광운대학교 화학과

A new conjugated conductive polymer containing heteroatomic unit in the main chain has been successfully synthesized by Stille cross-coupling reaction. It has been characterized by ^{1}H-NMR, ^{13}C-NMR, FT-IR spectrometers. Also, the properties of this polymer have been measured by GPC, UV-vis spectrometer, cyclic voltammetry and thermogravimetric analysis. This polymer has good solubility in organic solvents such as n-hexane, THF, chloroform and chlorobenzene. The λ_{max} of the polymer approximates 820 nm and the λ_{edge} of the polymer approximates 1060 nm in chloroform solution. Thus, this polymer has very low band gap and the polymer is expected to be applied to the active layer of the polymer solar cells.

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Synthesis, characterization and properties of a new conjugated conductive polymer containing pyrrole derivative

조태종 김인태*

광운대학교 화학과

A new conjugated polymer containing pyrrole derivative has synthesized by stille’s reaction and has good solubility in organic solvent. The polymer was characterized by ^{1}H NMR and UV-vis spectroscopy. The polymer's properties was measured by Gel permeation chromatography, UV-spectrometer, cyclovoltametry, conductivity and thermogravimetric analysis. The new synthesized polymer shows good absorbance over the solar spectrum, hence it can be used further for solar cell devices.

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Synthesis, characterization and comparison of properties between a polymer containing benzobisoxazole unit and another polymer containing benzobisthiazole unit

차주현 김인태*

광운대학교 화학과

A conjugated polymer containing benzobisoxazole unit in the main chain was successfully synthesized by Sonogashira cross-coupling reaction. Another polymer with the benzobisthiazole derivatives was also synthesized by Sonogashira cross-coupling reaction. The structures of polymers were identified by ^{1}H-NMR and ^{13}C-NMR. The thermal stability of these polymers was investigated by Thermogravimetric Analysis(TGA) and molecular weight were measured using Gel Permeation Chromatography(GPC). The polymer containing benzobisoxazole unit was compared with the polymer containing benzobisthiazole unit by UV-Vis spectroscopy and photoluminescence.

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Synthesis and Characterization of Alternating Terpolymer Containing bithiophene and biselenophene as two different donors

이지형 이대희 신지철 조민주 최동훈*

고려대학교 화학과

Until now low bandgap donor-acceptor (D-A) type conjugated molecules and polymers have displayed promising characteristics in organic semiconductors. Remarkably, terpolymer structures containing three different monomers in the polymer repeating unit is promising candidates for electronic and optoelectronic devices. Furthermore, conjugated terpolymer can control the energy level and their optical properties relying on different acceptor and donor units respectively. By virtue of these advantages, diketopyrrolopyrrole-based alternating conjugated terpolymer was designed and synthesized, which bears different donating units. Also, thermal analysis, electrochemical analysis and absorption spectroscopy were employed to identify their intrinsic properties.

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Two-Dimensional Network Polymers: Poly(isocyanate) from Self-Polymerizable Monomers

김석진 백종범*

울산과학기술대학교(UNIST) 에너지공학부

The COFs (Covalent Organic Frameworks) are a crystalline porous polymer. It can be used that gas storage, gas separation, optoelectronic application catalysis, absorbent and catalysis. Especially, 2D COFs have potential for developing new type ???? ? electronic. We tried to synthesis two-dimensional network polymers from self-polymerizable monomers. Without any solvent, the monomer shows a change just from applied heat. So, we analyzed a product by using the expected structure.

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Synthesis of functionalized filaments PCL fiber with Gadolinium oxide (III) to absorb neutrons

조대형 신관우[1,*] 김희석[*] 조애리[*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

The 3d printing market is emerging dramatically past 30 years. As increasing of 3d printing market, the need of functionalized filaments is also increased. Many researches are interested in conductive filaments which can make possible to change the plastic industries. Shown by this phenomenon, creating new functionalized filaments for 3d printing can change our industries and life styles more than expected. Not only conductive filaments, filaments which can absorb neutrons also take important role such as nuclearreactors or neutron barrier blocks. To achieve this goal,adoptgadolinium oxide(III),Gd2O3,well known material which can absorb neutrons into PCL(polycaprolactone) fiber. Even it contains under 5% of Gd2O3In PCL weight percent, this new functionalized fiber shows effective neutron absorption ability. Based on this fiber, neutron absorbing applications which can be made from 3d printers are possible.

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Development of target molecule detection and capture system utilizing fluorogenic polymer based DNA hydrogel

이지현 김원종*

포항공과대학교(POSTECH) 화학과

We suggest fluorometric sensor system for target molecule capture and detection utilizing polymer based DNA hydrogel (PD-hydrogel). The fluorescent PD-hydrogel composed by acrylamide, bis-acrylamide and dsDNA (hybridized with DNA and fluorophore modified partially hybridizable cDNA (fl-pcDNA)) were prepared by simple radical polymerization process and applied to detect DNA mismatch and small molecule as ATP (adenosine 5'-triphosphate). Target molecule detection utilizing PD-hydrogel would be successfully confirmed by both fluorescence decrement of PD-hydrogel and fluorescence increment of remained solution since the fl-pcDNA in PD-hydrogel were detached and released into the remained solution. Our developed PD-hydrogel platform would be easily applied to not only detection but also capture of target molecule selectively, by fluorogenic method.

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In situ cross linkable random copolymer containing triethoxyvinylsilane as a novel polymeric binder for high performance of Li batteries

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The electro chemical performance of Li ion battery (LIB) can be highly tuned by various factors which include morphology of anode material, nature of electrolyte and binding material, percentage of conducting materials etc. Among them, binding material have been attracted by researchers over decades, which results in the introduction of different polymeric binder, originated from nature, such as poly acrylic acid, carboxy methyl cellulose, alginic acid etc. for Si anode of LIBs. Recently several synthetic and structural modifications of these conventional polymeric binders, for example, random co polymer of polyacrylic acid with vinyl alcohol, porous scaffold of CMC, etc. has been developed by many researchers. However, the challenges of further development of Li ion rechargeable batteries still exists because of some unique property possessed by Li batteries, such as high energy density, high specific capacity and light weight to carry. Inspired from these advantages of LIBs, here in, we introduce a novel polymeric binder for Si anodes in LIB as an effort to improve the columbic efficiency and cycle durability of LIBs. We report a novel random copolymer, poly(tert-butyl acrylate-co-triethoxyvinylsilane) as an efficient binder with high ICE of 91% for LIBs. The binder form in situ cross linking by the removal of protective tert-butyl groups, demonstrated by FT-IR, helps to minimize the pulverization of Si nano particle in the anode. Moreover, the Silane group in the polymer exhibits high adhesive property with the electrode surface. In this present work we tried to find the optimum percentage of triethoxyvinylsilane in the random co polymer by analyzing the electro-chemical-mechanical properties of series of synthesized random copolymer.

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Fabrication and characterization of porous hollow nanoparticles based on colloidal silica

박은지 정일두*

부산대학교 고분자공학과

Porous, hollow, and polymeric nanoparticles were prepared using colloidal silica(CS) as a template. These nanoparticles were prepared by initially coating the silica with 3-methacryloxypropyltrimethoxysilane (MPS) and forming a shell by the polymerization of a mixture of styrene and methyl vinyl ketone (MVK). After the crosslinking of the polymeric shell with divinylbenzene (DVB), the silica core was removed by etching with hydrofluoric acid. The resulting polymeric shell was then made porous by photodegrading poly(MVK) component of the nanoparticle with ultraviolet (UV) irradiation. The porous, polymeric shell was characterized by 13C NMR and FT-IR. The morphology and the size distribution was determined with FE-SEM, TEM, and DLS. These nanoparticles could be applied for many biomedical and industrial applications.

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Characterization of Silica based Nanohybrids for Dental Composite Resin Restoratives

박은지 정일두*

부산대학교 고분자공학과

Silica nanoparticles are most often synthesized by the sol-gel process, in which alkoxysilanes are allowed to undergo hydrolysis and condensation reactions. Resin composites have been successfully used in dentistry as esthetic filling restoratives for decades with their high mechanical strengths. However, lack of direct chemical adhesion to tooth and slow degradation make them not very useful without applying extra bonding agents. BisGMA based composite resin restoratives are known for their excellent esthetics, easy handling and improved mechanical strength, and wear resistance. In the present study, we use polymerizable silicananoparticles with BisGMA in order to achieve a higher mechanical strength as well as durabilities.

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폴리(스타이렌-co-스타이렌 술포네이트) 아이오노머의 임의 상처 크기의 변화

김은희 김준섭[1,*] 소인섭[1]

조선대학교 신재생에너지융합학과 [1]조선대학교 응용화학소재공학과

본 연구에서는 다양한 양이온으로 중화한 폴리(스타이렌-co-스타이렌 술포네이트)(SPS) 아이오노머에 임의로 상처를 낸 후 그 상처 크기에 대해 조사하였다.SPS 공중합체를 Li+, Na+, K+, Cs+으로 중화하여 아이오노머 시료를 얻었다.폴리스타이렌(PS) 시료는 150℃에서, 아이오노머 시료들은 180℃에서 각각 열처리 하였다.일반 커터날이 장착된 350g 하중의 장치를 사용하여 열처리한 시편의 표면에 상처를 내 후 이 상처의 간격을 알기 위해 현미경으로 관찰하였다. 각각의 상처 간격의 평균값은 PS 가 약 104 ㎛, Li-SPS 가 약 76 ㎛, Na-SPS 가 약 84 ㎛, K-SPS 가 약 87 ㎛, Cs-SPS 가 약 87 ㎛로 측정 되었다.이상의 결과에서 아이오노머의 상처 간격이 비이온성 PS 고분자 보다 좁아짐을 알 수 있었다. 또한 Li+로 중화된 아이오노머의 경우에 상처 간격이 다른 양이온으로 중화된 아이노머의 경우 보다 좁다는 것을 알 수 있었다.

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Plasma Bonding of PDMS Microfluidic Chip with PEGDA Nano Mold for Modulus Controllable Polymeric Hierarchical nano-membrane

탁동하 방석영 강명우 나상철 JEON NOO LI[*]

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The performance of silicon and metal foil membrane based bio-inspired microfluidic and energy device such as organ on a chip, photovoltaic and fuel cell is limited by mechanical rigidity and fabrication complication. We report a facile method for the fabrication of modulus controllable free-standing membrane with multiscale geometry. Our method is based on plasma bonding of post designed PDMS (Polydimethylsiloxane) microfluidic chip with PEGDA (polyethylene glycol diacrylate) nano mold. PDMS is well known material about the plasma bonding system by dehydration reaction mechanism. PEGDA allow a replicate from the nano patterned silicon master. PEGDA surface is easily generated hydroxyl group when the plasma treatment due by oxygen atoms contained in the molecule. These two materials easily bonded through same dehydration reaction mechanism. Different kinds of UV curable resin with various viscosities from 57 cP to 2600 cP fill in the channel of bonded fluidic chip by capillary force. The PDMS and PEGDA bonded chip are separated by cohesive mechanical failure of PDMS after curing a UV curable resin. After that, the free standing multiscale membrane was peeled off from the PDMS channel. The bonding area of PDMS micro post with PEGDA nano mold is membrane area and the other fluidic area is supporting material for whole membrane. The various mechanical properties of free standing membrane depend on different kinds of UV curable resin. The soft or rigid membrane has a range of elastic modulus from 2 MPa to 320 MPa. Meanwhile, it has a hydrophobic or hydrophilic surface properties by different surface energy. This new method doesn't require pressurizing during whole fabrication process and it guarantees the highly uniform membrane over 2 cm^2 area.

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Development and structure/property relationship of new electron accepting polymers based on thieno[2',3':4,5]pyrido[2,3-g]thieno[3,2-c]quinoline-4,10-dione for all-polymer solar cells

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Several electron accepting polymers having weak accepting-strong accepting (WA-SA) and strong accepting-strong accepting (SA-SA) monomer alternation were synthesized for studies of structure/property relationship in all-polymer solar cells. As weak accepting monomers (WA), we developed two kinds of cyclic amide monomers, 4,10-bis(2-butyloctyl)-thieno[2',3':5,6]pyrido[3,4-g]thieno-[3,2-c]isoquinoline-5,11-dione (TPTI) and 5,11-bis(2-butyloctyl)-thieno[2',3':4,5]pyrido[2,3-g]thieno[3,2-c]quinoline-4,10-dione (TPTQ). As strong electron accepting monomers (SA), we designed difluorinated TPTQ (FTPTQ) and well-known perylene diimide (PDI) monomers. All of the accepting polymers exhibited sizable molecular weights and excellent solubility in common organic solvents. Among those polymers, PQP having TPTQ monomer exhibited best photovoltaic performance with power conversion efficiency (PCE) of 3.52 % (Voc = 0.71 V, Jsc = -8.57 mA/cm2, FF = 0.58) at a weight ratio of PTB10:PQP = 1:1, under AM 1.5G. The device performance of PFP containing difluorinated TPTQ (FTPTQ) was much lower than the other polymers due to the diminished internal polarization between SA-SA monomers. We found that space-charge limited current (SCLC) mobility is more important than field effect transistor (FET) mobility for determining the photovoltaic performance because the electron pathway of SCLC devices is similar to that of photovoltaic cells. By using 1-chloronaphthalene (CN) as a co-solvent, the morphology of the polymer blended films can be finely tuned to achieve better ordering toward face-on mode and favorable phase separation between electron donor and acceptor, resulting in great enhancement of short circuit current (Jsc) and fill factor (FF).

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Effects of temperature on the water absorption of poly(styrene-co-methacrylate) ionomer

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공유결합으로 이루어진 비극성 주 사슬에 이온기를 15 mol% 이내로 함유하고 있는 고분자를 아이오노머라고 통칭하는데, 본 연구에서는 온도가 아이오노머의 물 흡수도에 미치는 영향에 대해 알아보았다. 먼저 스타이렌과 메타크릴산을 공중합하여 poly(styrene-co-methacrylic acid) 공중합체를 만들었는데, 이 공중합체의 산 작용기의 함유량은 21.3 mol%였다. 이 공중합체를 아이오노머로 만들기 위해 산 작용기를 0.4N NaOH 표준용액으로 중화했다. 만들어진 아이오노머를 지름 13mm, 두께 1.35mm 동전 형태로 성형했다. 동전 형태의 아이오노머를 40°C, 60°C, 80°C, 100°C 의 물에서 중탕하여 20 분 간격으로 10 시간동안의 흡수도를 저울과 버니어 캘리퍼스로 측정했다. 또한 물의 온도가 높을수록 초기 흡수도 기울기와 최대 흡수도가 커지고, 최대흡수도에 도달하는 시간이 줄어드는 경향을 확인 할 수 있었다.

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키토산을 이용한 바나듐 레독스 흐름 전지 이온교환막 연구

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물을 용매로 사용하므로 인해 여러 가지 한계를 갖고 있는 수계 바나듐 레독스 흐름 전지에 비하여 비수계 바나듐 레독스 흐름 전지는 다양한 용매 선택 가능성에 의해 여러 가지 장점을 갖고 있다. 하지만 현재까지의 비수계 바나듐 레독스 흐름 전지를 위한 이온교환막에 관한 연구는 수계에 비하여 부족한 수준이다. 그에 따라 본 연구에서는 OH- 작용기를 가진 키토산을 응용한 필름을 제조하여, 비수계 바나듐 레독스 흐름 전지 이온교환막으로의 사용 가능성에 관한 연구를 수행하였다. 키토산은 대표적인 천연고분자라는 장점을 갖는 동시에 기존 연구들을 통해 비교적 높은 이온전도성을 나타내는 물질로 알려져 있다. 따라서 키토산의 이러한 장점들에 의해 바나듐 레독스 흐름 전지에 응용 가능할 것으로 생각된다. 완성된 필름의 이온교환막으로서의 사용 가능성을 확인하기 위하여 Electrochemical Impedance Spectroscopy 를 측정하여 필름의 이온전도도를 확인하였고, 바나듐 레독스 전지 single cell test 기를 이용하여 에너지 효율을 확인하였다.

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CO_2 선택적인 MOF와 poly(amide-6-b-ethylene oxide)을 이용한 CO_2 촉진수송 분리막 연구

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Metal Organic Frameworks (MOF)s 와 고분자를 이용하여 제조하는 Mixed Matrix Membrane (MMM)은, CO_2 대한 선택성이 있는 물질인 MOF 와 이와 혼화성이 뛰어난 고분자를 이용하여 제조된다. 본 연구에서는 MMM 의 CO_2 선택성을 증가시키기 위해, CO_2 선택성이 큰 poly(amide-6-b-ethyleneoxide) (PEBAX 1657)을 matrix 로 이용하였다. 촉진 수송막의 carrier 로 사용할 $\{Cu_2(Glu)_2(?\text{-bpa})\}?(CH_3CN)]_n$ (Cu-MOF) (Glu = glutarate, bpa = 1,2-bis(4-pyridyl)ethane)를 합성하여 PEBAX 1657 용액에 분산시켜 혼합물을 제조하고, 이 혼합물을 polysulfone support 위에 코팅하여 MMM 을 제작하였다. 10wt% Cu-MOF 를 포함한 PEBAX 용액을 도포하여 제작된 MMM 의 CO_2 투과도 값은 106 GPU, CO_2/N_2 선택도 값은 43 이다. 이는 PEBAX 1657 의 CO_2 투과도 값 13 GPU, 선택도 값 13 에 비해 높았다. Robeson's upper bound 와 비교하였을 때, Cu-MOF 를 포함한 MMM 의 선택투과도가 upper bound 의 위에 위치하는 것으로 보아, CO_2 배출농도가 높은 공정에 실질적으로 적용시킬 수 있는 가능성을 보여주었다. 또한, PEBAX 1657 에 도입한 Cu-MOF 가 CO_2/N_2 선택분리에 시너지효과를 제공했음을 확인하였다. Cu-MOF 도입으로 인한 PEBAX 1657 의 morphology 변화를 X-ray diffraction pattern 으로 확인하였고, MMM 의 선택투과도가 MMM 의 d-spacing 변화에 의존한다는 것을 확인할 수 있었다. 추가적으로, PEBAX 1657 의 어떠한 block 이 Cu-MOF 의 도입으로 인해 morphology 가 변화하고, CO_2/N_2 선택분리에 시너지효과를 제공했는지 확인하기 위해 polyethylene oxide 와 nylon 6 로 분리하여 MMM 을 제작하고 선택투과도를 확인하였다.

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비수계 바나듐 레독스 흐름 전지의 Celgard 막의 전류밀도에 따른 특성 연구

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바나듐 레독스 흐름전지(Vanadium redox flow battery, VRB)는 대용량 전력저장 시스템의하나로써 전해질을 반영구적으로 사용할 수 있다는 친환경성, 바나듐 전해질의 반영구적인 사용으로 인한 전지의 긴 수명, 또한 전기를 액체 상태인 전해질에 저장하기 때문에 용량 확장의 자유로움, 빠른 반응시간, 높은 충 방전 효율이라는 다양한 장점들로 인해 전해질, 전극, 멤브레인 등 VRB 의 다양한 분야에 관한 관련연구가 진행되고 있다. VRB 에서 멤브레인은 VRB 구성 핵심 물질이며, VRB 에 응용되는 멤브레인의 특성으로 높은 이온전도도, 낮은 이온 투과성, 그리고 우수한 화학적 안정성과 기계적 강도가 요구된다.본 연구에서는 수계 레독스 흐름 전지보다 넓은 범위의 작동 전압과 온도를 보장하는 비수계 레독스 흐름 전지에 적합한 멤브레인의 특성을 확인하기 위하여 다공성 멤브레인(Celgard)의 전류 밀도에 따른 에너지 효율을 확인하였고, 막의 성능은 VRB single cell test 기를 사용하여 충 방전 실험을 진행하였고, 흡수도와 전기저항, Electron Impedance Spectroscopy 를 이용하여 이온전도도를 통하여 확인하였다. 다양한 전류밀도에서 에너지 효율을 확인한 결과 높은 전류밀도에서 테스트를 할수록 효율이 높아지는 것을 확인 하였다. 결과적으로 비수계 바나듐 레독스 흐름전지가 수계 바나듐 레독스 흐름전지에 비해 넓은 전류밀도에서 응용이 가능한 장점을 확인하였다.

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Chitosan을 코팅한 상용 양이온 교환막의 특성 및 바나듐 레독스 흐름전지의 이온교환막으로의 응용 연구

조경현 방호선 원종옥*

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Redox flow battery(RFB)는 전해질에 포함된 활물질의 산화환원반응을 통하여 전기에너지를 충?방전하는 대용량 에너지 저장 시스템으로, RFB 구성 중 이온교환막은 두 전해질에 있는 활물질을 격리시키고 이온 전도를 통해 배터리 내부의 전기회로를 담당하는 역할을 한다. 따라서 이온교환막은 이온 전도성이 좋아야 하고, 활물질의 투과도가 낮아야 한다. Vanadium redox flow battery(VRB)는 산화수가 다양한 바나듐을 활물질로 사용하여 양극과 음극의 산화환원 물질을 모두 바나듐 만으로 사용할 수 있다는 장점을 가진다. 현재 VRB 의 양이온 교환막으로 많이 사용되고 있는 Nafion 은 높은 이온 전도성, 높은 내산성, 높은 내산화성과 낮은 수분 흡수 등 VRB 의 이온교환막으로서 우수한 특성을 가지고 있지만, 바나듐 이온의 투과도가 높아 VRB 시스템의 에너지 효율을 떨어뜨린다. 이를 보완하기 위하여 Nafion 막 표면을 다른 고분자로 코팅하여 바나듐 이온에 대한 막의 투과도를 감소시키고자 하였다. 코팅을 하기 위한 고분자로는 chitosan 을 사용하였고, 막 표면에 있는 이온들 간의 charge interaction 에 의한 self-assembly 를 이용하여 Nafion 112 의 표면에 chitosan 을 코팅하였다. 바나듐 이온 투과도, 수소이온 전도도, OCV 변화를 측정하여 기존의 Nafion 막과 코팅된 Nafion 막의 특성을 비교?분석하였다. 코팅 막을 적용한 VRB 단위전지의 성능을 평가하는 실험을 통하여 VRB 충?방전 곡선, 에너지 효율 등을 분석하였다.

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Fabric-Hydrogel Composite Membranes enhanced mechanical property and permeability for Microalgae Mass Culture

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인하대학교 고분자공학과

Our new fabric-hydrogel composite membranes which have good mechanical property, toughness and high performance ion-transporting is developed. These membranes are employed to culture marine microalgae for the production of bio fuel. Semi-permeable membranes made of cellulosic materials have already been commercialized in market, but they have limited ion permeability and are difficult to find for a low price. So we prepare the new concept of “fabric-hydrogel composite membranes” to overcome these drawbacks as like desirable ion permeability, transparency and mechanical properties. In particular, by introduction cotton fabric inside the hydrogel framework, it was possible to achieve superior mechanical properties to cellulosic membranes. Adding fabric frame inside network is key factors in casting thin membranes in large size and using them for cell culture in harsh marine conditions. Fabric-hydrogel composite membranes showed 1.20 x 10-8 m2 min-1 of nitrate anion permeability. Finally, we confirmed that composite hydrogel membranes can be applied to constructing bioenergy harvesting photobioreactors better than those of cellulosic materials.

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Hierarchical Striped Walls Constructed by the Photopolymerization of Discotic Reactive Building Blocks in the Anisotropic Liquid Crystal Solvents

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A triphenylene-based reactive mesogenic molecule (abbreviated as HABET) was newly designed and synthesized as a programmed building block to construct the stripe walls by the photopolymerization in the anisotropic liquid crystal (LC) solvents. On the basis of thermal, scattering and microscopic analyses, it was found that HABET formed three ordered structures: a columnar hexagonal LC phase, a tilted columnar hexagonal LC phase and a highly ordered columnar oblique crystal phase. The microscopic molecular orientations in the hierarchical superstructures were controlled in the anisotropic LC solvents with the help of surface anchoring forces, while the dimensions of the striped wall morphologies were determined by the patterned photomasks. The long axis of self-assembled columns in the striped walls was perpendicular to the surface alignment direction regardless of the photomask direction. Additionally, it was realized that the shapes of water drops as well as the surface water angles can be tuned by the hierarchical superstructures and morphologies of the polymerized HABET networks. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), BK21Plus Program, Korea.

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tricyanomethanide 이온젤을 이용한 기체 분리막의 성능 향상 연구

조은해 원종옥*

세종대학교 화학과

기존에 사용되고 있는 이온성 액체는 이산화탄소와의 높은 선택성과 낮은 휘발성으로 인해 기체 분리 막으로의 역할을 하고 있다. 하지만 이 막은 기체를 분리할 때 압력에 의해 안정성이 약해진다는 문제점을 갖고 있다. 이러한 단점을 보완하기 위해 고분자를 첨가하여 젤을 만듦으로써 막 안정성을 향상시키는 효과를 가지게 할 수 있다. 5 가지 이온성 액체인 1-ethyl-3-methylimidazolium tricyanomethanide, 1-butyl-3-methylimidazolium tricyanomethanide,1-hexyl-3-methylimidazolium tricyanomethanide, 1-butyl-1-methylpyrrolidium tricyanomethanide, 1-butyl-4-methylpyridinium tricyanomethanide 와 tri-block copolymer 인 poly(styrene-block-ethylene oxide-block-styrene) [SEOS]를 용매 methylenechloride 에 섞어 지지체인 나일론 막 위에 뿌려 supported ionic gel membrane [SIGM]을 만들었다. 만들어진 SIGM 을 bubble meter 를 사용하여 4 가지 기체 (질소, 이산화탄소, 산소, 메탄)들의 투과도와 선택도를 측정하였다. 또한 SIGM 의 내구성을 확인하기 위해 supported ionic liquids membrane [SILM]을 만들어 투과도와 선택도를 측정하여 SIGM 과 비교하였다.

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발표분야: 고분자화학

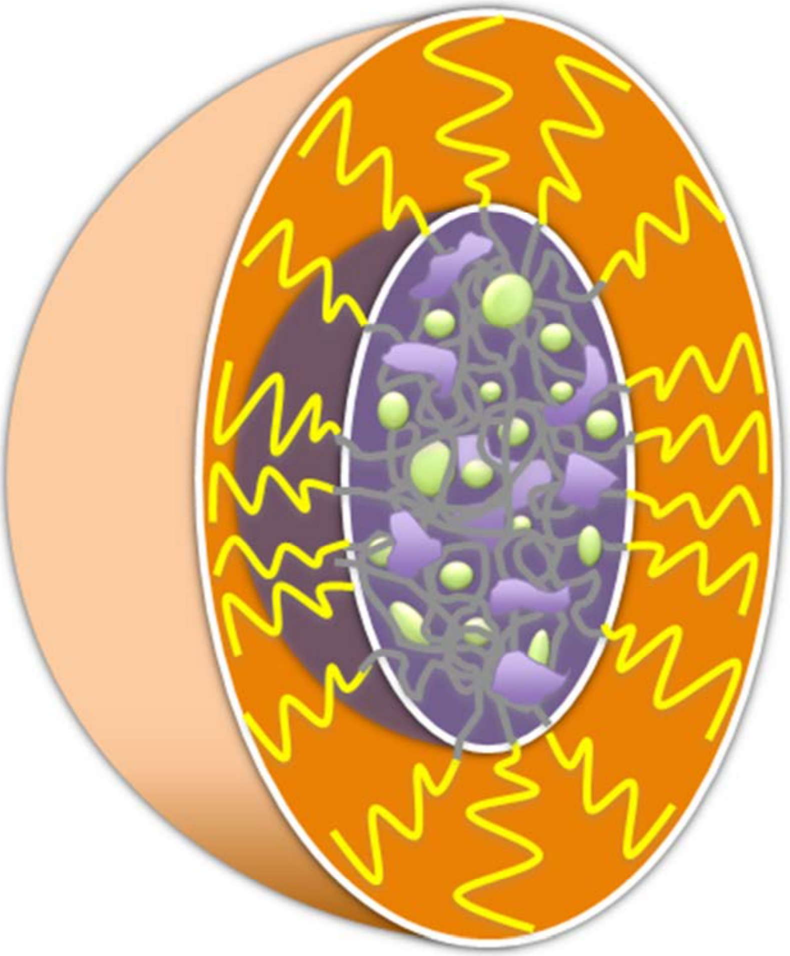
발표종류: 포스터, 발표일시: 수 16:00~19:00

Converting F127 Micelles to Stabilized Soft Particles by Semi-Interpenetrating Network

곽민석* **Listiana Oktavia**

부경대학교 화학과

We present a method to efficiently stabilize micelles of F127 by semi-interpenetrating networks (sIPN) formation. First, pentaerythritol tetraacarylate (PETA) loaded in the core was crosslinked to form sIPN resulting in stabilized particles. We characterized size and stability of the particles by fluorescence, UV-Vis spectroscopies, and dynamic light scattering. In addition, rheological behavior of the particles was investigated by large amplitude oscillatory shear. Furthermore, a number of chemical compositions and experimental conditions were tested to optimize sIPN formation of the polymer.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-47**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

SERS on DNA-Functionalized Nanohole Substrates

곽민석* <u>Andry Ongko Wijoyo</u> 이승현[1] 양승윤[1]

부경대학교 화학과 [1]부산대학교 바이오소재과학과

We fabricated a nanohole-based surface-enhanced Raman scattering (SERS) active substrate by selective patterning of polymer films with an ultrathin anodized aluminum oxide (AAO) etching mask followed by Au deposition. The surface of Au nanohole was functionalized by DNA and the subsequent addition of complementary Cy5-DNA exhibited SERS signals as anticipated. The improvement of DNA detection on patterned surfaces is a potential candidate for sensing applications.

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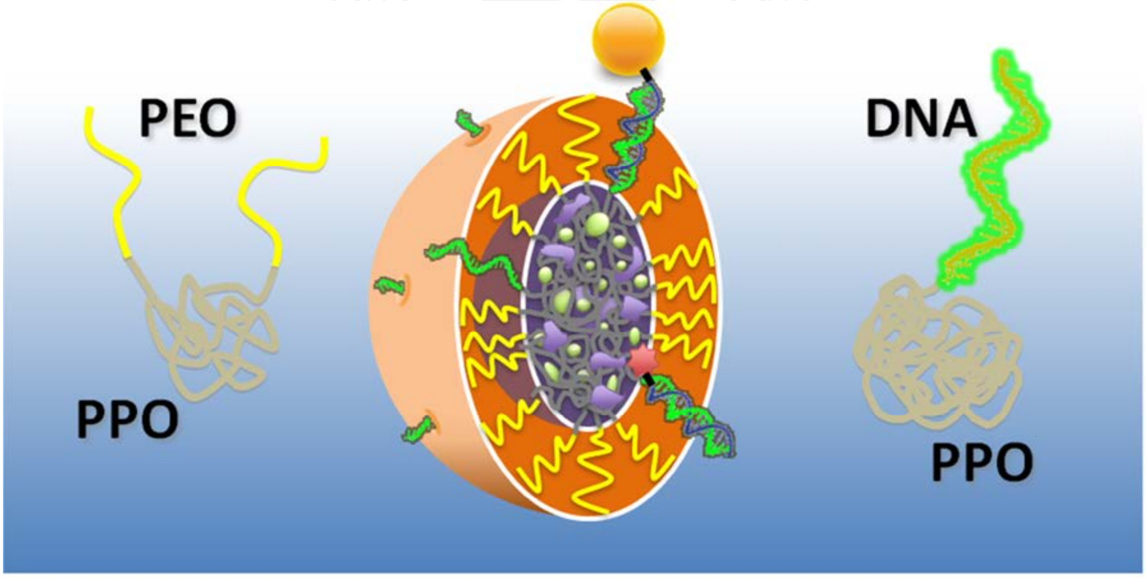
발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA Functionalized Polymeric Nanoparticle: Blending DNA Block Copolymer and F127

곽민석* 황주영

부경대학교 화학과

Here we present the formation and characterization of easily functionalizable mixed micelles with DNA/PEO corona and hydrophobic core which can be loaded with hydrophobic molecules and stabilized by the formation of cross-linked nanodomains. Furthermore, the corona is functionalized by hybridization either with dye-modified complementary DNA or with DNA-labelled gold nanoparticles.



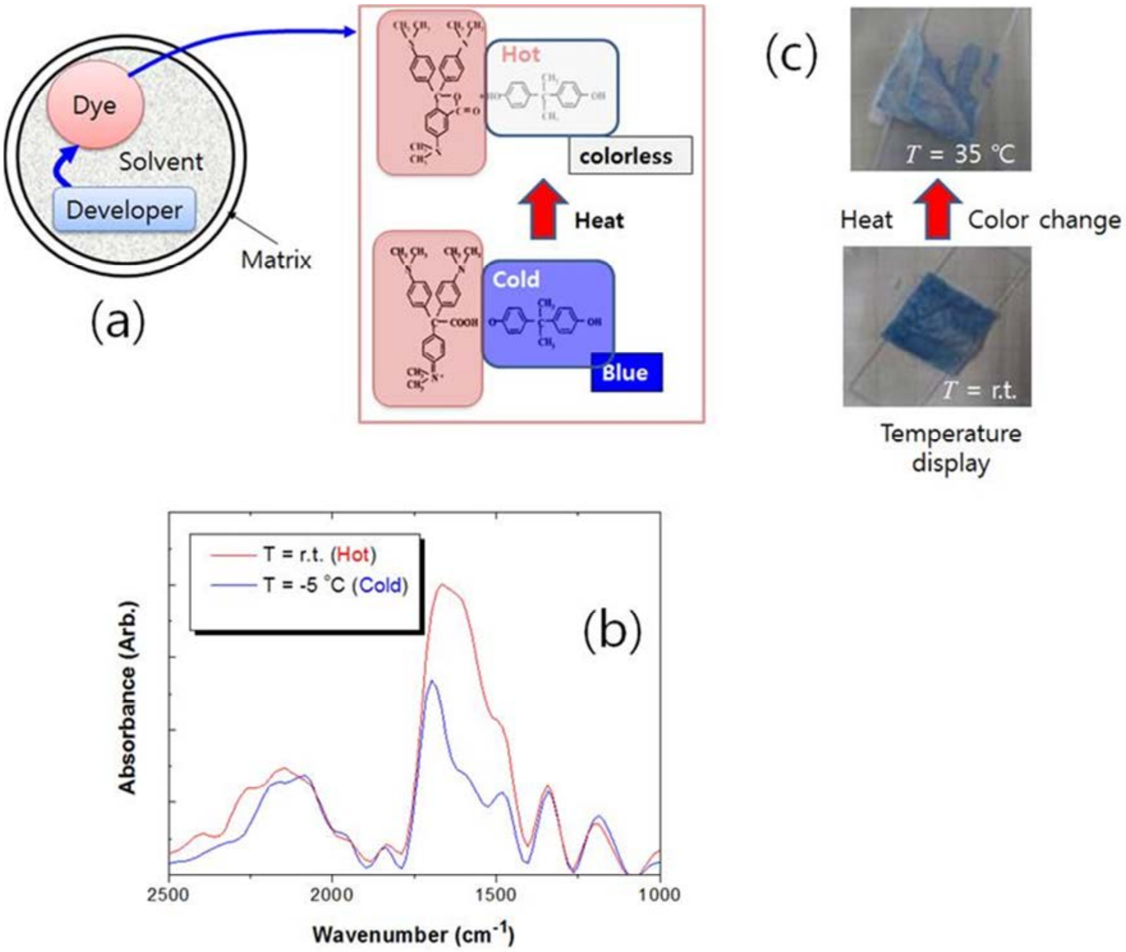
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-49**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabric-based display with thermochromatic dye for a simple temperature sensor

김도현 채희도[1] 백승휘[1] 유수련[2] 권오선[*] 신관우[3,*]

서강대학교 화학과 [1]서강대학교 화학과 대학원 [2]서강대학교 화학과,바이오계면연구소 [3]서강대학교 화학과 및 바이오융합과정

Smart fabric pertain to wearable technologies such as electrodes, sensors and other electronic devices has been rapidly developed especially due to not only the booming of smartphone market but also strong seeking new material for artistic fashion. Although textile displays is essential to present informative data acquisition gained from sensors or devices the direct display on surface of fabric platform for wearable devices has not been studied enough. Herein we will show a simple direct fabric display based on thermochromatic dye to switch the thermochromatic structure related to color change, without any electrical power supply. In this experiment, we only test one temperature sensing dye as shown in the inset of Fig. 1a. The solvent of the thermochromatic dye, which was purchased from Nano I&C, has phase changed at room temperature (r.t.). As the temperature was raised by heat, the color changed gradually from blue to white, indicating that the phase changes as shown in Fig. 1a. We observed the phase change by using Fourier transformed infrared spectroscopy (FT-IR) (Fig. 1b). After the thermocromatic ink was printed on silk fabric, the disappearance of color by heat was observed as we expected. We will develop the temperature display using the various temperature sensing thermocromatic inks in future. References1.P. Wang, Z.-G. Liu, X. Chen, F.-L. Meng, J.-H. Liu and X.-J. Haung, J. Mater. Chem. A. 2013, 1, 9189.2.N. Ruecha, et al. (to be published). Figure 1. Temperature sensing fabric using thermochromatic dye: (a) Schematic structure diagram of microcapsuled thermchromatic ink composed of dye, developer and solvent. (Inset) As the solvent is heated, the developer donates a proton to dye, resulting in rearrangement of molecule losing the color, (b) FT-IR spectra for thermochromatic dye as a function of temperature, showing the phase change apparently and (c) Fabric temperature display with one ink without any external power.


(a)
Dye
Solvent
Developer
Matrix
Hot
colorless
Heat
Cold
Blue
(c)
T = 35 ℃
Heat
Color change
T = r.t.
Temperature display
(b)
T = r.t. (Hot)
T = -5 °C (Cold)
Absorbance (Arb.)
Wavenumber (cm^{-1})
2500
2000
1500
1000

일시: 2015년 4월 15~17일(수~금) 3일간

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Injectable calcium phosphate/thermogel scaffolds for promoting osteogenesis of tonsil-derived mesenchymal stem cell

문효정 **PATELMADHUMITA** 정보경 고두영 정병문*

이화여자대학교 화학나노과학과

Understanding the effect of calcium phosphate on tonsil-derived Mesenchymal Stem Cell (TMSC) differentiation is important for enabling new biomedical applications. We prepared calcium phosphate with monetite and brushite structure which regulated by controlling the concentration of F127. The TMSCs are cultured in the 3D matrixes of in situ formed Poly (ethylene glycol)-poly(L -alanine-co-L-phenyl alanine) thermogel with different structure of calcium phosphate (calcium phosphate/PEG-PAF). The osteogenic differentiation was compared in thermogel scaffolds containing calcium phosphate with different morphology

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Synthesis and characterization of water soluble polymer and doped by ionic compound (Cs2CO3) for polymer solar cells(PSCs)

이자민 박동규*

경성대학교 화학과

We have fabricated a bulkheterojunction solar cell (BHJ-SC) from the conventional active polymer blend, P3HT:PCBM, by constructing a polymer multilayer structure with novel electron transporting while the one without water-soluble polymer (WSP), poly(fluorene-co-benzothiadiaziole), and doped water-soluble polymer by ionic compound(Cs2CO3), which is used as an electron transport layer on the top of commercially available active layer, P3HT:PCBM. All device characteristics show short circuit current density (Jsc), open circuit voltage (Voc), fill factor (FF) and power conversion efficiency (PCE).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural effects of thiophene-based copolymers on molecular packing, orientation of backbone, and kinetics of charge transport in organic field effect transistor

손성윤 박태호*

포항공과대학교(POSTECH) 화학공학과

Regioregular poly(3-hexylthiophene) (P3HT) readily self-assembles to form a well-ordered two-dimensional lamellar structure that displays an excellent charge carrier mobility (up to 0.1 cm2/(Vs)), as measured in an organic field effect transistor (OFET). It is well known that optoelectronic properties of P3HT are attributed to well-ordered lamellar structures which are formed by interdigitation of hexyl side chains and face-to-face packing of backbones because high degree of π-orbital overlap can be achieved through the structure. Here, we intended to reduce crystallinity of P3HT by incorporating thiophene units which do not have hexyl side chains into P3HT chains at random resulting in decreased structural regularity. The resulting copolymers were investigated to observe the effects of structural regularity of thiophene-based copolymers on molecular ordering and charge transport in OFET.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly efficient perovskite hybrid solar cells employing a novel hole transporting polymer

김관우 박태호*

포항공과대학교(POSTECH) 화학공학과

Perovskite hybrid solar cells have recently been the subject of extensive investigations. Mixed perovskites, such as CH3NH3PbI3-xClx, display a long electron diffusion length and a high light absorption profile. Generally, perovskite solar cells consist of the structure: transparent fluorine-doped SnO2 (FTO) substrate / compact layer / perovskites / hole transport material (HTM) / Au electrode. Here, We report a novel D?A type conducting polymeric HTM (TTB-TTQ) based on thiophene and benzothiadiazole as an alternative to spiro-MeOTAD. The resulting polymer was highly soluble in many organic solvents and exhibited excellent film formability. We demonstrated a perovskite solar cell with the highest power conversion efficiency yet achieved in such cells, 14.1 %, which is 22.6 % greater than that of a device employing a spiro-MeOTAD.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Perovskite Solar Cells based on New Polymeric Hole Transporting Materials and a Novel Measurement Method of Charge Density Dependent Hole Mobility

강경호 박태호*

포항공과대학교(POSTECH) 화학공학과

Recent developments in light absorber materials based on lead halide perovskite nanocrystals have yielded power conversion efficiencies exceeding 15% in hybrid solar cells. Alternative HTM materials with excellent electrical properties may be used in place of spiro-MeOTAD; however, few such materials are available. In this work, Solid-state organic?inorganic hybrid solar cells based on a CH3NH3PbI3 perovskite and a Poly[2,5-bis(2-decyldodecyl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione-(E)-1,2-di(2,2'-bithiophen-5-yl) ethene] (PDPPDBTE) hole transport polymer was successfully prepared. The excellent optical and electrical properties of organo-lead halide perovskite nanocrystals used as a light harvester yielded a 9.2% power conversion efficiency for the best-performing cell that exceeded the value (7.6%) obtained from the best hole conductor yet reported spiro-MeOTAD. The high PCE was attributed to the optimal oxidation potential (5.4 eV) and excellent charge carrier mobility of the polymer. The hydrophobicity of the polymer prevented water permeation into the porous perovskite heterojunction. As the result, the long-term stability of the PDPPDBTE devices, as measured over 1000 hours under a humid atmosphere, guarantees the practical applicability of these solid-state hybrid solar cells under outdoor working condition. These results suggest a broad strategy for developing efficient organic semiconductors, and further enhancements may potentially be realized by carefully tuning the energetic distributions of the HTP and perovskite.

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발표코드: **POLY.P-55**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Manipulating fabric temperature and colors by ink-jet printed electrode patterns

김희주 김용준[1] 신관우[2,*] 권오선[1,*] 박종진[3,*]

서강대학교 화학 [1]서강대학교 화학과 [2]서강대학교 화학과 및 바이오융합과정 [3]전남대학교 고분자융합소재공학부

Wearable electronics requires precise patterned electrodes on the various fabrics, which are highly stretchable, and often cause the electric breakdown. Approaches to print electrodes on fabrics are often by metal-wiring, or layer-stacking. Although each technique has own advantages, yet complex process and damageable weakness after vigorous washing processes are inevitable. We produced a micro-scale electrode patterns, using by ink-jet printing process. We demonstrated that CNT-based ink and silver-based ink-jet printing process can provide variously patterned electrodes. Depending on the printing times, and composition, we could tune the conductivity, leading to tunable temperature locally. With this capability, we would like to build color-varying fabrics, which might be utilized as smart camouflage fabrics.

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발표코드: **POLY.P-56**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparing conductivity of functional filament made of thermoplastic polymers and additives for making 3D printing

조애리 조대형[*] 김민정[*] 김용준[*] 권오선[*] 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Recently, three-dimensional (3D) printing has been emerged as an attractive technology, since it promises opening a new era of the second printing revolution following the pressing printing which was evented in Korea in 14 C. In fact the gear of technical developing progress has been already changed because the 3D printing relies on the additive manufacturing process being capable to complement to the current subtract technologies depended with pressing and milling processes for manufacture. There are alreadty a lot of reseaches about producing functional filament going keeping track of 3D printer wave. In order to obtain functional filament which can be made from FDM type, we conducted researches mixing thermoplastic polymer with a varity of additives to give conductivity. Polyethylene, polypropylene, poly strene, polyacrylonitrile butadiene sterene, polyurathane, polyolefin elastomers were in plastic. Silver nanoparticles, silver flake, carbon black, MWNTs were used as additives.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of density varied all carbon structures with CNT and iodine using dry powder mixing

김민정 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Density varied all carbon structures can be fabricated from a mixture of powder of single-walled or multi-walled bulk carbon nanotube and iodine. They can also be manufactured in diverse shape and scale with pelletizer. Several ultra-light carbon materials such as CNT aerogels and graphene aerogels have been made because of their wide range of application, for example, thermal insulator and storage of material like oil. However, manufacturing methods of these materials require comparatively complex pre-treatment. Great advantage of dry powder mixing method is its simplicity. It is possible because iodine is prone to sublime at room temperature. Iodine facilitates CNT network while two powders are mixing. As sublimation of iodine occurs, the density of solid reduces. Owing to the low mechanical strength of the obtained material, it requires additional research to reinforce and prevent it from shattering.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical study of structure-property relationship of a series of BDT-TPD polymers for polymer solar cells

정규관* 정조[1]

전북대학교 과학교육학부 [1]장곡고등학교 생활인권부

A variety of benzodithiophene (BDT) derivatives were developed and Suzuki or Stille couplings of them with various thieno[3,4-c]pyrrolo-4,6-dione (TPD) derivatives gave very promising class of conjugated polymers for solar cells. Many of them gave high power conversion efficiencies and still intensively investigated for synthesis of new polymers and applications for polymer solar cells in order to improve PCE and stability. However, randomly synthesizing and applying new polymers for solar cells not only takes great effort but is time-consuming process. In this paper, we computed a series of BDT-TPD polymers based on Gaussian 9 based software and the results such as HOMO-LUMO energies, bandgaps, π-electron delocalization, optimized molecular strucutures, and UV-Vis spectra were analyzed and compared with experimental data if available. The combined analyzed results gave useful insight for designing new class of conjugated polymers.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of hyperbranched poly(amidoamine) particles for heavy metal binding via inverse suspension polymerization

이상화 김상율*

한국과학기술원(KAIST) 화학과

Hyperbranched polymers have received much research attention because of their unique properties based on three-dimensional shape. Especially, hyperbranched polyamidoamine(PAMAM) which possess functional amine and amide groups can bind and separate various kinds of heavy metal ions in aqueous solution. In this study, we developed a process to fabricate 50~300μm PAMAM particles. These particles were prepared via inverse suspension polymerization with N,N'-methylenebisacrylamide, ethylenediamine. Detailed synthesis and characterization of the particles and their swelling ratio and metal ion absorption behavior will be presented.

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발표코드: **POLY.P-60**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of fluorinated benzothiadiazole-based small molecules for solution-processable organic photovoltaic cells

황수진 박상혁*

공주대학교 화학과

Because of the unique properties of fluorine atom, fluorinated organic molecules exhibit a lot of distinctive feature such as high thermal and oxidative stability, elevated resistance to degradation, enhanced hydrophobicity. Thererfore, for the development of stable and rugged solar cell devices, fluorinated materials are considered to be one of the promising candidates for the organic photovoltaics (OPVs). Furthermore, obtaining low bandgap materials are important for effective absorption of photons from the sun. It is well-known that the fluorine atom is a strong electron-withdrawing substituent, the introduction of F into the conjugated backbone would lower both the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) energy levels of the conjugated organic molecules. In this work, we have designed and synthesized fluorinated benzothiadiazole- and carbazole dimer-based organic small molecules. Because of the substituted two fluorine (F) groups to the benzothiadiazole unit, a larger open cirquit voltage (Voc) was observed by the decreased LUMO and HOMO energy levels.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of A1-π-A2-D-A2-π-A1 type small molecules based on carbazole dimer and benzo[c][1,2,5]thiadiazole component for solution-processable solar cells

황준연 박상혁*

공주대학교 화학과

Because of their potential to enable mass production of flexible, cost-effective, and large-area device applications, organic photovoltaic (OPV) devices which can be fabricated by simple solution processing techniques are under intense investigation in academic and industrial laboratories. However, most of the research has been focused on solution-processed polymer bulk-heterojunction (BHJ) solar cells. Compared with polymer-based OPVs, small molecule OPVs (SM-OPVs) possess some important advantages, including (1) uniform and defined molecular structures, resulting in less batch-to-batch variation; (2) generally higher open-circuit voltage (Voc); (3) higher hole mobility than the corresponding polymer materials; and (4) structural flexibility with simple control of energy levels via slight chemical structure modifications. In this work, to resolve problems of polymeric materials, we have designed and synthesized new low bandgap A1-π-A2-D-A2-π-A1 type small molecules, which terminal electron-withdrawing octyl cyanoacetate group is connected to a carbazole dimer core through another electron-accepting benzo[c][1,2,5]thiadiazole unit, for solution-processable SM-OPVs.

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Soluble Aromatic Polyamides Derived from Unsymmetrical Diamine with Two Trifluoromethyl Groups

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Aromatic polyamides(PA) are widely used as a high-performance polymer in advanced technologies due to their outstanding thermal and mechanical properties. Nevertheless, PAs have a problem like poor solubility in most organic solvents leading to limitation on their application. To overcome this problem, many research efforts have been made to enhance its solubility by introducing bulky pendant groups or flexible linkage into polymer backbone. Ether linkage is easily considered as a flexible linkage and offers enhanced solubility, color, and melt-processing properties. In addition, incorporation of CF_3 pendant group can also be considered as an effective means to improve the polymer solubility without deteriorating their properties. In this study, we designed unsymmetrical diamine monomer containing ether and CF_3 groups as a linkage and pendant moieties, respectively, and synthesized a series of PAs from the monomer. The synthesis and characterization of the PAs will be presented.

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Kinetic study for the reaction of TDI and alcohol

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TDI 와 -OH(alcohol) 작용기는 우레탄 결합을 하며, 많은 고분자 재료를 형성하는 반응이다. 우레탄 수지의 물리적 성질이 반응속도나 열역학 함수에 따라 변하기 때문에, 반응상수, 메커니즘 규명 등은 물성조절을 위한 중요 과제이다. 본 연구에서는 TDI 와 alcohol 반응에 대한 반응속도론적 연구를 통하여, 반응속도 상수와 활성화 에너지를 측정하였다. FT-IR 을 이용하여 isocyanate peak 의 intensity 변화를 이용하여 속도상수를 측정하였으며, 반응온도 변화시켜 가며, 활성화 에너지를 측정 하였다.

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The study for the MALDI-MS spectrum interpretation for the TDI and TMP reaction

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산업용도로 단열재, 의료용 패치 등 다양한 분야에 이용되는 고분자 제조시 cross-linker 로 사용하는 TDI(toluene diisocyanate)와 TMP(trimethylolpropane)의 urethane 반응을 MALDI-MS 를 이용하여 연구하였다. 반응 조건별, 시간 별로 다르게 나타나는 MALDI spectrum data 중 이론적으로 예측된 mass 값을 비교하여 반응 조건이 변할 때 생성되는 생성물을 확인 및 검증 하는 방법으로 prepolymer 형성에 대한 reaction monitoring 을 하였다. 그리고 LC-MS, IR 등을 이용하여 실험적으로 분석한 결과와 비교 함으로써 MALDI-MS 만으로도 prepolymer 생성 반응을 설명 할 수 있음을 보였다.

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Polyketone/polyamide-6 블렌드의 상용성 및 결정화 거동 연구

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결정성 고분자인 polyketone 은 우수한 열적, 화학적, 기계적 성질을 가지고 있지만, 열에 의한 분해가 잘 일어나고 가공범위가 좁다는 단점이 있다. 이러한 단점을 보완하기 위하여 공중합이나 블렌드에 대한 연구가 많이 진행되고 있다. Polyketone 과 다양한 고분자와의 블렌드를 통하여 성질을 개선하는 연구가 진행되었지만, 대부분의 고분자와 상용성이 없으나 polyamide-6 와의 경우는 상용성이 있는 것으로 알려져 있다. Polyketone/polyamide-6 블렌드의 상용성에 관한 연구에서 결정화 거동 및 상호인력에 관한 상세한 연구는 보고되지 않고 있다. 본 연구에서는 polyketone/polyamide-6 블렌드의 상용성을 Tg 분석과 자외선 분광법, 녹는점 강하법으로 알아보았다. Polyketone/polyamide-6 블렌드 조성에 따른 결정화 거동은 등온결정화와 비등온결정화 방법으로 조사하여 결정화 속도, Avrami 상수 등을 구하였으며, spherulite 형상 및 성장 속도와 등온결정화에서 구한 결정화 속도와 비교하였다. Polyketone/polyamide-6 블렌드의 Tg 는 전 조성헤서 하나로 관찰되었으며, 각각의 Tg 값의 중간 값을 가지는 것을 보아 비결정성 영역에서의 상용성을 확인하였고, 자외선 분광분석에서의 특정 피크 이동을 통해 수소결합 형성을 확인하였다. 녹는점 강하법으로 얻은 상호인력지수 값이 음의 값을 나타내어 결정성 영역에서의 상용성도 확인하였다. Polyketone/polyamide-6 블렌드의 결정화 거동은 등온결정화법을 통해 Avrami 상수와 결정화 속도를 구하였다. 또한 spherulite 의 형상과 성장속도를 관찰하여 등온결정화법과 비교하였다. 블렌드의 결정화속도 변화와 spherulite 형상의 변화 없이 크기가 작아지고 그 수가 증가하는 것으로 보아 polyamide-6 는 polyketone 의 결정화 메커니즘 변화는 일어나지 않으면서 결정성장 속도를 가속시키는 것을 확인하였다. 비등온결정화법은 변형 Avrami-Ozawa 모델을 적용하였을 때 등온결정화법과 일치하였다. 이 모델의 속도상수인 F(t)는 polyketone 의 값보다 낮았으며, 동일한 결정화도에서 polyamide-6 의 함량이 증가할수록 감소하였다.

상수는 거의 일정하였으며 이는 polyketone 에 polyamide-6 를 첨가하여도 결정의 성장이나 핵생성 메커니즘에 영향을 주지 않는 것으로 판단된다.

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Synthesis and Characterization of organic photovoltaic polymer

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A new organic photovoltaic polymer, a tetrathiafulvalene (TTF)-based main-chain polymer and contained fullerene (C60), was successfully synthesized via a condensation polymerization. TTF can work as an electron donor (D) and C60 can act as an electron acceptor (A). Therefore, the chemical component of TTF-DA-polymer is a DA dyads system. The chemical structure of TTF-DA-polymer was characterized by spectroscopic techniques such as FT IR, 1H and 13C NMR spectroscopes, and its thermal transition behavior was also monitored by DSC. Moreover, the electrochemical properties and photoelectric properties were researched by cyclic voltammetry, photoluminescence, and ultraviolet-visible spectrometer. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), the Converging Research Center Program (2013K001428), SW Fusion Components R&D Program (MOTIE-10047806) and BK21Plus Program, Korea.

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Striped Pattern of Fullerene-containing Reactive Mesogen

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The self-organization of fullerenes has gathered much attention in developing various functional nanostructures with controlled dimensionality and tailored properties. We proposed an advanced patterned Fullerene-containing reactive mesogen (FCRM) through mixed in cholesteric liquid crystalline medium without external agents, FCRM particles were micro-oriented resulting from phase separation between FCRM and the cholesteric liquid crystal. A novel fullerene-based molecule (FCRM) was newly synthesized. The self-assembled striped FCRM patterns with regular intervals were successfully prepared via the one-dimensional (1D) pattern-forming state of an elastically anisotropic cholesteric liquid crystal as a template. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), the Converging Research Center Program (2013K001428), SW Fusion Components R&D Program (MOTIE-10047806) and BK21Plus Program, Korea.

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Polypropylene/GO nanocomposites processing using GO-supported Ziegler-Natta catalyst via master batch technique

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Graphene, which is a two-dimensional sp2 carbon material with one atom thickness, has shown great promise in electronic devices, as energy-storage materials, in chemical/bio-sensors, for bio-medical applications, and as nanofillers in composites, due to its excellent electrical, thermal, and mechanical properties and high surface areas. A few examples of chemically modified graphenes showed interesting performances as a catalyst or as a support in catalytic reactions.The highly isotactic PP prepared with GO-supported TiCl4 catalysts by in situ polymerization. The I.I, molecular weight, MWD were influenced by internal donors and external donors. With introduction of internal donor and external donor, the I.I was dramatically improved and the GPC curves are shifted higher molecular weight region. The shift of GPC curve could be ascribed to the internal donor were replaced by the silane compound lead to increase the molecular weight of PP. PP/GO nanocomposites were prepared by using the obtained PP as a master batch with commercial PP using a twin screw mixer. The modulus of PP/GO nanocomposites increased by addition of GO dispersed PP, that is prepared by GO-supported TiCl4 catalysts. Thermal stability of nanocomposites are much higher than that of commercial PP. The in-situ polymerization processes are promising techniques for preparation of well dispersed GO nanocomposites by using GO-supported catalysts.

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Magnetotactic Self-Assembled Peptide Architectures

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Biological molecular machines capable of converting chemical energy into mechanical work regulate a wide variety of biological processes in living organisms. Motor proteins, one of the most well-known biological machinery, perform their essential motile functions such as cargo transport, muscle contraction. Over the past few decades, inspired by the protein machines, considerable advance has been made in controlling the motions of synthetic molecules by virtue of the pioneering efforts of organic chemists. In most precedent studies, movable parts of the synthetic machines were shepherded by using nonbiological molecular scaffolds with unique structural constraints such as mechanical interlocking, overcrowded alkenes. However, de novo design of a well-defined, artificial molecular machine from biological elements still poses a great challenge due to the inherent complexities such as unpredictable folding and agglomeration. Protein-based molecular machines, in particular, are highly complicated supramolecular ensembles obtained from the sophisticated integration and precise positional displacement of subunit structures. And therefore it is inevitably difficult to rectify the subtle motions at the molecular level from protein-based molecular assemblies. Here we show a very simple, ingenious demonstration that the assemblies of peptide foldamers, artificial mimicry of protein fragments, are able to be directly utilized as molecular machines biased by external magnetic field.

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패턴화된 reduced graphene oxide(RGO) 전극을 이용한 분자각인 고분자 박막 제작 및 특성 분석

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분자각인 고분자는 주형분자, 기능성 단위체, 가교제의 공중합으로 제작하고 주형분자의 제거를 통해 주형분자와 상호 보완적인 공극을 형성하여 주형분자의 인식이 가능하다. 따라서 주형분자의 선택적인 인식이 가능한 분자각인 고분자는 분리분석, 약물전달 시스템, 센서 등에 광범위하게 이용되고 있다. 최근, 분자각인 고분자의 응답 특성을 향상시키기 위해 graphene, nanowire 와 같은 전기 전도성이 우수하고 넓은 비표면적을 가지는 물질을 사용한 분자각인 고분자에 관한 연구가 진행되고 있다. 따라서 본 연구에서는 평면 분자각인 고분자와 달리 향상된 응답 특성을 위해 패턴화된 reduced graphene oxide(RGO) 전극을 이용한 분자각인 고분자 박막의 제작과 그 특성을 분석하고자 한다. Colloid 와 surfactant 의 정전기적 상호작용에 의해 형성된 hexagonal close packed polystyrene colloidal array 에 전기화학적 방법을 통해 graphene oxide(GO)를 증착하고 이를 환원 시켜 패턴화된 RGO 전극을 제작한다. RGO 전극은 전기화학적 증착과정에서 가해주는 전압의 세기, 전압을 가하는 시간 등을 통해 최적화하고 패턴화된 RGO 전극 위에 전기화학적 방법으로 분자각인 고분자 박막을 제작한다.

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콜로이드 리소그래피를 이용한 마이크로 패턴화된 분자각인 고분자 박막의 제작

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경북대학교 고분자공학과

분자각인 고분자는 특정 물질을 공유결합 또는 비 공유결합을 통해 고분자 매트릭스에 각인시키는 기술로서 쉽게 특정 물질의 인식이 가능하며 온도, PH 의 영향을 받지 않으므로 반영구적으로 사용 가능하기에 화학, 고분자학, 생명공학 및 의학관련 센서 분야에서 많은 관심을 받고 있다. 최근 화학 센서 분야에서는 특정 물질에 대한 분자각인 고분자의 센서 응답 특성을 향상시키기 위해 정렬된 마이크로/나노 구조를 제작하기 위한 연구가 진행되고 있다. 한 예로 음이온성 콜로이드와 계면활성제의 정전기적 상호작용을 이용한 정렬된 2 차원 결정 형성에 관한 연구가 보고된 바 있다. 따라서, 본 연구에서는 콜로이드 및 계면활성제의 상호작용을 통해 제작된 특정 패턴화된 콜로이드 템플릿을 사용하여 2,4-dinitrotoluene (DNT) 탐지용 분자각인 고분자 박막을 제작하고 그 특성을 분석하고자 한다. 콜로이드 템플릿은 dip-coating 방법과 열 전이를 통해 평면의 기판상에 전이된 콜로이드를 polydimethylsiloxane (PDMS)로 복제하여 제작한다. 패턴화된 기판의 홈 폭, 콜로이드 입자의 크기, 콜로이드 및 계면활성제의 농도를 조절함으로써 제작된 다양한 구조의 콜로이드 템플릿을 사용하여 poly (methacrylic acid-co-ethylene glycol dimethacrylate) (PMAA-co-EGDMA)로 구성된 분자각인 고분자 박막을 제작한다.

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탄소나노 섬유를 이용한 2,4-Dinitrotoluene 검출용 분자각인 전도성 고분자 박막 제작 및 특성분석

이태권 양진철 곽진원 박진영*

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분자각인 고분자는 주형분자(template)를 제거함으로써 생성되는 상호보완적인 공극을 통해 특정물질을 선택적으로 인식하는 고분자 물질로써 특정물질에 대한 높은 선택도와 높은 친화도를 가지기에 단백질, 아미노산, 약물 등을 검출하는 센서로 많이 사용되고 있다. 최근, 이러한 센서의 인식능력을 향상시키기 위해 다양한 기판 상의 분자각인 고분자에 마이크로/나노 패턴을 형성하는 연구가 진행되고 있다. 그 예로 본 연구팀에서는 수정진동자 위에 콜로이드 리소그래피를 통해 패턴을 형성한 뒤, 폴리피롤 공중합체의 전기중합으로부터 제조된 분자각인 고분자 박막의 특정물질에 대한 향상된 응답특성을 보고한 바 있다. 따라서, 본 연구에서는 탄소나노 섬유 기판에 마이크로 공극 패턴을 가진 2,4-dinitrotoluene 검출용 분자각인 전도성 고분자 박막을 제작하고 센서응답 특성을 분석한다. 공극 패턴은 콜로이드 리소그래피를 이용하여 탄소나노 섬유에 콜로이드 단일막을 패턴하고 분자각인 물질(2,4-dinitrotoluene)을 가진 폴리피롤 공중합체를 전기중합한 후 콜로이드 층을 제거함으로써 형성된다.

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장소: 일산 KINTEX
발표코드: **POLY.P-73**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Crosslinkable Nafion film for DMFC by using Layer by Layer self assembly

윤미선 허아람 조창기*

한양대학교 유기나노공학과

Layer by Layer self-assembly (LbL) method is a very useful way to make a polymeric thin film by using electrostatic attraction. And a polymer electrolyte membrane (PEM) for direct methanol fuel cell (DMFC) can be prepared by using the LbL method. Nafion® is most commonly used electrolyte in PEM fuel cells, because of their high proton conductivity and chemical stability. Although the Nafion has many benefits it is not satisfactory in many aspects; fuel crossover when fueled with alcohols. In this research, we converted some sulfonic acid group of the Nafion into alkyne in order to crosslink the Nafion with another polymer which contains azide group by click reaction. LbL method was used for the preparation of fuel cell film by using the Nafion and azide modified cationic copolymer, and subsequent click reaction Obtained film was characterized by H-NMR, IR, IEC, water uptake, proton conductivity, and methanol permeability. Uncrosslinked LbL film was used as a reference.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Evaporation Characteristics of the Distilled Sulfur Mustard (HD) from Ground Substances using a Laboratory-Sized Wind Tunnel

정현숙

국방과학연구소 화생방부

In this study, we demonstrate a robust method for the evaporation characteristics of the distilled sulfur mustard from ground substances (sand, soil, and concrete) with temperatures, drop sizes, and airflow rates. We use a 5-cm wind tunnel and thermal desorption (TD) in connection with gas chromatograph and mass spectrometry detection (GC/MSD). Drops of neat HD, ranging in size with 1, 6, and 9 microliter, are applied to small subsrate coupons. The temperatures are either 18, 25, or 35 oC and the airflow rates are either 22, 175, or 375 SLPM. The vapors of HD are quantitatively collected using thermal desorption tubes. The data obtained here will be eventually incorporated into the software program NBC-RAMS which predicts the hazard of chemical agents under various environmental conditions.

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발표코드: **IND.P-75**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis of Diketo-Pyrrolo-Pyrrole(DPP) Colorants and Investigation of Their Color Change Properties

김헌수 김승희[1] 박수열[*]

한국화학연구원 계면재료공정연구그룹 [1]단국대학교 화학과

Diketopyrrolopyrroles(DPP) are bicyclic pigment containing two units. The DPP represent high performance red pigment because of their excellent light and thermal stability. The typical DPP derivatives have melting point over 350℃, a very low solubility in most solvent, an absorption in the visible region with maximum between 500 nm and 600 nm. In our research, the synthesis of DPP pigments are discussed and chromatic characteristics of these pigment synthesized are analyzed by a spectrophotometer. DPP derivatives have been traditionally used in coloring of fibers, plastics, automotive coatings and recently have gained much attention in synthesis of LEDs, color filters, NIR Dyes.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

preparation and characterization of hydrophilic lens materials containing various benzophenone group

김득현 성아영*

세한대학교 안경광학과

The optical and physical characteristics of hydrogel lens polymerized with various hydroxybenzophenone group in the basic hydrogel lens material were evaluated. 2-Hydroxybenzophenone, 2,4-dihydroxybenzophenone and 2,4,4- trihydroxybenzophenone were used as additives and also, the mixture containing 2-hydroxyethyl methacrylate and additive was copolymerized in the presence of AIBN as an initiator. The polymer by using thermal polymerization process for hydrogel lens was produced and the physical properties showed that the contact angle of sample containing 2-hydroxybenzophenone, 2,4-dihydroxybenzophenone and 2,4,4-trihydroxybenzophenone was in the range of 65.16~60.85°, 61.59~53.45° and 61.09~54.43°, respectively. The optical properties of produced the hydrogel lens including 2-hydroxybenzophenone showed that the UV-A transmittance was 86.8~72.2%, the UV-B transmittance was 84.2~70.4%, Also, in case of the hydrogel lens including 2,4-dihydroxybenzophenone and 2,4,4-trihydroxybenzophenone, the results showed that the UV-A transmittance was 76.20~16.80%, 61.80~11.60%, and the UV-B transmittance was 66.80~2.00%, 50.80~1.40%, respectively. The addition of 2,4-dihydroxybenzophenone and 2,4,4-triyhydroxybenzophenone allowed the hydrogel lens to block UV.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of water-soluble copolymers using modified maleic anhydride

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Generally, the water-soluble polymer is synthesized using maleic anhydride and olefin. It is very difficult to synthesize maleic anhydride copolymer having long carbon chain. In this study, new water-soluble polymers containing polyoxyethylene groups were prepared using modified maleic anhydride. The modified maleic anhydrides were synthesized by maleic anhydride and MPEG (polyethylene glycol monomethyl ether) and then, modified maleic anhydride were polymerized with polybutene. The cmc of synthesized copolymers are 0.0010~0.0017 mol/L

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

High performance material containing siloxanyl group for hydrogel ophthalmic lens

김동현 성아영*

세한대학교 안경광학과

The gas permeability, optical transparency, mechanical properties and biocompatibility, physical and chemical are significant physical properties of hydrogel ophthalmic lens for this study, the physical and optical characteristics of hydrogel ophthalmic lens copolymerized with addition of siloxanyl methacrylate and cross-linking agent ethylene glycol dimethacrylate in the basic hydrogel ophtalmic lenses material were measured. And also in particular, the utility of siloxanyl methacrylate as a high gas permeability and high visible light transmittance material for ophthalmologic devices by measuring the oxygen permeability and spectral transmittance were investigated. The copolymerized hydrogel ophthalmic lenses of all combinations showed flexible and soft characteristics after being hydrated for standard saline-solution. The oxygen permeability value of the lenses ranges from 50.05 to 54.21 x 10-11(cm2 x mlO2)/(sec x ml x mmHg). The visible light tansmittance of copolymerized ophthalmic lenses, was in the range 89~ 91%. The material containing siloxanyl methacrylate is expected to be able to be used usefully as a material for high oxygen permeability hydrogel lens.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of asymmetrical ionic liquids

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동국대학교 화학과

Ionic liquids (ILs) are generally formed by an organic cation and a weakly coordinating anion. They have received vast research interests in recent years because of their unique properties such as high thermal stability, non-volatility, nonflammability, high ionic conductivity, wide electrochemical window and miscibility with organic compounds. A new series of novel asymmetrical ionic liquids (ILs) consisting of tributylalkyl phosphonium and alkylimidazolium, trimethylamine or triethylamine were synthesized in batch and micro-reactor. various asymmetrical ionic liquids were investigated about their thermal stability, specific conductivity, electrochemical window and solubility. among them, the best asymmetrical ionic liquid was selected as redox electrolyte of dye-sensitized solar cells(DSSC).

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Emission properties of triphenylamine-o-carborane dyads induced by twisted intramolecular charge transfer

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고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 신소재화학과 [2]서울여자대학교 화학과

We developed unique electron donor-π-acceptor dyad systems with diphenylamino at para- and meta-position of phenyl, and ortho-carborane. The para- and meta-substituted D- π -A systems showed three kinds of emission originated from the local excited (LE) state, a twisted intramolecular charge transfer (TICT) state and an aggregation induced emission (AIE). The TICT emission showed strong solvent-polarity dependency, which is attributed to the dipole moment changes in excited TICT state. The strong AIE emission is observed in extremely nonpolar solvent such as n-hexane, because the association between solutes caused by low-solubility. Contrast to these, the steric hindrance between donors in para-substituted of D- π -A- π -D system prohibited the formation of TICT state, hence the LE and AIE emissions were observed dominantly.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rationally Designing Bimetallic Complexes for Light-Driven Redox Catalysis: How to Assign Specific Functions to Each Metal in a Bimetallic Ir(III)-Pt(II) Complex

조양진 강상욱* 조대원[1] 손호진*

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 신소재화학과

최근 자연계에 존재하는 광합성 안테나 복합체들의 원리를 모방한 인공광합성 연구가 세계적으로 활발히 진행되고 있다. 광에너지를 흡수, 에너지 전달, 그리고 반응점(Reaction Center)에서의 전자전달현상으로 이어지는 자연계 내 촉매반응공정은 실질적인 인공광합성 연구에서 요구되는 다음의 세가지 (1) 집광능력 및 전하분리, (2) 에너지 (엑시톤) 전달, 그리고 (3) 촉매활성점에서의 효과적인 전자이동과 밀접한 연관성을 가지며 광변환 효율을 높이는 결정적인 요인이 된다. 이에 본 연구에서는 효과적인 광변환촉매시스템 개발의 한 방법으로서 집광, 엑시톤 전달, 및 촉매 역할들을 한 분자 내에서의 구현되도록 디자인하였다. Polypyridyl 이리듐 (Ir) 착화합물을 집광체로 백금(Pt)착물을 수소발생환원촉매로서 사용하였으며 집광체와 촉매사이의 효과적인 에너지전달을 위하여 2,3-bis(2-pyridyl)pyrazine (dpp) 단위체가 bridge unit 으로 사용되었다. 준비된 다기능 촉매의 광물리적, 전기화학, 그리고 이론계산을 통한 들뜬 전자의 거동 및 촉매작용의 메커니즘 연구가 세밀하게 수행되었으며 수중수소발생 실험을 통한 광촉매 효율이 평가 되어졌다. 효과적인 에너지 이동에 최적화된 화합물이 성공적으로 합성되었으며 이는 질량분석법 및 핵자기공명 분광법 등에 의해 확인 되었다. 화합물의 광물리적, 전기화학적 특성이 측정 되어졌다. 배위화합물에 따른 분자내 에너지 이동 및 분석을 제시함으로써 추후 태양전지 및 인공광합성 등 광화학 분야의 분자 설계의 방향성에 도움을 줄 것이다.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

High value-added production of MFB : a novel synthesis of intermediates for Imatinib

김선호 김석찬*

국민대학교 화학과

Crude Methyl 4-formylbenzoate (c-MFB) is an industrial waste, which is generated from Dimethyl terephthalate (DMT) manufacturing process. DMT is well-defined raw material for PET production. Commercial DMT has been synthesized from p-xylene. In this process, partial oxidation of p-xylene is mainly causative of the major impurities. MFB is major by-product of DMT manufacturing process. The component ratio of by-product (c-MFB) is MFB 80%, DMT 14%, MMB 6% and the quantity of c-MFB is annually 1000MT. Until the present, all c-MFB have been discarded by burning it. And it generates huge amount of CO2 gas from burning waste, which it causes environmental pollution.To solve this problem, we have developed new application area of MFB. MFB is applicable as starting materials in synthesis of imatinib intermediate. As it known, Imatinib is widely used as tyrosine kinase inhibitor. The U.S. FDA(Food and Drug Administration) has approved imatinib as first-line treatment for CML(chronic myelogenous leukemia). In 2001, Novartis launched Gleevec based on imatinib.The methyl 4-((4-methylpiperazin-1-yl)methyl)benzoate (MMMB) are used as the intermediate material of imatinib. This medicine give us the idea for the new application of MFB as the starting material of imatinib. Because it can be synthesized from MFB by using the method of reductive amination. For these reasons, we have developed the new synthetic method of imatinib.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Purification of AMCA from Industrial Waste

김종천 김선호 김석찬*

국민대학교 화학과

c-MFB(methyl 4-formylbenzoate) is generated from process of DMT(dimethyl terephthalate), DMT is generated by oxidization of *p*-xylene and its esterification. In this process, partially oxidization of *p*-xylene produce major impurities, which are MFB and MMB(methyl 4-methylbenzoate). The compornant ratio is MFB 80%, DMT 14%, MMB 6%. c-MFB is produced 1000ton every year. c-MFB is burned out. However, the problems associated with environmental pollution. Therefore we found application of MFB. It is applicable as starting materials in synthesis of AMCA((4-aminomethyl)cyclohexanecarboxylic acid)

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장소: 일산 KINTEX

발표코드: **IND.P-84**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Etherification of glycerol using alkali metal-acetate salts as catalysts

한태열 이제승* 정민석 박서경

경희대학교 화학과

Glycerol has emerged as a renewable bio-resource for the synthesis of polyglycerols which have various application fields. Diglycerol and triglycerol have been used as useful additives for food, cosmetic, and pharmaceutical emulsifiers. The etherification reaction of glycerol was conducted in the presence of alkali metal-acetate salts as catalysts. Alkali metal-acetate salts showed high catalytic activities with corresponding selectivities for diglycerol and triglycerol. The influences of various reaction variables including the nature and loading amount of catalyst, reaction time, and reaction temperature on the etherification of glycerol were investigated

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발표코드: **IND.P-85**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Etherification of glycerol using heterogeneous catalysts

한태열 이제승* 박서경

경희대학교 화학과

Diglycerol and triglycerol are useful compounds for various industrial fields including food, cosmetic, and pharmaceuticals. Alkali metal embedded zeolites were used as catalysts and they showed high selectivities for diglycerol and triglycerol. In order to examine the reactivities of the catalysts, several reaction variables including the amount of catalysts, reaction time and reaction temperature were investigated.

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발표코드: **IND.P-86**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ammonia activation of porous carbons using 2,2-biphenol and their application for carbon capture

박서경 이제승* 한태열

경희대학교 화학과

Novel micro- and mesoporous carbon materials have been prepared by soft template method using 2,2’-biphenol as a precursor. The porosity of prepared porous carbon materials could be controlled by the amount of block copolymer used as a soft template. The surface areas of carbonized phenolic resin were measured as 598 $m^2 g^{-1}$ with a pore volume of 0.37 $cm^3 g^{-1}$. The surface areas further increased up to 1778 $m^2 g^{-1}$ with a pore volume of 0.78 $cm^3 g^{-1}$ by the heat treatment under ammonia atmosphere. The CO_2 adsorption capacity of pristine carbons increased from 2.15 to 2.98 mmol g^{-1} after ammonia activation.

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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

CO_2 activation of porous carbons using 2,2-biphenol and their application for carbon capture

박서경 한태열 이제승*

경희대학교 화학과

Porous carbon materials have been prepared by a soft-template method using 2,2'-biphenol as a precursor. Porous carbons activated at high temperature under carbon dioxide environment exhibited large surface areas and high CO_2 adsorption capacities. The surface area of carbonized phenolic resin was measured as 598 m^2 g^{-1} with a pore volume of 0.37 cm^3 g^{-1}. Interestingly, after the carbon dioxide activation process, the surface areas and pore volumes of carbons increased as high as 2614.8 m^2 g^{-1} with a pore volume of 1.39 cm^3 g^{-1}. The CO_2 adsorption capacities of carbon dioxide activated carbons increased up to 4.60 mmol g^{-1}.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and activation of porous carbons from biomass and their application for carbon capture

박서경 이제승* 한태열

경희대학교 화학과

Porous carbon materials have been prepared using biomass as a precursor by heat treatment under nitrogen atmosphere followed by the heat treatment under ammonia atmosphere. The experimental results showed that the temperature of carbonization and activation significantly affect the pore structure and CO_2 adsorption capacities of porous carbon materials. The specific surface areas of porous carbon derived from alginic acid were measured as high as 258.2 m^2 g^{-1} with a pore volume of 0.15 cm^3 g^{-1}. The surface area of pristine cabons increased up to 1032.0 m^2 g^{-1} with a pore volume of 0.65 cm^3 g^{-1} by the ammonia activation at high temperature. The CO_2 adsorption capacity of ammonia activated carbon derived from alginic acid were measured as high as 2.20 mmol g^{-1} at ambient temperature and pressure.

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Structural and Morphological Transformations of Metal-Organic Framework

김태호 최소라 이희정 오문현*

연세대학교 화학과

Coordination polymers (CPs) including metal-organic frameworks (MOFs) have received a great deal of attention due to their many applications in gas storage, catalysis, and separation. Structural topologies and compositions of CPs are quite important factors that define their porosities and properties. For example, several CPs have similar compositions, but have different structural topologies and so have different properties. Herein, we report the structural and morphological transformations of three-dimensional Kagom?-like structured (In-MIL-68, [In(OH)(BDC)]n) hexagonal lumps to three-dimensional quartz structured (QMOF-2, [InH(BDC)2]n) pointed hexagonal rods.

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Highly Effective Heterogeneous Sensors Based upon Coordination Polymers

이일랑 조원 이희정 오문현*

연세대학교 화학과

In general, heterogeneous sensors display low sensitivity and weak signals; however, there are many demands for heterogeneous solid sensors due to their excellent chemical stability and outstanding recyclability. Thus, the development of effective heterogeneous sensors is a very important and challenging area. Herein, we wish to report highly effective heterogeneous sensors in the form of core-shell microspheres based upon luminescent lanthanide coordination polymers. The small size and excellent dispersity of core-shell type coordination polymer microspheres result in an extremely sensitive and selective sensing on Cu2+ ions.

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Nanocomposites of Au NPs/Pt replica and their SERS effect

홍다영 권영욱[1,*] 곽진수[1] 김강영[1] 조승익[1] 김근오[1]

성균관대학교 자연과학부 화학과 [1]성균관대학교 화학과

We report the nanocomposites of Au nanoparticles (NPs) on ordered Pt nanorods with varying sizes or assemblies of Au NPs and the investigation of their plasmon coupling properties for surface enhanced Raman spectroscopy (SERS) effect. Nanostructured Pt thin films were chosen as SERS substrates because they can have surface plasmon resonance (SPR) mode due to their well-ordered structures with controlled gap. When 4-aminobenzenethiol (4-ABT) was used as probe molecules, our nanocomposites showed strong SERS signals than that of Au NPs on Si wafer. So-called 'hot spot' in an interlayer of Au NPs and nanostructured Pt thin films makes strong electromagnetic fields and it can lead SERS effect. This SERS effect was confirmed through the computational results, which were applied by the finite difference time domain (FDTD). FDTD calculations indicated that the electric field enhancement experienced by Au NPs/nanostructured Pt thin films is much enhanced at certain region. Based on experimental and theoretical results, we demonstrate that Au NPs/nanostructured Pt thin films for SERS substrate were formed on enhancement of electromagnetic field with the junction.

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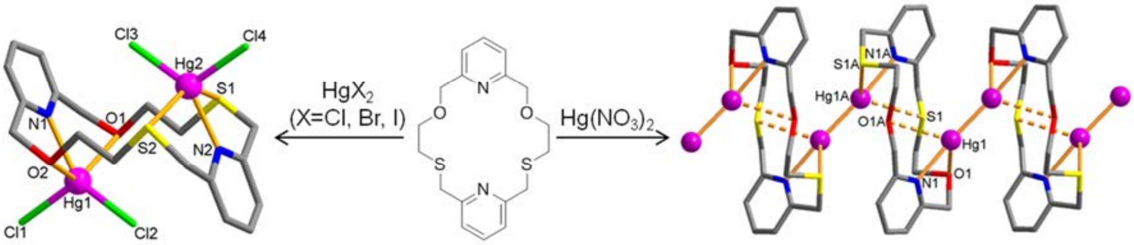
Synthesis of an $N_2O_2S_2$-Donor Macrocyclic Ligand and Its Supramolecular Silver(I), Mercury(ll), Copper(II), and Nickel(ll) Complexes

서수진 이은지 이심성*

경상대학교 화학과

A ditopic macrocycle L which employs NO_2 and NS_2 donor sets in each side to accommodate one hard and/or one soft metal ion(s) in the cavity was synthesized. First, the reactions of L with Ag(I) salts afforded exocyclic 1D coordination polymers of type $\{[Ag(L)]X\}_n$ (1: X = ClO_4^- and 2: X = BF_4^-) with different coordination modes. The treatment of L with mercury(II) halides yielded isostructural endocyclic dinuclear complex, $[Hg_2(L)X_4]$ (3a: X = Cl, 3b: X = Br, and 3c: X = I). Notably, mercury(II) nitrate gave a 1D coordination polymer with an Hg-Hg contact, $\{[Hg(L)]NO_3\}_n$ (4) (*see below*). While, the reaction of HgI_2 with L in the presence of CuI afforded an endocyclic monocopper(II) complex, $[Cu(L)][Hg_2I_6]$ (5), in which the square-type dimercury(II) hexa-iodide cluster exists as a separated counter anion. The reaction of L with $Ni(NO_3)_2{\cdot}6H_2O$ afforded an endocyclic complex, $[Ni(L)](NO_3)_2{\cdot}2H_2O$ (6). The results of the metal complexation behaviors of L both in solid and solution states are discussed.



3, Dimercury complex

L

4, 1D Polymeric complex via Hg-Hg contact

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Solvent-induced single-crystal to single-crystal transformation from heteronuclear 2D to homonuclear 2D coordination polymers via removal of Hg_2I_4 cluster and rearrangement

김슬기 박인혁 이심성*

경상대학교 화학과

Stimulus single-crystal to single-crystal (SCSC) transformation is one of the most fascinating methodologies for the creation of novel materials. A significant SCSC transformation of a heteronuclear coordination polymer (CP) to a homonuclear CP by removal of a partial inorganic unit followed by rearrangement is reported. The O_2S_2-macrocycle L^1 with a longer $S\cdots S$ distance reacts with a mixture of CuI and HgI_2 to yield the heteronuclear CP, $[Cu_2(\mu_2\text{-}Hg_2I_4)(L^1)_2(CH_3CN)_2I_2{\cdot}C_6H_5CH_3]_n$ (1), in which L^1-Cu-L^1-Cu 1D chains are cross-linked by a μ_2-Hg_2I_4 bridging cluster, giving rise to an infinite 2D structure. Notably, exposure of the yellow single crystals of 1 in methanol induces the SCSC transformation resulting in a colorless homonuclear 2D CP, $[(\mu_2\text{-}Cu_2I_2)(L^1)]_n$ (2) formed through removal of the μ_2-Hg_2I_4 bridging part couple with the rearrangement of the metal coordination sphere. Furthermore, a conventional direct reaction of L^1 with CuI afforded two 1D CPs, $[(Cu_3I_3)(L^1)_2]$ (3) and $[(Cu_4I_4)(L^1)_2]$ (4), whose structures are totally different from that of 2 obtained from the removal-rearrangement process.

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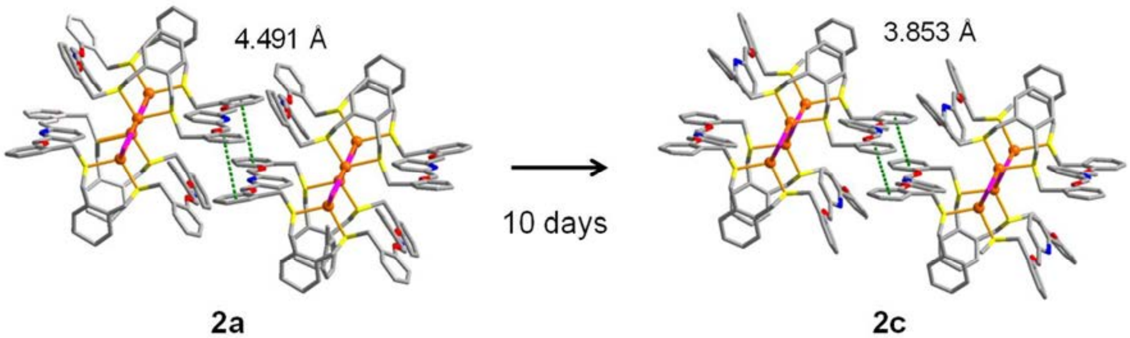
An Extra-Large Macrocycle: Its Double Decker Type Complex Exhibiting Single-Crystal to Single-Crystal Transformation in Air

강윤지 박인혁 이심성*

경상대학교 화학과

There is a growing interest in a large macrocyclic ligand system that can form binuclear complexes exhibiting electron transport, charge transfer, and allosteric behavior. In this presentation, a 19-membered $N_2O_2S_2$-macrocycle (L^1) and a 38-membered $N_2O_4S_4$-macrocycle (L^2) obtained as a mixture via respective [1:1] and [2:2] cyclization reaction were separated and their coordination behaviors with copper(I) iodide were investigated. When CuI was reacted with L^1, we also obtained an endocyclic mononuclear complex featuring three separated units of formula $[Cu(L^1)]I_3{\cdot}$ether (1). The notable product is a copper(I) iodide complex, $[(Cu_2I_2)_2\,(L^2)\,_2]{\cdot}2toluene{\cdot}2CH_3CN$ (2a), with the large macrocycle L^2. In 2, two macrocycles are doubly linked by two Cu_2I_2 squares via Cu-S bonds resulting in the formation of a large double decker. Most notably, when the single crystals of 2a were undisturbed in air for 10 days, the CH_3CN molecules in the lattice were removed to form $[(Cu_2I_2)_2\,(L^2)_2]{\cdot}2toluene$ (2c) in a single-crystal to single-crystal (SCSC) manner inducing the interligand π-π interaction to be more stronger.



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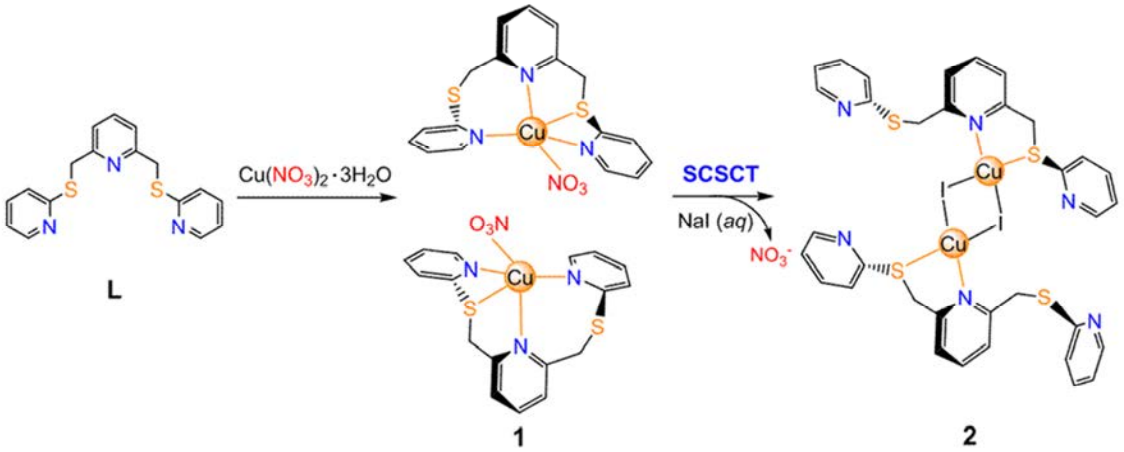
Anion-Exchange Induced Single-Crystal-to-Single-Crystal Transformation Accompanying Monomer to Dimer and Copper(II) to Copper(I)

이형환 박인혁 이심성*

경상대학교 화학과

Anion-exchange induced single-crystal-to-single-crystal transformation (SCSCT) accompanying monomer to dimer and copper(II) to copper(I) are reported. A flexible tripyridyl disulfide ligand, L, reacts with copper(II) nitrate to give a monocopper(II) complex $[Cu(L)NO_3]\cdot(NO_3)\cdot$toluene (1) adopting a distorted square pyramidal geometry. Interestingly, when the dark-blue single crystals of 1 were immersed in 3 M NaI aqueous solution, the sample was transformed to a pale yellow dimeric copper(I) complex $[Cu_2(L)_2I_2]$ (2) in which two ligands are linked by Cu_2I_2 square-type cluster. This result is noteworthy because the conventional reaction of L with CuI yielded a mixture of four products, $[(Cu_4I_4)(L)_2]$ (3), $[(Cu_4I_4)(L)_2]\cdot 2CH_2Cl_2$ (4), $[(Cu_4I_4)(L)_2]\cdot CH_2Cl_2$ (5), and $[(Cu_4I_4)(L)_2]$ (6) adopting a similar bis(ligand) complex type linked with a stepped cubane cluster whose structures are totally different from that of 2. Furthermore, compound 2 is the first example of the copper(I) iodide complex prepared by the anion-exchange approach.


Cu(NO3)2·3H2O
SCSCT
NaI (aq)
NO3-
L
1
2

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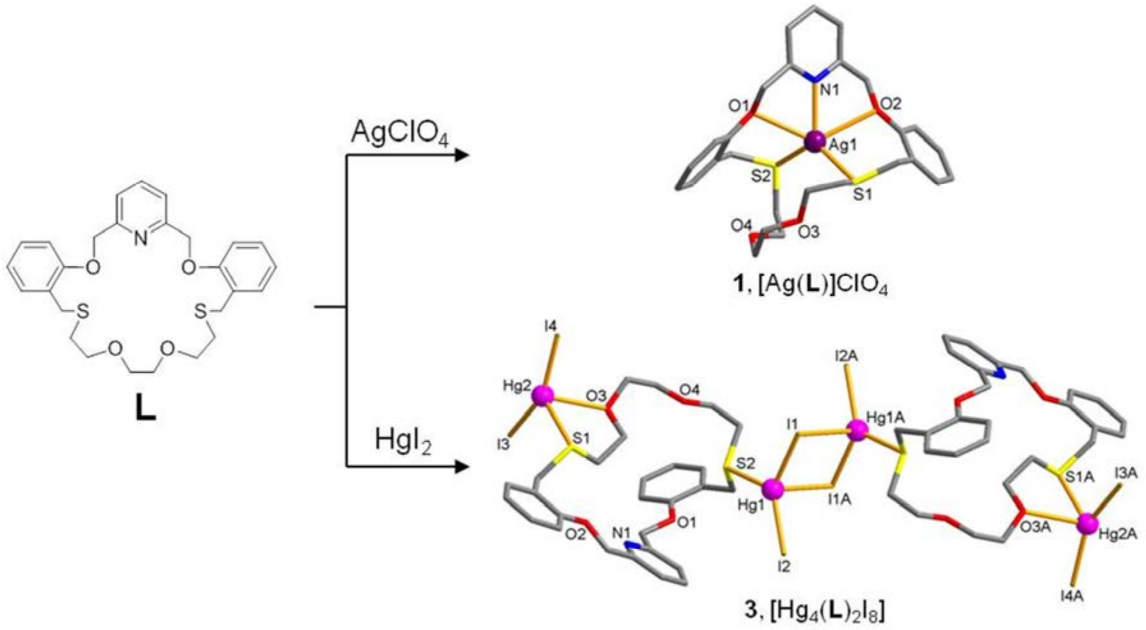
Tight and Loose Fits: Silver(I), Copper(I), Mercury(II), and Cadmium(II) Complexes with an Over-Size Macrocycle

신민경 주희영 이심성*

경상대학교 화학과

We propose a 23-membered NO_4S_2-donor macrocycle, L, which employs a pyridine subunit to accommodate metal cation inside the cavity and two benzo subunits to enhance the structural rigidity. L is somewhat semi-flexible due to the consecutive SOOS segment including the bridge heads for the exocyclic coordination. As mentioned, L incorporating the tight fit and loose fit parts toward a wide range of metal ions could be expected as a candidate for uptake and releasing processes for the metal species. In this presentation, synthesis and structural characterization of L and its complexes are reported. First, reactions of L with $AgClO_4$ and $Cu(ClO_4)_2 \cdot 3H_2O$ afforded typical endocyclic 1:1 complexes $[Ag(L)]ClO_4$ (1) and $[Cu^I(L)]ClO_4$ (2). An NMR titration of the formation of 1 confirmed that the Ag^+/L stoichiometry of 1:1 found in the solid state is also maintained in solution. The reaction of mercury(II) iodide with L yielded a unique discrete 4:2 (metal-to-ligand) complex of formula $[Hg_4(L)_2I_8]$ (3, see below). When a mixture of CdI_2 and HgI_2 was used in the reaction with L, a discrete type complex with two separated parts of formula $[Cd(L)I]_2[Hg_2I_6]$ (4) was isolated.



L

1, [Ag(**L**)]ClO$_4$

3, [Hg$_4$(**L**)$_2$I$_8$]

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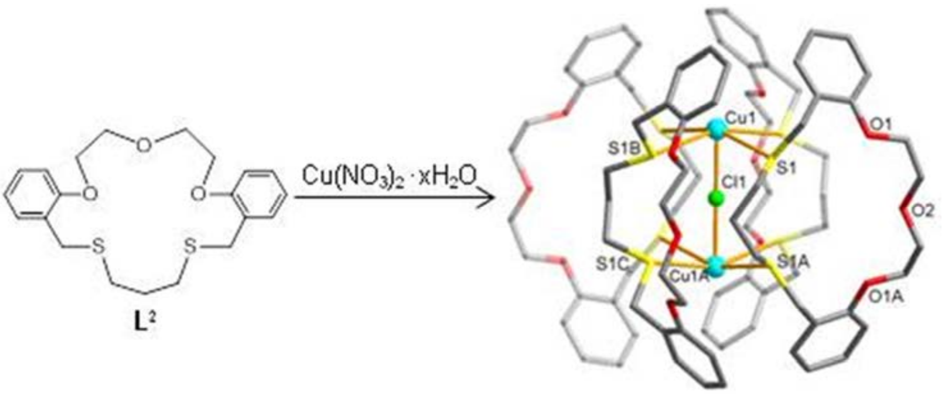
Ligand-Directed Supramolecular Complexes of O_3S_2-Macrocycles with Different Exo-Coordination Modes

최한별 류현수 이심성*

경상대학교 화학과

As a programmed approach toward the self-assembly of new types of metallosupramolecules of macrocyclic ligands, a 17-membered (L^1) and an 18-membered (L^2) O_3S_2-macrocycles with different $S\cdots S$ distances were synthesized. In the complexation of L^1 with HgI_2, a 1:2 complex $[Hg(L^1)_2I_2]$ (1) and a 1:1 complex $[Hg(L^1)I_2]$ (2) with different coordination environments were isolated as a kinetic (1) and a thermodynamic controlled (2) products. Reaction of L^1 with CuI yielded a 2:2 complex $[(Cu_2I_2)(L^1)_2]$ (3), with two macrocycles sandwiching an exodentate rhomboid dimer cluster, Cu_2I_2. Reactions of L^2 with mercury(II) halides yielded isostructural 1-D coordination polymer of type $[Hg(L^2)X_2]_n$ (4a: X = Br and 4b: X = I). While, same reaction with CuI afforded an emissive double-stranded 1-D polymeric complex, $[(Cu_4I_4)(L^2)_2]_n$ (5), in which ligands are linked by a cubane-type Cu_4I_4 cluster. Unlike 4 and 5, copper(II) nitrate gave a unique 2:4 complex $[Cu_2(L^2)_4Cl](NO_3)_3$ (6) (see below). The dicopper(II) shaft and each macrocyclic blade are doubly connected by Cu-S bonds to generate a four-bladed windmill structure with C_4 symmetry.



6,
Four-bladed windmill
type 2:4 complex

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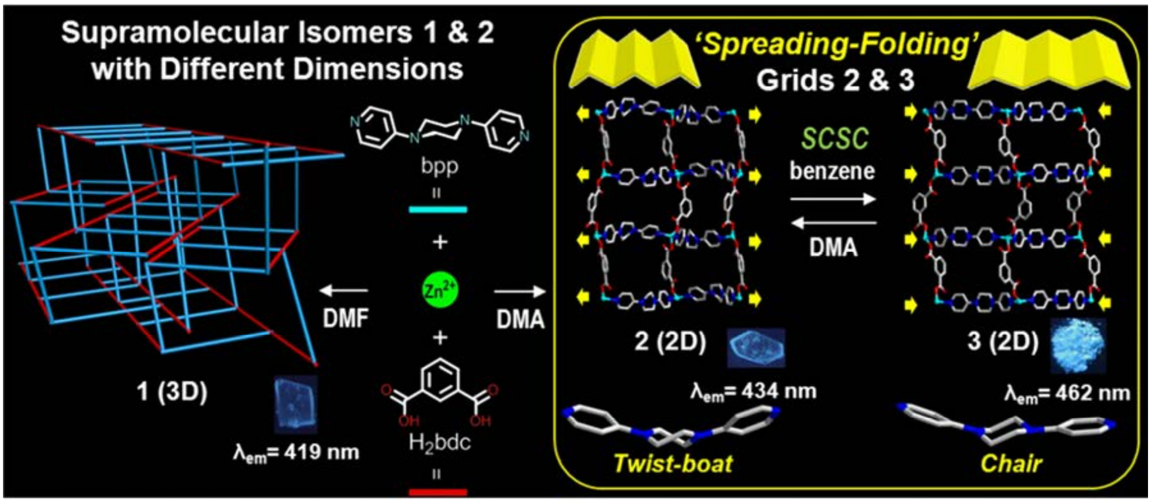
Supramolecular Isomers Accompanying Dimensional Change and Reversible Single-Crystal to Single-Crystal Transformation

주희영 박인혁 이심성*

경상대학교 화학과

Due to the intrinsic semi-flexible nature of the piperazine subunit, 1,4-bis(4-pyridiyl)piperazine (bpp) as a bischelating ligand can possess several conformations. Since the bpp ligand is multitopic, it could provide excellent potential for the construction of the new types of coordination frameworks. In connection with this reason, bpp was chosen as organic building blocks. Solvent-directed formations of a two-dimensional (2D) and a 3D supramolecular isomers and a reversible single-crystal to single-crystal (SCSC) transformation of the former one by solvent-exchange are reported. Solvothermal reaction of $Zn(NO_3)_2 \cdot 4H_2O$, bpp, and benzene-1,3-dicarboxylic acid (H_2bdc) in DMF afforded a self-penetrated 3D MOF, $\{[Zn_2(bpp)_2(bdc)_2] \cdot 4DMF \cdot 4H_2O\}_n$ (1), adopting a firewood pilling structure. When the above synthetic procedure was repeated employing DMA as a solvent, a 2D coordination polymer, $\{[Zn_2(bpp)_2(bdc)_2] \cdot 4DMA \cdot 6H_2O\}\}_n$ (2) was obtained whose structure shows a square grid topology as a supramolecular isomer of 1. The solvent-exchange-mediated SCSC transformation induced by benzene or DMA reversibly converts 2 into another square grid $\{[Zn(bpp)(bdc)] \cdot 2.5C_6H_6\}\}_n$ (3), which accompanies the spreading-folding motion of the square grid structure associated with the conformational change of bpp from twist-boat to chair form.


Supramolecular Isomers 1 & 2
with Different Dimensions
bpp
+
Zn2+
+
H2bdc
DMF
DMA
1 (3D)
λem= 419 nm
'Spreading-Folding'
Grids 2 & 3
SCSC
benzene
DMA
2 (2D)
λem= 434 nm
3 (2D)
λem= 462 nm
Twist-boat
Chair

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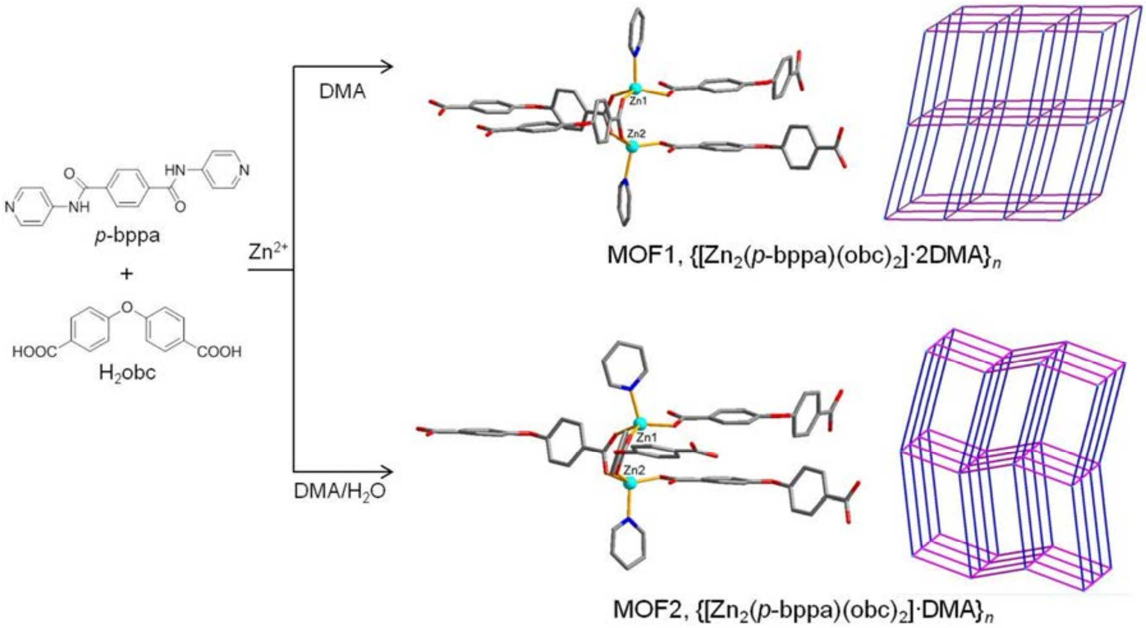
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-Dependent Supramolecular Isomers of 3D Zn(II) MOFs Derived from Binary Ligands

이은지 박기민[1] 이심성*

경상대학교 화학과 [1]경상대학교 기초과학연구소

We report the solvent-dependent zinc(II) supramolecular isomers MOF1 and MOF2, derived from a mixture of bis(amidopyridine) ligand (*p*-bppa) and dicarboxylate ligand (H_2obc= 4,4′-oxybisbenzoic acid). MOF1, $\{[Zn_2(p\text{-bppa})(obc)_2]\cdot 2DMA\}_n$, isolated from DMA shows a 3-fold interpenetrated 3D pillared-layer framework in which the Zn-obc square-grid layers are pillared by *p*-bppa ligands. Interestingly, when DMA/H_2O (2:1) was used instead of DMA solvent, we isolated MOF2, $\{[Zn_2(p\text{-bppa})(obc)_2]\cdot DMA\}_n$, which also shows a similar pillared-layer structure but its 3D framework is much more distorted than that in MOF1 due to the different orientation of one obc ligand in the dinuclear zinc(II) SBU (*see below*). In addition, MOF1 and MOF2 exhibit bright-blue emission (λ_{em} = 439 and 472 nm, respectively) originated from metal-ligand charge transfer (MLCT).


p-bppa
+
H2obc
HOOC
COOH
NH
HN
N
O
Zn2+
DMA
DMA/H2O
Zn1
Zn2
MOF1, {[Zn2(p-bppa)(obc)2]·2DMA}n
MOF2, {[Zn2(p-bppa)(obc)2]·DMA}n

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발표분야: 무기화학
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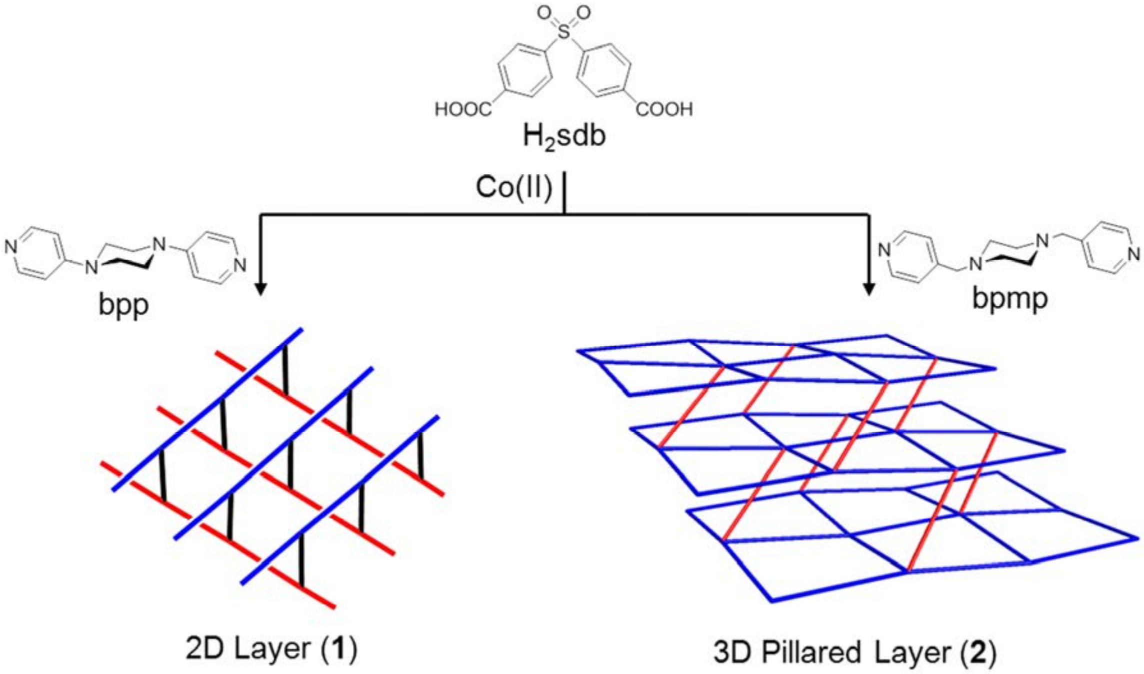
Co(II) and Zn(II) Coordination Polymers based on Dipyridyl Piperazine Ligands with Different Flexibility

주희영 이심성*

경상대학교 화학과

The flexibility effect of dipyridyl piperazine ligands, bpp and bpmp, on the resulting MOF structures is reported. Under the solvothermal condition, the reactions of H_2sdb with cobalt(II) or zinc(II) in the presence of bpp or bpmp afforded four coordination polymers (1-4). Complex 1, $\{[Co_3(Hbpp)_2(sdb)_4(\mu_2\text{-}H_2O)_2]\cdot 4H_2O\}_n$, shows a 2D structure in which a trinuclear cobalt(II) cluster SBU and sdb ligands are extended to generate a grid-type layer (see below). Notably, one side of bpp ligand is monoprotonated and acts as monodentate ligand which occupies the axial position of the terminal Co atom. While, bpmp forms a 3D pillar-layered complex 2, $\{[Co_2(bpmp)_{1.5}(sdb)_2(DMF)(\mu_2\text{-}H_2O)]\}_n$, with the 2D layers being pillared by bpmp on the skew. In zinc(II) complexation, bpp gave a self-catenated 3D complex 3, $\{[Zn_2(bpp)_2(sdb)_2]\cdot 2DMA\}_n$. While, bpmp resulted in the formation of a 3D pillar-layered framework $\{[Zn(bpmp)(sdb)]\cdot DMF\cdot 2H_2O\}_n$ (4) in which the 2D layers formed by Zn(II), bpmp, and sdb are further pillared by bpmp ligands.


HOOC
COOH
H$_2$sdb
Co(II)
bpp
bpmp
2D Layer (**1**)
3D Pillared Layer (**2**)

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Silver(I) Coordination Polymers of an NO_2S_2-Macrocycle: Anion-Controlled Dimensional Changes and Anion-Exchange

이은지 박기민[1] Mari Ikeda[2] Shunsuke Kuwahara[3] Yoichi Habata[3,*] 이심성[*]

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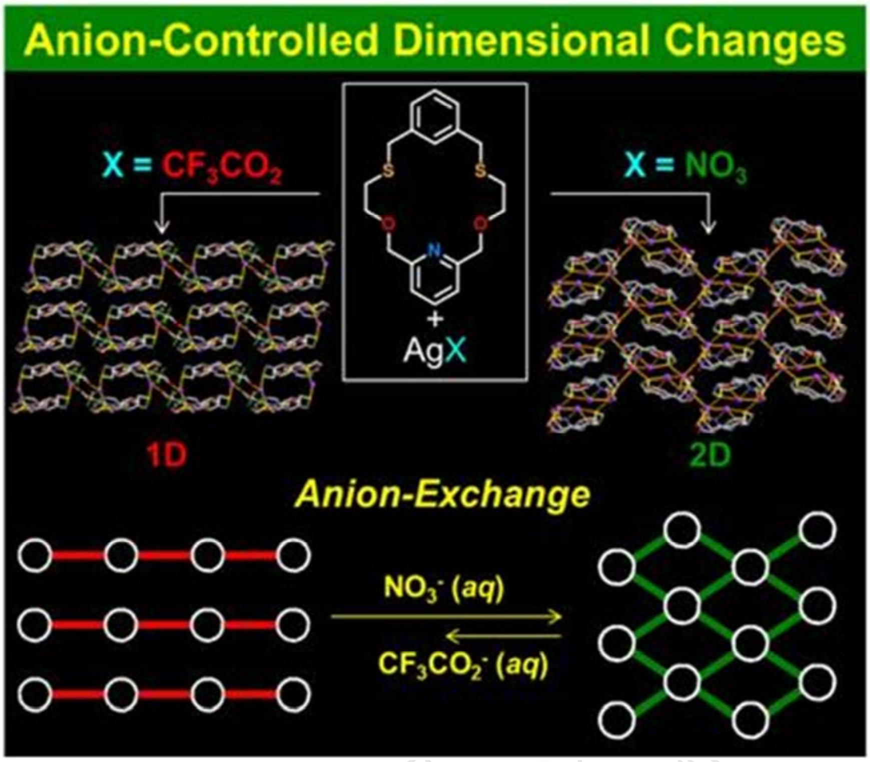
A rationally designed NO_2S_2-macrocycles L which employs an NS_2 donors in one side to accommodate a metal cation in the cavity (endo-coordination) and the two sulfur donors for the exo-coordination was synthesized. The proposed approach allowed us to prepare endo/exocyclic multidimensional coordination polymers. As might be expected, reaction of L with AgX (X= PF_6^-, $CF_3CO_2^-$, NO_3^-, and $CF_3SO_3^-$) afforded the complexes $[Ag_2L_2](PF_6)_2$ (1), $[Ag_4L_2(CF_3CO_2)_4]_n$ (2), $[Ag_4L_2(NO_3)_4]_n$ (3), and $\{[Ag_3L_2(CF_3SO_3)_2]CF_3SO_3\}_n$ (4) that adopt cyclic dimer, 1D-, 2D-, and pseudo 3D network structures, respectively, with the structure adopted depending on the coordination ability and coordination modes of the anion used. Interestingly, quantitative anion-exchange accompanying an irreversible structural conversion from 2, 3, or 4 to 1 was observed in the crystalline state by the powder X-ray diffraction (PXRD) and IR spectroscopy. The anion-exchange of $CF_3CO_2^-$ in 2 with NO_3^- to yield 3 is noteworthy because it undergoes quantitatively in the crystalline state, accompanying the dimensional increase from 1D to 2D. Thus, a mechanistic process from 2 ($CF_3CO_2^-$, 1D) to 3 (NO_3^-, 2D) was also proposed (see above Scheme).


Anion-Controlled Dimensional Changes
X = CF_3CO_2
X = NO_3
S
S
O
O
N
+
AgX
1D
2D
Anion-Exchange
NO_3^- (*aq*)
$CF_3CO_2^-$ (*aq*)

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Supramolecular Isomers Exhibiting Different Photoreactivity of [2+2] Cycloaddition: Double and Single Dimerizations

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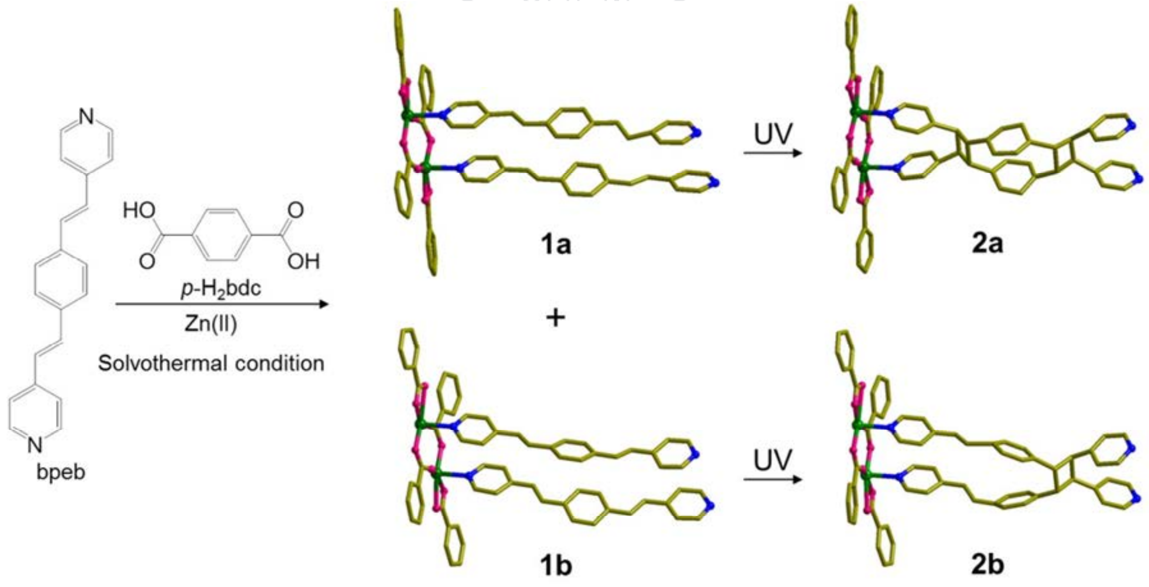
We describe two 3D Zn(II) supramolecular isomers (1a and 1b) derived from an olefinic dipyridyl ligand 1,4-bis[2-(4'-pyirdyl)ethenyl]benzene (bpeb) and 1,4-benzenedicarboxylic acid (H_2bdc) showing different photoreactivity. A mixture of pale yellow plate-shaped crystals of $[Zn_2(bdc)_2(bpeb)_2]\cdot 4DMA$ (1a) and pale yellow needle-shaped crystals of $[Zn_2(bdc)_2(bpeb)_2]\cdot 2DMA$ (1b) adopting 2-fold interpenetrated 3D MOFs were obtained from solvothermal condition. The bpeb ligands aligned in an in-phase manner in two-fold interpenetrated isomers 1a and 1b undergo [2+2] cycloaddition reaction via single-crystal to single-crystal (SCSC) manner to the double dimerized 2a and the single dimerized 2b, respectively.



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Dipyridyl-N_4-Macrocyclic Pillar Ligand for Discrete and Polymeric Complexes

류현수 Leonard F. Lindoy[1,*] 이심성[*]

경상대학교 화학과 [1]School of Chemistry, The University of Sydney

Dipyridyldibenzotetraaza[14]annulene[1] (H_2L) has an extended 14-membered dibenzomacrocyclic structure bearing two appended terminal pyridyl groups. It is potentially ditopic towards metal binding since it incorporates both an in-ring N_4-donor set and the exo-ring pyridyl donors.[2,3] Six complexes have been synthesized and structurally characterized: $[Ni(L)]_2$ (1), $[Co(L)]_2$ (2), $[Co(L)]_n$ (3), $\{[Co_4(L)_2(bpdc)_2]\cdot 3DMF\cdot H_2O\}_n$ (4), $\{[Cd_2(H_2L)_2(bpdc)_2]\cdot xSolvent\}_n$ (5), and $\{[Zn(H_2L)(bdc)]\cdot DMF\cdot 3H_2O\}_n$ (6) all based on the ditopic macrocyclic ligand, H_2L in the absence and presence of dicarboxylate coligands. Complexes 1 and 2 are isostructural and square-planar metal ions occupying the macrocyclic cavity bound to the N_4-donor set of the macrocycle in its doubly deprotonated form. In 3, the Co(II) center again occupies the macrocyclic cavity, but in this case one axial site is occupied by a pyridyl nitrogen from a second ligand complex, resulting in the formation of an infinite zigzag 1D structure. In addition, the reaction of H_2L with $Co(NO_3)_2\cdot 6H_2O$ in the presence of H_2bpdc resulted in a pillar-layered 3D framework (4). In 4, the 3D framework was generated by pillaring the 2D layers formed by H_2bpdc with two macrocyclic complex units arranged side by side. Same reaction with $Cd(NO_3)_2\cdot 4H_2O$ resulted in a pillar-layered 3D framework (5), but in this case each Cd(II) center does not occupy a macrocyclic cavity. Reaction of H_2L with $Zn(NO_3)_2\cdot 4H_2O$ and H_2bdc afforded a 2D coordination polymer (6) in which the H_2L units link 1D $[(bdc)\text{-}Zn\text{-}(bdc)\text{-}Zn\text{-}]_n$ backbones.

References

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[2] Mulyana, Y. *et al.*, *J Incl Phenom Macrocycl Chem* 2011, *71*, 455.

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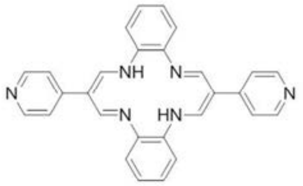
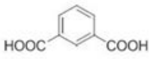
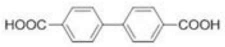


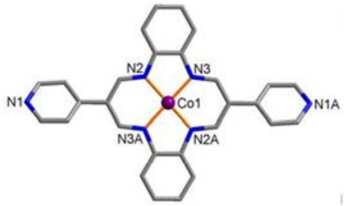
H$_2$L



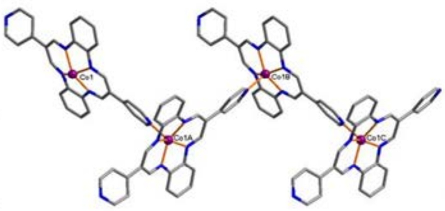
H$_2$bdc



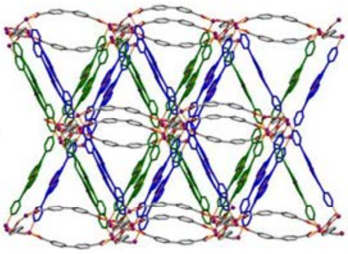
H$_2$bpdc



Endocyclic Monomer Complex (**2**)



Zigzag 1D Polymer (**3**)



Pillar-layered 3D Framework (**4**)

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal growth and structural and magnetic phase transitions of $(C_6H_5CH_2CH_2NH_3)_2(Mn_xCu_{1-x})Cl_4$ (Mn,Cu-PEA) mixed crystals

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고려대학교 화학과 [1]한국원자력연구소 중성자과학연구부 [2]한국원자력연구원 중성자과학연구부

$(C_6H_5CH_2CH_2NH_3)_2MnCl_4$ (Mn-PEA) and$(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) belong to the layered inorganic-organic systems of the general formula AMX_4 , where A = organic cation, M = divalent metal, and X = halides. These systems are of special interest because of their low-dimensional magnetic properties (de Jongh, 1986). Although both crystals are crystallized in a same orthorhombic Pbca structure (No.61), with a = 7.2099(9), b = 7.2664(9), c = 38.238(5), and Z = 4 at room temperature for Cu-PEA (Polyakov et al., 2012) and with a = 7.2075(9), b = 7.3012(14), c = 39.413(6), and Z = 4 at room temperature for Mn-PEA, respectively. However, the magnetic properties are significantly different (Cu-PEA is ferromagnetic and Mn-PEA is antiferromagnetic). To test the miscibility of the two different crystals and to check the magnetic properties and the phase transition temperature changes, we tried to synthesize the mixed crystals of (Mn,Cu)-PEA with various chemical ratio. In this presentation, we will briefly report the results of the thermal analysis and magnetic properties.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Plasmon Resonance Effects of Pt Nanoparticles on Light-driven Hydrogen Photoproduction from Rh-H Species

김진흥

이화여자대학교 화학·나노과학과

Although the decomposition of formic acid using molecular metal complexes has been poorly studied previously, several reports in this area have been published recently. Most studies with molecular metal catalysts reported the non-photochemical decomposition of formic acid, and often use thermal energy to achieve high conversion rates and yields. More studies of photochemical systems containing molecular metal catalysts for the HCOOH decomposition are required to understand their photocatalytic mechanisms and develop efficient catalytic systems utilizing one of the major sources of hydrogen. Photochemical hydrogen production is carried out using molecular Rh complexes and formate in the presence of platinum nanoparticles (PtNPs) in aqueous solution. Visible light-driven photocatalytic reactions for hydrogen production with and without NAD+ follow two different pathways. The chemically generated NADH is sequentially oxidized by PtNPs upon photoactivation of eosin Y to produce hydrogen. However, hydrogen is also produced in photoreactions of the Rh catalyst and PtNPs with formate in the absence of NAD+ and eosin Y. The sencond pathway for hydrogen production in the absence of NAD+ derives from a direct proton-coupled electron transfer of the Rh(III)-hydride intermediate generated from the Rh catalyst and formate upon photoactivation of PtNPs.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric Assay of Cyanide Ions Using a Thioamide-based Probe Containing Phenol and Pyridyl Groups

김진홍* 김 철[1]

이화여자대학교 화학·나노과학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

The selective assay of cyanide ions with a thioamide compound (HNPTU) containing phenol and pyridine as a chemosensor is reported using absorbance changes in a buffered aqueous solution (50 mM HEPES, pH 7.4) containing ethanol. Upon treatment with cyanide ions, the colorless solution of HNPTU turned to yellow. No significant changes were observed with other comparable anions, such as F-, Cl-, Br-, I-, and CH3COO-. The color change of HNPTU upon treatment with CN- was maintained even in the presence of the comparable monovalent anions. The complex stability constant (Ka = 2.6 x 103) for the stoichiometric 1:1 complexation of HNPTU with cyanide ions was obtained based on absorbance titrations. The interaction of HNPTU with cyanide ions was proposed to be deprotonation, as shown by NMR and Cu(II) treatment experiments.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Single Crystal Neutron Diffraction techniques for Crystal Structure Investigations

오인환

한국원자력연구소 중성자과학연구부

Single crystal neutron diffraction has attracted special interest to acquire detailed information on both crystal structures and magnetic structures. The high resolution in the reciprocal space is necessary to determine the accurate structure parameters which are essential for the understanding of structure research of complex systems, for example, anhamornic effects in ionic conductors, dynamic and static mean-square displacement parameters in real crystals, detailed hydrogen distribution in hydrogen bonds, dynamical and static hydrogen atoms disorder, molecular-group rotations. Magnetic neutron diffraction on single crystals can give an opportunity to investigate magnetic structures including non-collinear and helical spin structures and spin densities as well as magnetic phase transitions. Several single crystal neutron diffraction results are presented in order to show the scientific potential of the neutron single crystal technique.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Current Status of Supramolecular Crystallography Beamline in Pohang Light Source

신종원 김대웅[1] 문도현[*]

포항가속기연구소 빔라인운영부 생명화학소재팀 [1]경북대학교 자연과학대학 화학과

The Supramolecular Crystallography beamline at Pohang Light Source in Korea has been designed to operate in the photon-energy range of 6~20 keV (2.0 ~ 0.61 Å) based on a bending magnet in PLS II. It is dedicated to single crystal crystallography with inorganic/organic, supramolecule and MOF crystals. The experiment station is equipped with high speed and high sensitivity of an ADSC Quantum Q210 area detector containing a 210 mm^2(4096 x 4096 pixel) detection area, high accuracy three-axis air-bearing type goniometer, a cryojet for cooling sample using a liquid nitrogen controlled 90~500 K range. Recently, we install the high power laser (300~2100 nm) and xenon lamp (300 W) for catalytic and photoreactivity stduies. We will provide new technique and challenge works for your extreme researches. The status of beamline, equipments and several fabrication techniques will be presented on this poster.

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발표분야: 무기화학

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Solvent Dependent Structures of hexaazamacrocyclic copper complex with 2,7-naphthalenedicarboxylic acid

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The coordination chemistry of the macrocyclic ligands and their interaction with metal ions have attracted extensive interest due to their potential applications in chemistry, material science, and metalloenzymes. In particular, macrocyclic complexes involving vacant sites in an axial position are good candidate for assembling supramolecular materials, with potential application such as gas storage materials as well as catalyst for copolymerization of carbon dioxide and cyclohexene oxide. Thus, first, as building blocks for supramolecular chemistry, novel copper(II) hexaaza macrocyclic complex, $[Cu(C_{16}H_{18}N_6)(ClO_4)_2]$ (1), containing butyl pendant groups has been synthesized. Second, from the self-assembly of 1 with deprotonated 2,7-naphtalendicarbixylic acid, 2,7,-NDC^{2}-, mononuclear complex of $[Cu(C_{16}H_{38}N_6)(H_2O)_2](C_{12}H_6O_4)$ (2) and 1-D chain polymer of $[Cu(C_{16}H_{38}N_6)(C_{12}H_6O_4)]\cdot 2CH_3OH$ (3) have been prepared, respectively. Interestingly, when dipping 2 into a DMF/MeOH mixed solvent, 3 can be formed. In this poster, we will explain the detailed preparation, crystal structure, and magnetic properties as well as interesting coordination chemistry.

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In Situ Synchrotron X-ray Crystallography of CO_2 Adsorption/Desorption on Single Crystal of the Functionalized Coordination Polymer

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The studies on the coordination polymers have been attracted much attention in chemistry, material science and the chemical industry because of their potential and/or practical applications for molecular recognition, magnetism, gas sorption and heterogeneous catalysis. In particular, the well-defined porous channels found in coordination polymers are ideal for the uptake of guest molecules, such as CO_2, CH_4, N_2 and H_2 gases and can also show high selectivity for particular species from mixture materials. Sorption properties of coordination polymers or metal organic frameworks (MOFs) have been widely studied, however, researches related with sorption states of gas molecules in single crystal are very rare. Recently, new coordination polymer of zinc(II) complex, $[(tpmd)Zn(NCBH_3)_2]_n \cdot x$ guests (1) , has been prepared by the self-assembly of Zn(II) species and $NCBH_3$ counterions with *N,N,N´,N´*-tetra-4-pyridyl-methylenediamine (tpmd) in an oxygen-free dry box. The channels of 1 display internal voids, each being capable to accept several gas molecules. In particular, to investigate the CO_2 sorption sites and locations in 1, we have determined *in situ* the structure of 1 with sorbed CO_2 molecules at 1 bar and 196, 273 and 298 K, respectively.In this poster, we will explain the detailed preparation, crystal structure, and *in situ* gas sorption studies conducted on 2D beamline at Pohang Light Source by single crystal X-ray diffraction analysis as well as interesting coordination chemistry.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses, crystal structures, and magnetic properties of tetranuclear cobalt(II) complexes with *N*-(2-pyridylmethyl)iminodipropanolate

정아림 신종원[1] 민길식[2,*]

경북대학교 화학과 [1]포항가속기연구소 빔라인운영부 생명화학소재팀 [2]경북대학교 사범대학 화학교육과

The synthesis and characterization of multinuclear transition metal complexes have received much interested because of their chemical, electronic and structural properties. Recently, we have prepared two new cobalt(II) compounds, $[Co_2(pmidp)(OAc)_2]_2\cdot 2MeOH$ (1) and $[Co_2(pmidp)(NO_3)_2]_2\cdot MeCN$ (2), by the $Co(OAc)_2\cdot 4H_2O/Co(NO_3)_2\cdot 6H_2O$ with *N*-(2-pyridylmethyl)iminodipropanol (H_2pmidp) in MeCN/MeOH under an aerobic condition. These compounds have been investigated by single crystal X-ray diffractometry and magnetochemistry. The structures of 1 and 2 consist of a tetranuclear Co_4O_4 core in a cubane structure. In structure 1, two cobalt(II) ions are each coordinated with two N atoms and three O atoms from ligands and an O atom from an acetate anion. The others are each coordinated with three O atoms from ligands and three O atoms from acetate anions. Complexes 1 and 2 have same coordination environments but anions are different (OAc^- for 1, NO_3^- for 2). 1 displays antiferromagnetic interactions between the cobalt(II) ions. In this poster, we will present the detailed preparation of the ligand and cobalt compounds, crystal structures, magnetic properties.

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Phosphorescent Iridium(III) Cyclometalates with Substituted o-Carboranes

이영훈 박재영[1] 김민지[1] 이민형[1,*]

울산대학교 기초과학연구소 (EHSRC) [1]울산대학교 화학과

A series of [(C^N)$_2$Ir(acac)] complexes [{5-(2-RCB)ppy}$_2$Ir(acac)] (R= H, alkyl (Me, *i*Pr, *i*Bu), and aryl (Ph, $CF_3C_6H_4$, C_6F_5)) with various 2-R-substituted o-carboranes at the 5-position in the phenyl ring of the ppy ligand were prepared and characterized by X-ray diffraction studies, spectroscopic analyses and theoretical calculations. The phosphorescence efficiency varies from highly emissive (Φ_{PL}= 0.8 for R = H, alkyl) to poorly emissive (R = aryl) depending on the 2-R substituent and the polarity of the medium. Theoretical studies suggest the non-emissive nature of 2-arylsubstituted complexes is mainly attributed to the large contribution of the LUMO in the S1 excited state from CB unit and the variation in the C-C bond length between the S_0 and T_1states by steric effect of 2-substituent and the polarity of the solvent. The solution-processed EL devices incorporating the complexes with Me and iBu substituents, respectively as emitters also display good performance.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical and Fluoride Binding Properties of 2-R-Substituted *o*-Carborane?Triarylborane Dyads

이형동 이영훈[1] 김태원 이민형*

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Although fluoride anion plays an important role in dental care and osteoporosis therapy, the fluoride-ion recognition has attracted great attention due to detrimental effects on the body when it was taken in excess. One of challenging candidates for detecting fluoride ion selectively is to use triarylboranes because they have high Lewis acidity allowing for binding fluoride strongly. To increase the fluoride affinity of triarylborane, we introduced *o*-carborane on the *meta*-position of phenyl ring of the triarylborane. Furthermore, substitution effect of various alkyl (H, Me, ^{i}Bu) or aryl (C_6H_5, $CF_3C_6F_4$) groups incorporated in the 2-position of carborane unit was also investigated. Indeed, introduction of *o*-carborane into the triarylboranes enhanced the Lewis acidity along with high fluoride affinity. After degradation of the carboranyl cage from *closo*- to *nido*-form by fluoride, the emission bands of all triarylboranes were red-shifted, leading to turn-on sensing phenomena toward fluoride. All compounds were characterized by X-ray single crystal diffraction determination, spectroscopic analysis, and theoretical calculations.

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Synthesis and Lewis Acidity Enhancement of Triarylborane by Appended Phosphine Oxide Groups

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A series of mono-, di-, and tri-phosphine oxide substituted triarylboranes, Mes_2BAr (1), $MesBAr_2$ (2), and BAr_3 (3) (Ar = 4-(Ph_2PO)-2,6-Me_2-C_6H_2) were prepared to investigate the effect of a phosphine oxide group (Ph_2PO) on Lewis acidity enhancement of triarylboranes. An X-ray crystal structure of 3 revealed peripheral decoration of Ph_2PO groups with a C_3-axis perpendicular to the trigonal boron center. UV/Vis absorption and PL spectra indicated a significant contribution of π(Mes or phenylene)$\rightarrow p_\pi$(B) charge transfer in the lower-energy electronic transition. Cyclic voltammetry measurement showed apparent LUMO stabilization by introduction of phosphine oxide groups, the extent of which gradually increased with the increasing number of phosphine oxide groups. Lewis acidity enhancement was also supported by the gradual increase in fluoride ion affinity in the order 3 > 2 > 1. Details of synthesis, characterization, and fluoride binding properties will be discussed with theoretical calculations.

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Reactivity Comparison of Cobalt(III)-Peroxo and Cobalt(III)-Hydroperoxo Complexes

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Metal-dioxygen adducts, such as metal-peroxo and -hydroperoxo species, are key intermediates that observed in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. Previously, manganese(III)-hydroperoxo complex, $[Mn(III)(TMC)(OOH)]^{2+}$ (TMC=1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane) was characterized and reactivity of this intermediate has been shown electrophilic character. In this work, using Me_3-TPADP (Me_3-TPADP=3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane) ligand, $[Co(Me_3\text{-TPADP})(CH_3CN)_2]^{2+}$ was synthesized and characterized. Cobalt-peroxo complex, $[Co(Me_3\text{-TPADP})(O_2)]^{+}$, was synthesized with H_2O_2 in the presence of triethylamine. Upon protonation, Co(III)-peroxo complex was converted into a Co(III)-hydroperoxo complex, $[Co(Me_3\text{-TPADP})(OOH)(CH_3CN)]^{2+}$. Interestingly, the Co(III)-hydroperoxo complex shows both nucleophilic ans electrophilic reactivity. In addtion, nucleophilic reactivity of Co(III)-hydroperoxo complex is higher than that of Co(III)-peroxo complex.

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A new Zr (IV) based metal-organic framework comprising sulfur-containing ligand: Enhancement of CO_2 and H_2 storage capacity

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For better understanding of proton conduction mechanism, proton conduction dynamics was investigated by ^2H NMR study and spectroscopical analysis. For application of metal-organic frameworks (MOFs) in gas storage application, enhancement of gas sorption capacity is one of the most important issues for industrial application. It is belied that incorporation of strong gas sorption sites in the framework can increase gas sorption capacity in MOFs. Herein, we report a new MOF comprising a sulfur-containing ligand (Zr-btdc) for incorporation of electronegative heteroatoms as a strong gas-binding site. Interestingly, despite smaller surface area of the Zr-btdc, it showed higher gas (H_2 and CO_2) sorption capacity than a heteroatom free isostructural framework (UiO-67). It is expected that incorporation of a sulfur atom on ligand makes similar effect to sulfur doping on pore surface of the framework. Electrostatic potential analysis result showed that heteroatom incorporation in the ligand could increase electronegativity of framework surface. Therefore, the incorporation of sulfur atom on MOF can make sulfur-doping effect on framework surface resulting in enhancement of gas sorption capacity. Details of our recent work will be presented.

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Tuning the reactivity of zinc ion-bound iron(III)-peroxo complex by water molecule

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Redox-inactive metal ions play important roles in tuning chemical properties of metal-oxygen intermediates. Herein we report the effect of water molecules on the redox properties of nonheme iron(III)-peroxo complexes binding redox-inactive metal ions. The coordination of water molecule to Zn^{2+} ion in $(TMC)Fe^{III}-(O_2)-Zn^{2+}$ ($1-Zn^{2+}$) decreases the Lewis acidity of Zn^{2+} ion, resulting in the decrease of the one-electron oxidation and reduction potentials of $1-Zn^{2+}$. This further changes reactivity of $1-Zn^{2+}$ in oxidation and reduction reactions; no reaction occurs upon addition of an oxidant (e.g., CAN) to $1-Zn^{2+}$, whereas $1-Zn^{2+}$ coordinating water molecule, $(TMC)Fe^{III}-(O_2)-Zn^{2+}-(OH_2)_2$, releases the O_2 unit in the oxidation reaction. The present results provide the first biomimetic example showing that water molecule at the active sites of metalloenzymes may participate in tuning the redox properties of metal-oxygen intermediates.

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Synthesis, characterization and reactivity of a nonheme Mn(III)-acylperoxo complex

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Metastable Mn-acylperoxo species, which are the precursors of high-valent Mn-oxo species, are proposed to be a key intermediate in biological and chemical oxidation reactions. In the present study, a Mn(III)-acylperoxo intermediate was generated by reacting Mn(II)(C1)$(OTf)_2$ complex bearing a tetradentate N4 ligand (C1 = 1,2-bis(2-(1-methyl-1*H*-benzo[*d*]immidazol-2-yl)pyrrolidin-1-yl)ethane) with peroxybenzoic acid (PBA) and characterized with various spectroscopic techniques. The reactivity of Mn(III)-acylperoxo intermediate was investigated in the oxidation of thioanisole derivatives and styrene derivatives (i.e., oxygen atom transfer (OAT) reactions). The present study provides the biomimetic example demonstrating that Mn-acylperoxo species possesses an electrophilic character and is able to conduct directly the OAT reactions.

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Characterization and Reactivity of Ni(II)-Hydroperoxo Species Bearing macrocyclic TMC ligands

신선영 남원우[1,*]

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Mononuclear metal?dioxygen species ($M\text{-}O_2$) have been implicated as key intermediates in the catalytic cycles of dioxygen activation by heme and non-heme metalloenzymes. Previously, we have been reported that the synthesis and charectrization of metal-superoxo and -peroxo complexes by changing the ring size of the supporting TMC ligands. In this work, we will show the generation of Ni(II)-hydroperoxo species bearing 13- and 14-TMC ligands, by conversion of Ni(II)-surperoxo and Ni(II)-peroxo in presence of different base or/and acid. The characterization of Ni(II)-hydroperoxo species will be introduced with various spectroscopic methods such as UV-vis, ESI/CSI-MS, EPR, and resonance Raman spectroscopy. Furthermore, the reactivity of Ni(II)-hydroperoxo species bearing 13- and 14-TMC ligands will be here presented in the C-H bond activation (e.g., CHD) and oxygen atom transfer reaction(e.g., Ph_3P).

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Demonstration of Electrophilic as well as Nucleophilic Reactivity of Mononuclear Non-Heme Manganese(III)-Hydroperoxo Complex

전소현 이용민[1] 남원우[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 기초과학연구소 [2]이화여자대학교 화학과

Manganese(III)-peroxo and manganese(III)-hydroperoxo species have been invoked as key intermediates in the activation and formation of dioxygen (O_2) and the detoxification of reactive oxygen species by enzymes and their biomimetic compounds. We have shown that first example of dioxygen activation of manganese(II) complex bearing an N-tetramethylated cyclam (TMC) ligand in the presence of base, followed by protonation of an manganese(III)-peroxo to get the monomuclear manganese(III)-hydroperoxo complex $[Mn(III)(TMC)(OOH)]^{2+}$. Very recently, we have shown that the manganese(III)-hydroperoxo complex derived from protonation of an isolated manganese(III)-peroxo complex $[Mn(III)(TMC)(OOH)]^{2+}$. The Mn(III)-hydroperoxo intermediate is well characterized with various spectroscopic techniques like electronic absorption, resonance Raman, electron paramagnetic resonance, and X-ray absorption spectroscopy/extended X-ray absorption fine structure (XAS/EXAFS) as well as with density functional theory (DFT) calculations, showing the binding of a hydroperoxide ligand in an end-on fashion. Previously we have shown that $[Mn(III)(TMC)(OOH)]^{2+}$ is a competent oxidant in oxygen atom transfer (OAT) reactions. Now we have demonstrated that reactivity of Mn(III)-hydroperoxo complex in O-H bond activation by H-atom abstraction as well as the deformylation of aldehydes. These reactivity results demonstrate that the Mn(III)-hydroperoxo species are viable oxidants in both nucleophilic and electrophilic reactions by manganese-containing enzymes.

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Mechanistic Study on Non-Heme Iron Catalyzed Chlorine Dioxide Generation

박정민 남원우[1,*]

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The chlorine oxyanions (ClO_n^-, n = 1 - 4) spanning oxidation states of +1 to +7 have found diverse uses from bleaching agents to oxidizers in rocket fuels. Of chlorine oxyanions used for ClO_2 production, ClO_3^- is the common source. The primary commercial use of chlorine dioxide is as an oxidizing agent for pulp bleaching, water disinfection and treatment. However, because of the fault with instability of ClO_2, it is necessary for on-site production of ClO_2 for practical application. We have reported that non-heme manganese catalysts offer a new method for the preparation of pure chlorine dioxide for on-site use. In this work, we studied the reaction of non-heme iron complex, [Fe(III)(TAML)], with sodium chlorite in acetate buffer solution by spectroscopic methods. As the results, chlorine dioxide was produced in a good yield in the reaction of [Fe(III)(TAML)] complex with sodium chlorite and we found that the yield and rate of conversion from chlorite to chlorine dioxide by [Fe(III)(TAML)] complex is much greater than that obtained from manganese non-heme catalysts.

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Reaction of Salicylaldehyde with *N*-Cyanomethyl Groups Attached to a Tetraaza Macrocyclic Nickel(II) Complex

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대구대학교 화학과

Salicylaldehyde reacts with the *N*-CH_2CN pendant arms of $[NiL^1]^{2+}$ (L^1=2,13-bis(N-cyanomethyl)-3,14-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}0^{7.12}$]docosane) to produce $[NiL^2]^{2+}$ bearing both 1-hydroxy-2-aza-4-oxanaphthalene and 2-aza-4-oxanaphthalene rings. The heterobicyclic functional pendant arms of $[NiL^2]^{2+}$ are involved in coordination in the solid state and in various solvents. The nickel(Ⅱ) complex is quite stable in the solid state and in acidic aqueous solutions. In basic aqueous solutions, however, the complex is rapidly hydrolyzed to $[NiL^3]^{2+}$ bearing two *N*-CH_2CONH_2 pendant arms.

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Fused Heterocyclic N-donor Ligand Derived from Di(2-pyridyl)ketone and Its Coordination Mode towards Transition Metals

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이화여자대학교 화학나노 [1]이화여자대학교 기초과학연구소 [2]이화여자대학교 화학과

Multidentate N-donor ligands play many fundamental roles in chemical science. For example, often they are critical factors in transition metal-mediated reactions to achieve high efficiency, selectivity and robustness by providing the well-defined primary and secondary coordination sphere around the center of transition metals. From a viewpoint of bio-mimetic system, the well-defined coordination sphere given by a certain N-donor ligand is an essential requirement not only to maintain intrinsic functions of metalloproteins but also to reproduce the short-lived intermediates in synthetic systems. In particular, di(2-pyridyl)ketone has shown its versatility in developing the supporting N-donor ligands for bio-mimetic metal complexes. In this context, we have synthesized a fused heterocyclic multidentate N-donor ligand using the di(2-pyridyl)ketone as a starting material. We have also prepared transition metal complexes bearing the same ligand system to investigate their coordination mode and PL properties. In this presentation, structural characterization, spectroscopic properties and chemical reactivities of the metal complexes bearing a fused heterocyclic multidentate N-donor ligand will be discussed.

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Fabrication of Supported AuPt Alloy Nanocrystals with Electrocatalytic Activity through Exploitation of Conversion Chemistry of Layer-Deposited Pt2+ on Au Nanocrystal inside Silica Nanosphere

김성현 정화경[1] 김종원[1] 이인수[*]

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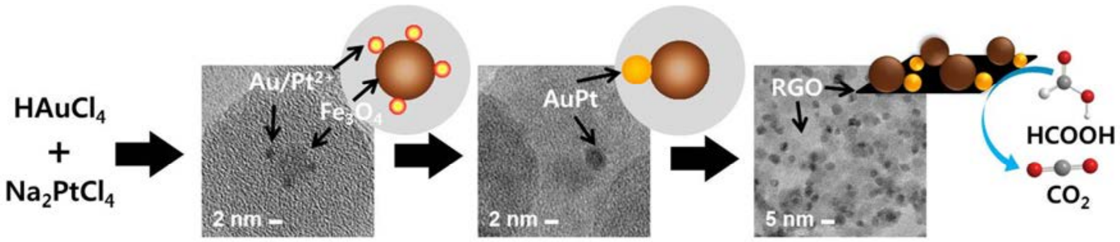
We report on the exploitation of the nano-confined conversion chemistry of the Au- and Pt-containing binary nanocrystal for developing the facile and controllable synthesis of surfactant-free AuPt nanocrystals with enhanced formic acid oxidation (FAO) activity, which can be stably and evenly immobilized on various support materials to diversify and optimize their electrocatalytic performance. In this study, an atomic layer of Pt^{2+} species was discovered to be spontaneously deposited *in-situ* on the Au nanocrystal generated from a reverse-microemulsion solution. The resulting Au/Pt^{2+} nanocrystal thermally transformed into a reduced AuPt alloy nanocrystal during the subsequent solid-state conversion process within the SiO_2 nanosphere. The alloy nanocrystals could be isolated from the SiO_2 in surfactant-free form and then dispersedly loaded on the carbon sphere surface, allowing for the production of a supported electrocatalyst that exhibits much higher FAO activity than commercial Pt/C catalysts. Furthermore, by involving Fe_3O_4 nanocrystal in the conversion process, the AuPt alloy nanocrystals could be grown on the oxide surface, improving the stability of supported metal catalysts, and then uniformly loaded on a reduced graphene oxide (RGO) layer with high electro-conductivity. This produced electrocatalytic $AuPt/Fe_3O_4/RGO$ nanocomposites whose catalyst-oxide-graphene triple-junction structure provides improved electrocatalytic properties in terms of both activity and durability in catalyzing FAO.


HAuCl$_4$
+
Na$_2$PtCl$_4$
Au/Pt^{2+}
Fe$_3$O$_4$
2 nm
AuPt
2 nm
RGO
5 nm
HCOOH
CO$_2$

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A colorimetric chemosensor for the sequential detection of copper(II) and cysteine

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A simple and easy-to-make colorimetric chemosensor 1 for the sequential detection of Cu^{2+} and cysteine was developed by combination of hydroxynaphthalene-2-carbaldehyde and diaminomaleonitrile. This sensor 1 exhibited an obvious color change from pale yellow to orange in the presence of Cu^{2+} in aqueous solution. Also, the resulting 1-Cu^{2+} complex sensed cysteine through naked-eye, showing recovery from 1-Cu^{2+} to 1, over other sulfur-containing amino acid and peptide. Moreover, the sensing ability of 1 for Cu^{2+} was supported by theoretical calculations.

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Multiple target chemosensor: a fluorescent sensor for Zn(II) and Al(III) and chromogenic sensor for Fe(II) and Fe(III)

김용성 김진아 유가림 이선영 김 철[1,*]

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A multifunctional fluorescent and colorimetric chemosensor 1, based on two juloidine moieties as a binding and signaling unit, has been synthesized in a one-step procedure. Receptor 1 showed prompt responses toward Zn^{2+} and Al^{3+} ions through selective fluorescence enhancement in dimethylformamide (DMF), while the presence of 5% water rendered 1 detect only Zn^{2+}. Moreover, 1 sensed the iron by “naked eye” with the clear color change. Upon the addition of Fe^{2+} and Fe^{3+} into each solution of 1, the color of the solutions changed from pale yellow to dark green for both Fe^{2+} and Fe^{3+}. The binding modes of the complexes were determined to be 1:1 complexation stoichiometry through Job plot, ^{1}H NMR titration and ESI-mass spectrometry analysis.

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Macrocyclic Zinc(II) Coordination Polymers Constructed from Aromatic Rigid and Flexible Cyclohexane Dicarboxylate Ligands

김태영 서성용 서초현 김주창*

부경대학교 화학과

With the purpose of finding out coordination polymers having fascinating structural features, we employed the macrocyclic Zn(II) complex as a metal ion connector, and dicarboxylic acid bpdcH_2 (4,4'-biphenyl dicarboxylic acid) and 1,4-chdcH_2 (*e*,*e*-1,4-cyclohyclo dicarboxylic acid) as bridging ligand linkers in basic solution, respectively. From the self-assembly processes of an appropriate combination of metal ion and bridging ligand, we have obtained two coordination polymers, $\{[Zn(L)(bpdc)]\cdot 0.75H_2O\}n$ (1) and $\{[Zn(L)(e,e\text{-}1,4\text{-}chdc)]\cdot 2H_2O\}n$ (2). In both complexes, the coordinataion geometries about the zinc(II) ions show a distorted octahedron, forming coordination polymers with bridging ligands. One of the pertinent features found in 1 is the presence of two kinds of 1D chain, running toward crystallographic b and c directions, respectively. Meanwhile, the structure 2 exhibits a simple 1D coordination polymer. In this presentation, the details of the structures 1 and 2 as well as their properties will be discussed.

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A selective colorimetric chemosensor for copper(II) ion and fluoride based on a diaminomalenitrile

이선영 이성열 이재준 김진아 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A new and simple colorimetric receptor 1, based on 2,3-diaminomaleonitrile moiety and julolidine moiety, has been synthesized and characterized. 1 showed a selective colorimetric sensing ability for copper (II) ion by changing color from yellow to colorless, and could be utilized to monitor Cu^{2+} over a wide pH range of 4-12. The detection limit (2.1 μM) of 1 for Cu^{2+} is much lower than that (30 μM) recommended by WHO in drinking water. Moreover, the receptor 1 can detect fluoride ions by color change from yellow to orange, distinguishing fluoride ion effectively from anions such as $CH3COO^-$ and CN^-. 1 showed the 1^- deprotonated by fluoride was reversible simply through treatment with a proper reagent such as HCl. The sensing mechanism for F^- was theoretically supported by DFT and TD-DFT calculations.

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Tetranuclear self-assembled *s*-tetrazine-ruthenium cages: the encapsulation of π-rich aromatic molecules

강혜지 최문근*

연세대학교 화학과

The interest of metallamolecules has been increased, because of easy shape modification with coordination geometry of transition metals and modulating functionalities introducing functional ligands. The preparation and binding constant study of metalla-cages bearing various ligands which show unique functionalities are required to understand host-guest systems for the applications, such as sensors, drug delivery, catalyst and stabilization of reactive intermediates.In this study, the tetraruthenium molecular-rectangles introducing 3,6-di(4-pyridyl)-*s*-tetrazine were synthesized. π-electron density and steric hindrance of ruthenocycles were modified by inverse Diels-Alder reaction and chloride substitution. The structures of synthesized metallacages were characterized by ^{1}H NMR spectroscopy and single crystal X-ray diffraction. The binding constants between ruthenocycle hosts and various aromatic guests were measured by ^{1}H NMR titration. The binding constant was increased that extend π- conjugation of aromatic guests showed higher association constant ruthenocycle hosts. Modification of ruthenium cage by inverse Diels-Alder reaction decreased the binding constant with π-electron rich aromatic molecules. In addition, the binding constants between ruthenocycle hosts based on dioxobenzoquinone with the aromatic guests were higher than ruthenium cages including dichlorobenzoquinone.

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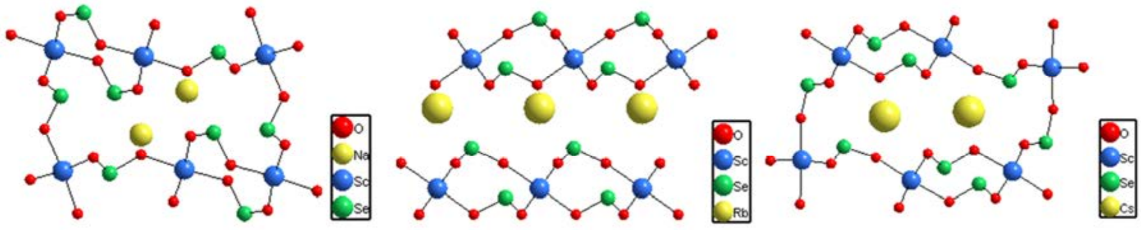
Hydrothermal synthesis and characterization of new quaternary scandium selenites

송승윤 옥강민*

중앙대학교 화학과

A series of new quaternary scandium selenites have been synthesized through hydrothermal reactions using alkali metal carbonates, scandium nitrates, and selenium dioxide, and water as reagents. The stoichiometrically similar materials reveal two- and three-dimensional framework structures consisting of ScO_6 octahedra and SeO_3 polyhedra. Detailed structural analyses suggest that the size of alkali metal cations and subsequent interactions between alkali metal cations and oxides strongly influence the direction of lone pairs on Se^{4+} cations. Thorough characterizations including X-ray diffraction, SEM/EDAX, infrared and UV-Vis diffuse reflectance spectroscopies, thermal analyses, and dipole moment calculations for the new alkali metal scandium selenites are presented. Nonlinear optical (NLO) property measurements on the NCS phase will also be presented.



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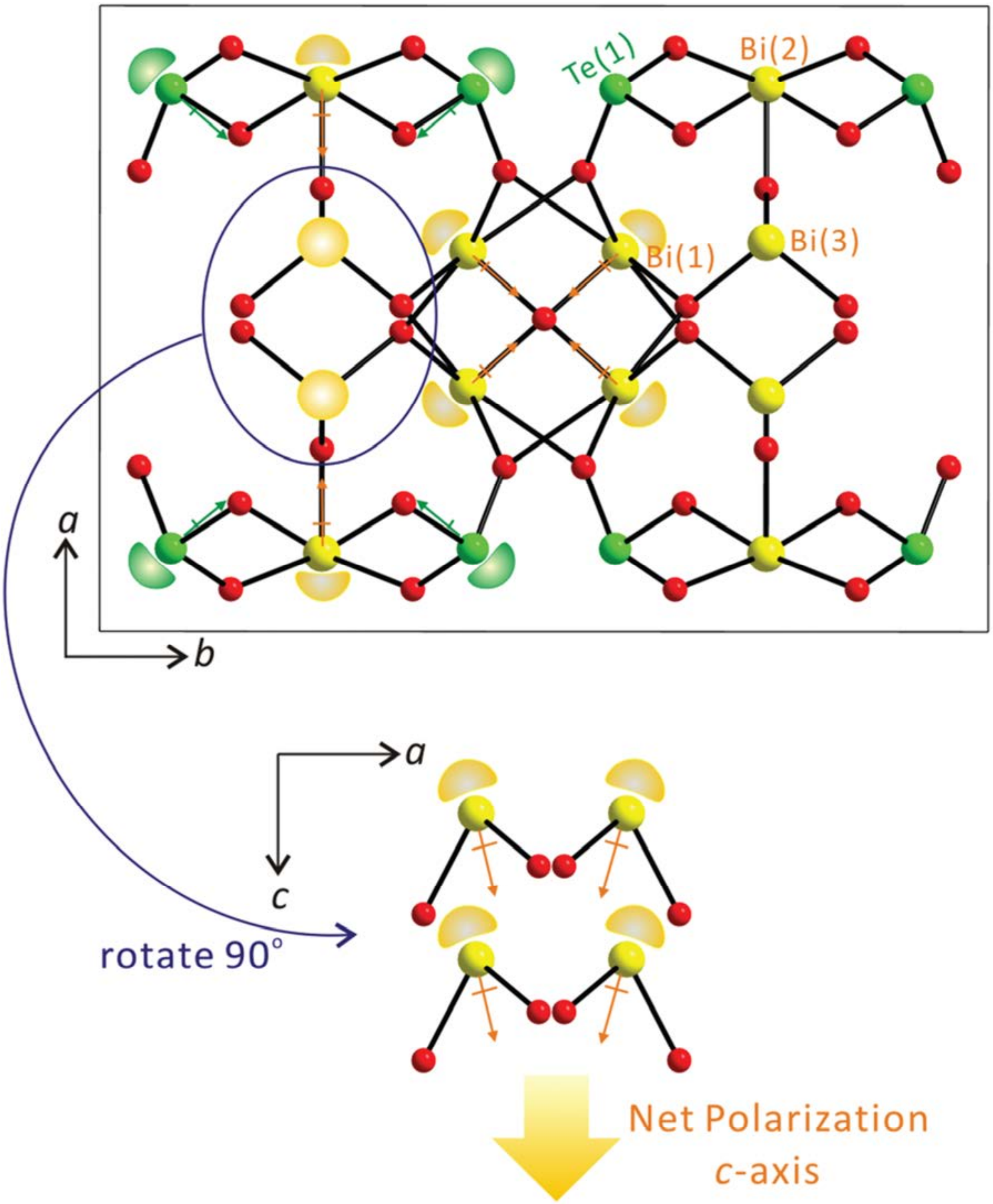
Effect of polarizable lone pair cations on the second-harmonic generation (SHG) properties of noncentrosymmetric (NCS) $Bi_{2-x}Y_xTeO_5$ (x = 0-0.2)

조홍일 옥강민*

중앙대학교 화학과

Bi_2TeO_5 that is containing two kinds of lone pair cations exhibits large second-harmonic generation (SHG) efficiency (300 × α-SiO_2). Structural analysis suggests that the alignment of the polarization of the asymmetric environment is extremely important for the SHG efficiency for the reported material. In this research, we have successfully doped a non-polarizable cation, Y^{3+} into the site of polarizable cation, Bi^{3+} with stereoacive lone pairs through standard solid-state reactions. Powder X-ray diffraction data show that pure phases of $Bi_{2-x}Y_xTeO_5$ (x = 0, 0.1, and 0.2) have been synthesized successfully. SHG properties measurements reveal that the NLO properties decrease as more Y^{3+} is doped into the Bi^{3+} sites. Detailed structure-SHG properties relationships along with other characterizations will be introduced.


Te(1)
Bi(2)
Bi(1)
Bi(3)
a
b
a
c
rotate 90°
Net Polarization
c-axis

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvothermal Synthesis and Characterization of Two New Barium-Organic Compounds: Reversible Solvent Exchange and High thermal Stability

HALAKESHOBHAKANTAPPA 옥강민*

중앙대학교 화학과

Two novel barium-organic coordination polymers have been synthesized under solvothermal conditions by employing two different organic linkers. The structures of these frameworks have been determined by single-crystal X-ray diffraction. The materials have been further characterized by powder X-ray diffraction (PXRD), elemental analyses, UV-visible and FT-IR spectroscopy, and thermogravimetric analysis (TGA). The structures of the materials reveal three-dimensional frameworks comprising inorganic motifs with one-dimensional chains connected through organic linkers. The PXRD and FT-IR confirm the reversible coordination of respective solvent molecules, DMF and H2O. Gas adsorption properties towards nitrogen, hydrogen, and carbon dioxide have been also investigated.

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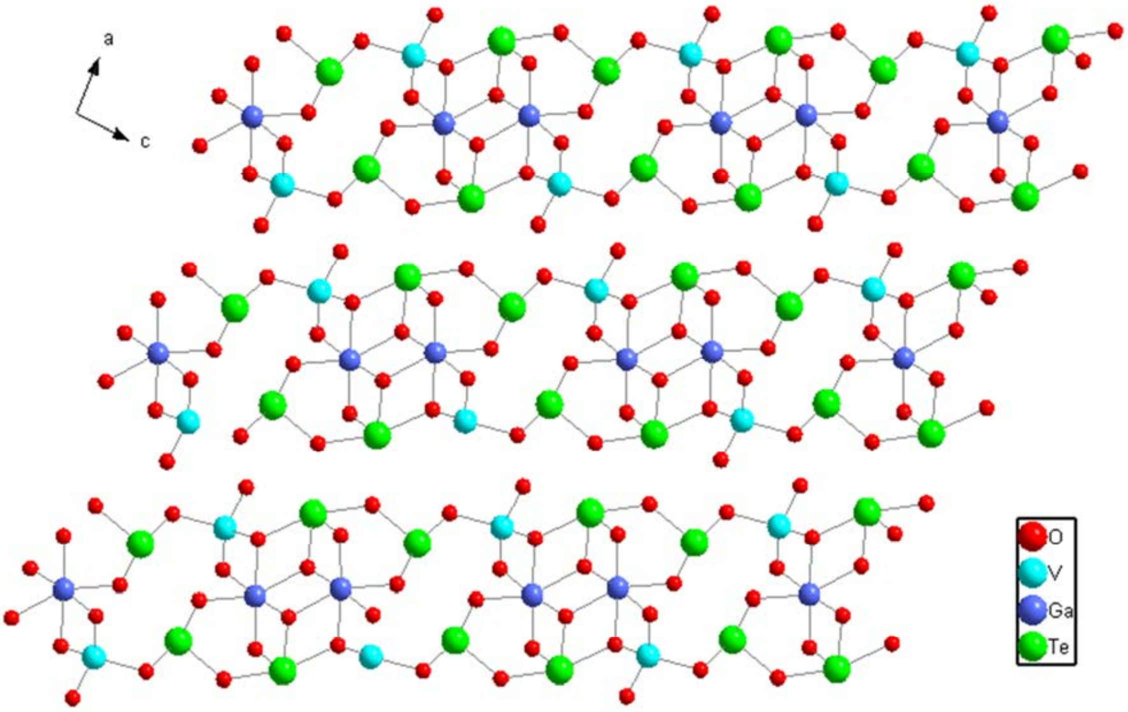
A New Quaternary Layered Tellurite with Asymmetric Polyhedra

배수환 옥강민*

중앙대학교 화학과

A new gallium vanadium tellurite compound has been synthesized through both standard solid-state and hydrothermal reactions. Single crystal X-ray diffraction reveals that the reported material has a layered structure consisting of asymmetric polyhedra such as TeO_3 and TeO_4. The local unsymmetrical coordination environment of the constituent polyhedra is attributed to the stereoactive lone pairs on Te^{4+} cations. The newly prepared compound has been fully characterized. UV-vis diffuse reflectance spectral data suggest that the band gap energy of this compound is 3.35 eV. Infrared spectra and thermal behavior of the compound will also be presented.


a
c
O
V
Ga
Te

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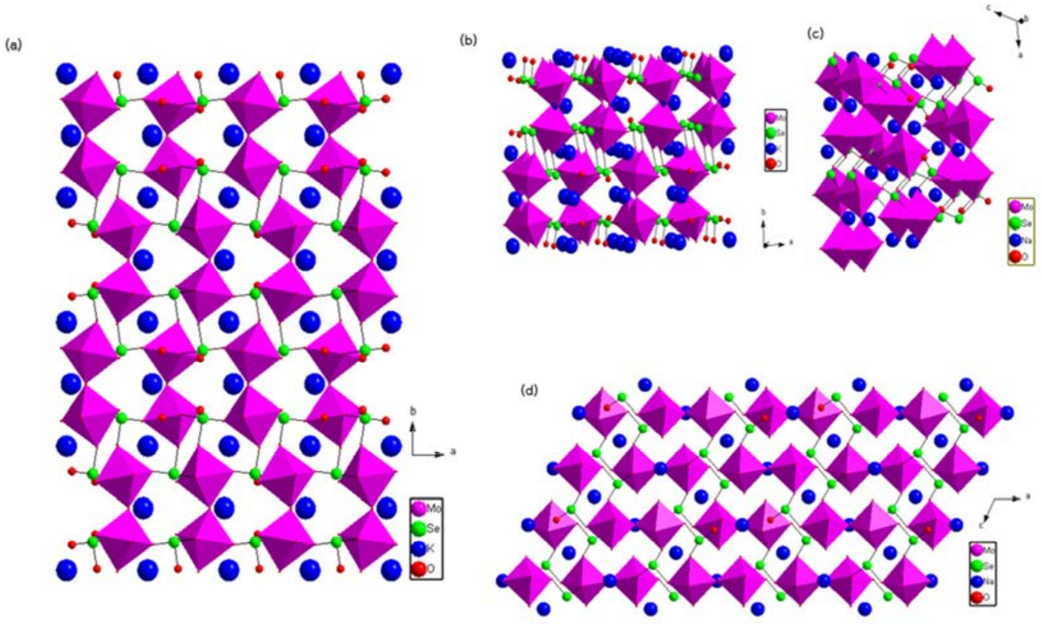
Synthesis, structure, and characterization of a series of new quaternary molybdenum selenites

방성은 옥강민*

중앙대학교 화학과

Single crystals and pure polycrystalline samples of new quaternary molybdenum selenites materials have been prepared through hydrothermal and standard solid-state reaction techniques using various alkali metal carbonates, MoO_3, and SeO_2 as reagents. Single-crystal X-ray diffraction reveals that the synthesized materials have three-dimensional structures. The frameworks of the reported materials are composed of corner-shared MoO_6 octahedra and SeO_3 polyhedra. Although the presented materials have similar stoichiometry, they crystallize in different space groups. Detailed structural analysis suggests that the slight structural difference mainly originates from the size of alkali metal cations and subsequent coordination environment. Further characterization including SEM/EDAX, infrared and UV-vis diffuse reflectance spectroscopies, and dipole moment calculations will also be presented.


(a)
b
a
Mo
Se
K
O
(b)
Mo
Se
K
O
b
a
(c)
c
b
a
Mo
Se
Na
O
(d)
a
c
Mo
Se
Na
O

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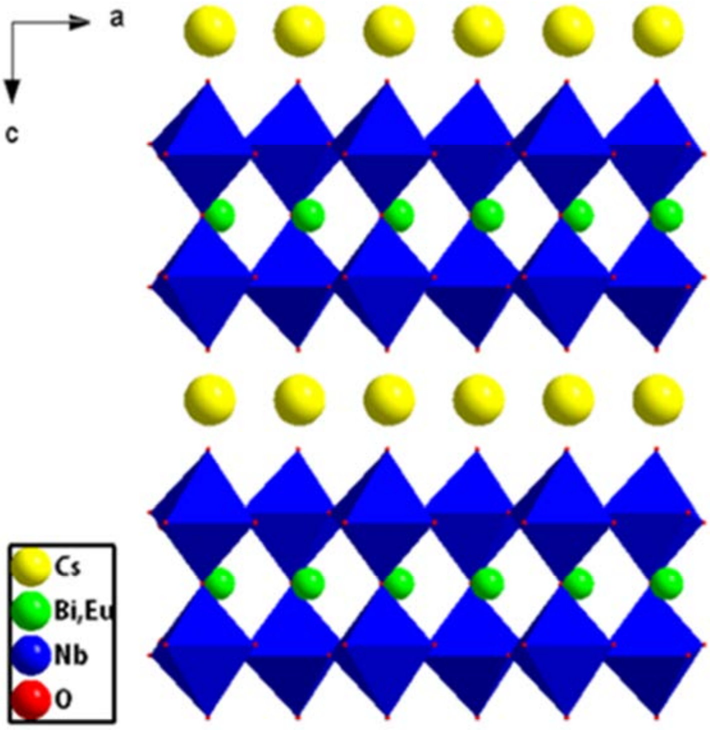
Second-Harmonic Generation (SHG) and Photoluminescence Properties of Dion-Jacobson Type Layered Perovskite Solid Solutions, $CsBi_{1-x}Eu_xNb_2O_7$ (x = 0-0.2)

김형구 옥강민*

중앙대학교 화학과

Hyung Gu Kim and Kang Min Ok*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, 156-756, Republic of Korea.A series of noncentrosymmetric (NCS) layered perovskite solid solutions, $CsBiNb_2O_7$, $CsBi_{0.9}Eu_{0.1}Nb_2O_7$, and $CsBi_{0.8}Eu_{0.2}Nb_2O_7$ were synthesized by solid state reactions. Powder X-ray diffraction studies reveal that the solid solutions adopt NCS polar orthorhombic space group, $P2_1am$ (No. 26). The structures are composed of corner-shared distorted NbO_6 octahedra and out of center A-cations, Bi^{3+} and/or Eu^{3+}. The SHG efficiencies of $CsBiNb_2O_7$, $CsBi_{0.9}Eu_{0.1}Nb_2O_7$, and $CsBi_{0.8}Eu_{0.2}Nb_2O_7$ are 50, 30, and 25 times that α-SiO_2, respectively. The decrease in SHG for Eu^{3+}-doped materials is due to the lack of net moment originating from the polyhedra of polarizable lone pair cation, Bi^{3+}. Photoluminescence (PL) spectra for $CsBi_{1-x}Eu_xNb_2O_7$ exhibit characteristic bands for f-f transitions and strongly suggest the asymmetric coordination environment of Bi^{3+}/Eu^{3+} site in $CsBi_{1-x}Eu_xNb_2O_7$ solid solutions.



$CsBi_{1-x}Eu_xNb_2O_7$ (x = 0–0.2)

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Nano-sized Li_2MnSiO_4/carbon as a high capacity cathode material for lithium-ion battery

황차환 이경구[1,*] 옥강민[*]

중앙대학교 화학과 [1]군산대학교 화학과

Lithium transition metal orthosilicates were proposed as possible cathode materials for the lithium ion battery. Among the candidates, Li_2MnSiO_4 (LMS) offers promise to deliver high energy density (333mAh g^{-1}) and thermal stability compared to lithium transition metal oxides. However, due to its poor electronic conductivity and slow Li-ion diffusion, particles of LMS are required to be nano-sized and carbon coated. By doing so, high rate capability and discharge capacity can be easily achieved. In this study, ultrasound-assisted reaction was adopted for the synthesis of LMS nanoparticles. The high power sonochemical reaction is able to induce an effective surface coating on template materials homogenously in a short reaction time. LMS precursors were prepared under ultrasound field for 20 min. The precursors were calcined at 700 ^{o}C for 8 h under Ar atmosphere to obtain carbon coated crystallites. The synthesized LMS/C nanoparticles (20~30nm) crystallized in orthorhombic space group, $Pmn2_1$. The synthesized LMS by ultrasound-assisted reaction has more regular shape and pore size in comparison to the sol-gel reaction compound. The first cycle discharge capacity of synthesized LMS/C was about 250 mAh g^{-1} in the voltage range of 4.8~1.5 V and the current density was 16.5 mAh g^{-1}.

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Synthesis and characterisation of Cu(II), Co(II) and Cd(II) complexes with *N*,*N*-bis((1H-pyrazol-1-yl)methyl)cyclopentanamine and *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)cyclopentanamine ligands

최성혜 남중관 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [L_nMCl_2] (L_n = L_A, L_B, M = Co, Cu, Zn) were synthesized by the reaction of the corresponding metal starting materials with *N*,*N*-bis((1H-pyrazol-1-yl)methyl)cyclopentanamine (L_A) and *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)cyclopentanamine (L_B), respectively. The X-ray crystal structure of [L_ACoCl_2], [L_BCoCl_2] and [L_ACuCl_2] were best described as a distorted trigonal bipyramidal geometry involving coordination of the nitrogen atom of the cyclopentanamine moiety and the metal center, resulting in the formation of an eight-membered chelate ring. [L_ACoCl_2] showed the highest catalytic activity for the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 7.67×10^4 g PMMA/molCo?h at 60°C among the others and compared to the reference complex [$CoCl_2$] (4.03×10^4 g PMMA/molCo?h).

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Conformational Control of Light-Emitting Properties: Reaction-Based Fluorescent Turn-On Probes

김세용 이동환*

서울대학교 화학부

Fluorescent probes represent an important class of stimuli-responsive molecules that detect specific chemicals via change in emission intensity, excitation/emission wavelength, or a combination of both. Such photophysical properties can be modulated by covalent or conformational control of extended π-conjugation. Recently, we have found that sterically-congested and conformationally-distorted *N*-aryl benzotriazole systems display remarkably different luminescence properties compared with typical planar *N*-aryl benzotriazoles. Taking advantage of this conformation-dependent fluorescence switching, we have developed fluorescent turn-on probes for palladium in solution samples. In this presentation will be discussed fundamental structure-property relationships that underpin this chemistry and their practical implications.

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Synthesis and Characterization of Copper(Ⅰ) Coordination Polymers Based on Pyridine Ligands with Thioether Substituents

권은진 전영은 강기행 박현진 김태호* 김진은*

경상대학교 화학과

Recently, we have focused on the development of luminescent copper(I) coordination polymers with N/S donor ligands. 3-(2-(*tert*-butylthio)ethoxy)pyridine (L^1) and 3-(2-(benzylthio)ethoxy)pyridine (L^2) have been synthesized. Three Cu(I) coordination polymers (CPs) $\{[Cu_4I_4L^1_2]\cdot CH_2Cl_2\}_n$ (1), $[Cu_4I_4L^1_2]_n$ (2), and $[CuIL^2]_n$ (3) based on L^1 and L^2 have been prepared. CPs 1 and 2 are composed of cubane Cu_4I_4 cluster node. CP 1-3 shows yellow, yellow-green, and blue light emission under UV irradiation. The results of our investigation including syntheses, structural characterization, thermal and photoluminescence properties of three new Cu(I) CPs 1-3 are presented.

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Stepwise Synthesis and Reversible Crystal Transformation of Cu(I) Coordination Polymers by Solvents

전영은 강기행 권은진 박현진 김태호* 김진은*

경상대학교 화학과

$[Cu_xI_x]$- based coordination polymers(CPs), $[Cu_2I_2L_2]_n$ (1), $[Cu_4I_4L_2]_n$ (2a), $\{[Cu_4I_4L_2]\cdot 2CH_3CN\}_n$ (2b), $\{[Cu_4I_4L_2]\cdot 0.5C_6H_6\}_n$ (2c), $\{[Cu_3I_3L]\cdot C_3H_6O\}_n$ (3) have been synthesized with 2-(2-benzylthio)ethyl)pyrazine (L). CPs 2a-2c shows supramolecular isomeric structures by solvent molecules. In CPs 1-3, the solvent-mediated reversible crystal-to-crystal transformation between them was achieved by exposing solvent vapor or soaking the crystalline sample in the diverse solvent (MeCN, benzene, acetone). CP 3 has been prepared by rearrangement of CP 2 in acetone by ultrasonication or solvothermal method. Interestingly, the crystal structure of 3 interconnected by long stair-step $(CuI)_n$ polymer units is two-dimensional. CP 5 has been stepwisely synthesized from CP 1 via CP 2 through the removal of ligand by solvent. Crystal transformation between topologically different Cu(I) CPs 2a,2b and 2b are reported.

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Crystal Structures and Photophysical Properties of Cu(I) Coordination Polymers Based on Pyridine Ligands with Thioether substituents

박현진 전영은 강기행 권은진 김태호[*] 김진은[*]

경상대학교 화학과

The pyridine ligands (L^1 and L^2) with thioether substituents were synthesized by the reaction of 2-chloroethyl cyclohexyl sulphide and 3-, or 4-hydroxypyridine. Three Cu(I) coordination polymers (CPs) $\{[\mathrm{CuIL}^1]\cdot\mathrm{MeCN}\}_n$ (1) $[\mathrm{CuIL}^1]_n$ (2), and $[\mathrm{CuIL}^2]_n$ (3) were prepared by the reaction of CuI and ligands. CPs 1 and 2 shows a 1D loop chain structure, based on a rhomboid Cu_2I_2 cluster node. CP 3 shows an interpenetrated 2D network structure. We report structures, thermal behaviors and photophysical properties of the CPs based on N/S mixed donor ligands.

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Solvent-Induced Crystal Transformation of Cu(I) Supramolecular Isomers

강기행 전영은 박현진 권은진 김태호* 김진은*

경상대학교 화학과

Solvent-responsive four 1D copper(I) coordination polymers (CPs), $\{[Cu_4I_4L(MeCN)_2]\cdot CH_2Cl_2\}_n$ (1), $\{[Cu_4I_4L(MeCN)_2]\cdot CHCl_3\}_n$ (2), $\{[Cu_4I_4L(MeCN)_2]\cdot 0.5\ p\text{-xylene}\}_n$ (3), and $[Cu_4I_4L(MeCN)_2]_n$ (4), have been prepared by self-assembly reactions between CuI and *N*,*N'*-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide (L). CPs 1-4 are interconnected by cubane Cu_4I_4 clusters, which are pseudopolymorphic supramolecular isomers by solvent molecules. Crystal transformations caused by reversible solvent exchange were observed under appropriate conditions such as solvent.

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Microporous organic polymer for carbon-mesoporous Cr_2O_3 anode materials for lithium ion batteries

홍석조 강다예 김의순 조경일 신영준 손성욱*

성균관대학교 화학과

This presentation will show the KIT-6 template synthesis of the highly ordered mesoporous chromium oxide materials, and microporous organic polymer coating on them. The KIT-6 silica has been used for templating the specific mesoporous structure. We obtained mesoporous chromium oxide materials using the KIT-6 as a template. Chromium oxide can be used as anode materials for lithium ion batteries, and has a large theoretical capacity of 1,058 mAh/g. However, in the practical application, it shows poor cycling performance and low capacity. To improve the electrochemical ability of chromium oxide, we introduced microporous organic polymer into its surface by Sonogashira coupling with tetra(4-ethynylphenyl)methane and 1,4-diiodobenzene. Microporous organic polymer has armophous structure and micropores (pore size < 2nm), even after carbonization. The resultant microporous carbon shell has good electrical conductivity. Carbon-coated chromium oxide resulted in reversible capacity of 480 mAh/g at 50 mAh/g current density after 50 cycles. It was more efficient compared to the bare chromium oxide materials. In this study, we show that microporous organic polymer can be used for the carbon coating on anode materials to enhance the electrical conductivity and cycling performance.

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MOFs bearing C_{2h}-symmetric terphenyl dicarboxylate linker

김현철 허성[*] 김성진[1] 김영미[2,*]

한국외국어대학교 화학과 [1]이화여자대학교 화학과 [2]이화여자대학교 나노바이오 기술연구소, 화학-나노과학과

We recently prepared a new C_{2h}-symmetric terphenyl dicarboxylate linker, terphenyl-3,3’-dicarboxylate (3,3’-TPDC), and a corresponding one-dimensional (1D) Cu(II) coordination polymers containing 3,3’-TPDC. Here we report two isostructural 3D MOFs with the general formula [M(TPDC)(DMF)] (M = Co (I) , Mn (II)) resulted from the assembling of a metal ion and the bridging ligand 3,3’-TPDC. MOFs I and II were structurally characterized by X-ray crystallography. Both MOFs are isostructural and crystallize in the monoclinic C2/c space group. The coordination geometry of a metal ion is distorted octahedral constructed by four $O_{carboxylate}$ (η^1:η^1:μ_2) and two μ_2-O_{DMF}. Because as-prepared MOFs do not have void volume we try to remove the weakly-coordinated bridging DMF molecules to generate void space. In order to remove bridged DMF molecules, I was heated at 180°C for 5 h. Pink-colored I was changed the color to violet (I_180) whose structure could not be determined due to lost its crystallinity. We inferred from the magnetic susceptibility data for both MOFs that there exist week antiferromagnetic interactions in a metal chain since the main magnetic interactions should happen between metal ions bridged by the short carboxylate-based ligand and DMF oxygen atoms. Removing the bridged DMF molecules can increase the distance of M…M in a metal chain of I and II and change the magnetic property, but similar magnetic behaviors for both MOFs tells us that the removing of the bridging DMF molecules could not significantly cause the changing of M…M distance and relevant magnetic properties.

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Double Helical Ag(I) Coordination Polymers Induced by Unsymmetrical Dipyridyl Ligand

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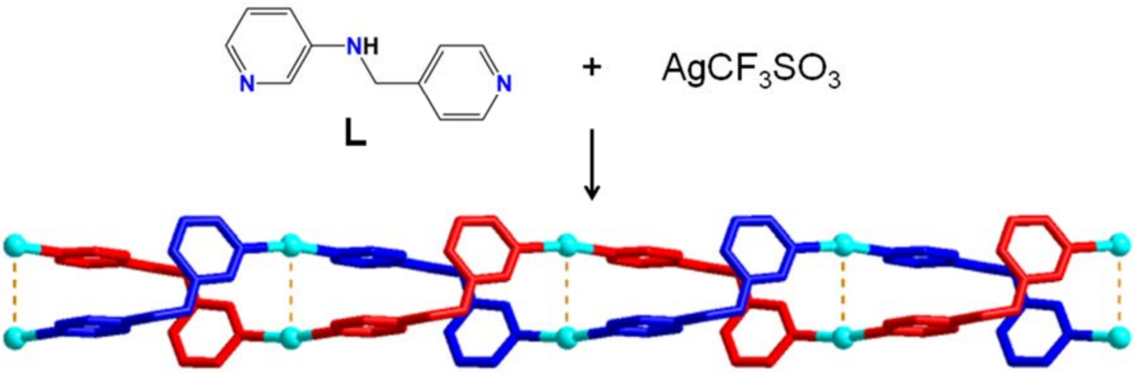
Helical structures have received much attention in supramolecular chemistry and materials science because of their fascinating similarities in biological systems to nucleic acids and proteins as well as their potential applications as functional materials in asymmetric catalysis and non-linear optical materials. Although many single-, double-, and multiple-stranded helical coordination polymers have been reported, however, the rational and desirable construction of supramolecular helical structure is still obstructed by the limited understanding of the structural constraints. In the preparation of the helical coordination polymers, much effort should be devoted to the careful design of organic ligands and the reasonable selection of metal ions with the rational geometries.

One of useful strategies constructing supramolecular architectures with helical structures is the employment of the flexible ditopic ligands and metal ions with linear geometry. In particular, unsymmetrical dipyridyl ligand L is one of good candidates for construction of helices because it is a nonlinear and flexible ligand and has two terminal pyridines with different substituted positions.

Herein, we report the crystal structure of a fascinating infinite double helical silver coordination polymer derived from the unsymmetrical and flexible dipyridyl ligand L and its physical properties including TGA and solid-state photoluminescence. To the best of our knowledge, infinite double helical structure is less common, whereas numerous discrete double helicates have been reported.


N
NH
N
L
+
AgCF₃SO₃

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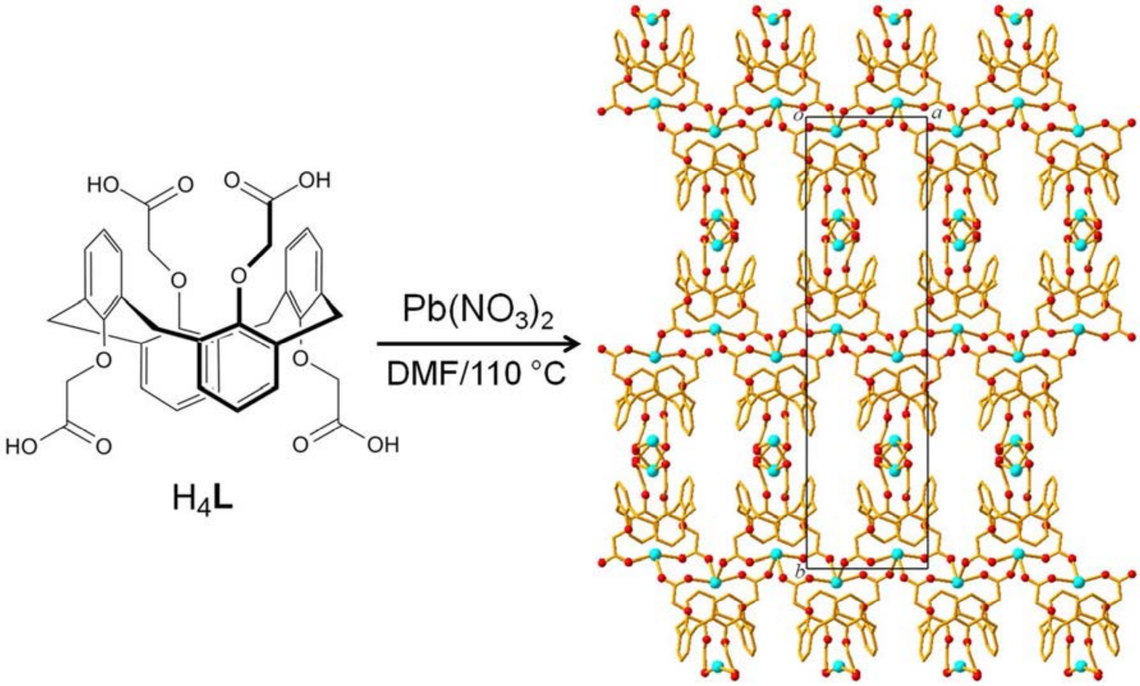
Calix[4]arene-based Metal Organic Framework: Crystal-to-Crystal Transformation on Lattice Solvent Removal

이은지 김영훈[1] 주희영 허정석[1,*] 박기민[2,*]

경상대학교 화학과 [1]충남대학교 화학과 [2]경상대학교 기초과학연구소

Metal organic frameworks (MOFs) are one of the fastest growing fields in supramolecular chemistry due to their great potential applications in catalysis, gas storage, and separation. Together with the development of MOFs, recently, calix[4]arene-based metal organic frameworks (calixMOFs) obtained through solvothermal reaction of calix[4]arene derivatives with metal ions become a rising subject of supramolecular chemistry. This is because the calixMOFs are able to possess the potential of the calix[4]arenes themselves such as gas uptake besides the porosities of the calixMOFs themselves. Most of them are two- and three-dimensional calixMOFs constructed from the reaction of upper-rim functionalized calix[4]arenes with the transition metal ions. In contrast, the examples of calixMOFs based on lower-rim functionalized calix[4]arenes are relatively rare.A tetracarboxylic acid calixarene derivative H4L with 1,3-alternative conformation as a potential anionic tetradentate ligand is a good candidate in the construction of three-dimensional porous calixMOF because not only the four pendant arms are directed outward from the calix[4]arene unit but also they can be coordinate to four or more metal ions. Herein, we report the preparation and crystal structure, and physical properties including TGA, photoluminescence and gas uptake of new 3D calix[4]arene-based MOF formed by the self-assembly of H4L and lead ion. Furthermore, Single-crystal to single-crystal transformation of the obtained calixMOF upon the removal of guest molecules will be discussed.


HO
O
O
OH
O
O
O
O
HO
O
O
OH
$H_4\mathbf{L}$
$Pb(NO_3)_2$
DMF/110 °C
o
a
b

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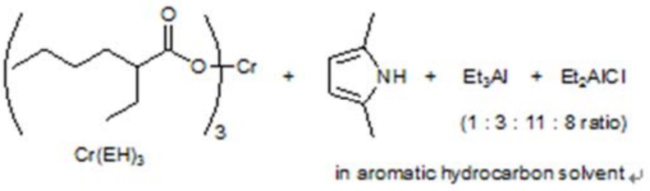
Improvement and Demystification of Chromium Precursor for Phillips Ethylene Trimerization Catalyst

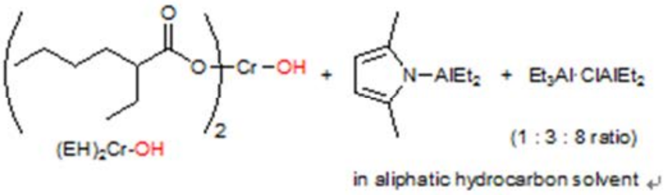
전종엽 이동환 이분열*

아주대학교 분자과학기술학과

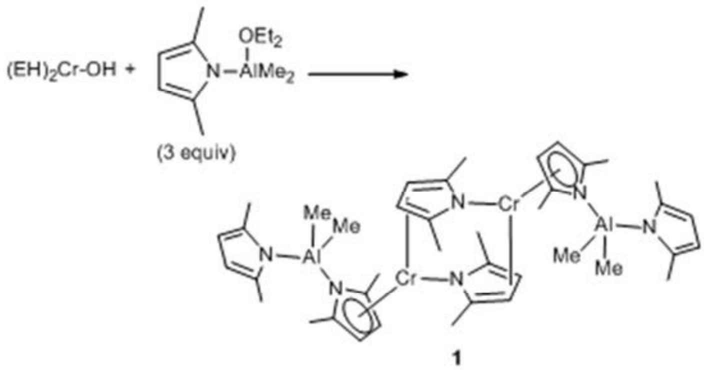
The production of linear α-olefin (LAOs) via ethylene oligomerization has recently emerged as a highly topical issue. A chromium catalyst that can selectively generate 1-hexene, discovered in Phillips in the early 1990s, has been applied to the commercial process since 2003 (Scheme 1). The Phillips catalyst prepared by reacting $Cr(EH)_3$ (EH=2-ethylhexanoate), 2,5-dimethylpyrrole ($Me_2C_4H_2NH$), Et_3Al, and Et_2AlCl in an aromatic hydrocarbon solvent was improved to a congener composed of a new chromium precursor $(EH)_2CrOH$, $(Me_2C_4H_2N)AlEt_2$, and $Et_3Al\cdot ClAlEt_2$ (Scheme 2). Reaction of $CrCl_3$ with 3 equiv Na(EH) in water did not generate $Cr(EH)_3$, but unexpectedly produced $(EH)_2CrOH$. Our improved system exhibited consistently high activity (54×10^6 g/mol-Cr·h), which is approximately three times higher than erratic catalytic performance of the Phillips catalyst system. Reaction of $(EH)_2CrOH$ with $(Me_2C_4H_2N)AlMe_2$ generate Cr(II)-complex which provided active species when activated with $Et_3Al\cdot ClAlEt_2$(1).



Scheme 1 Components of the original Phillips catalyst.



Scheme 2 The improved catalyst system prepared using $(EH)_2CrOH$.



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P-O and P-S Bond Formation/Cleavage Reactions at a Nickel Center Supported by an Anionic PPP Ligand; a New type of Metal-Ligand Cooperation

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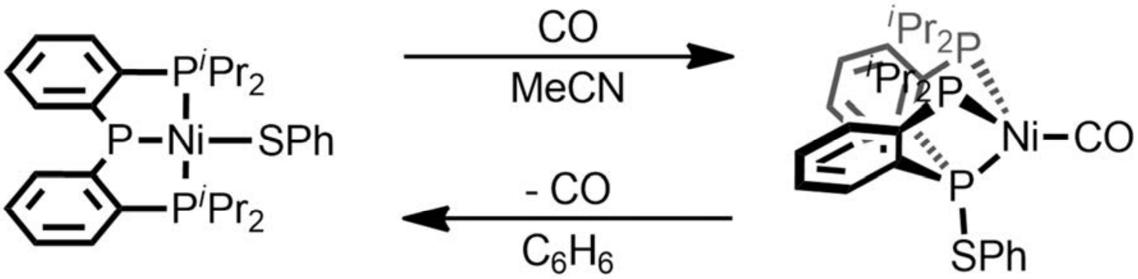
한국과학기술원(KAIST) 화학과

Metal-ligand cooperation based on non-innocent ligands is recently receiving attention as a unique methodology to utilize various oxidation states of the metal complexes for catalytic reactions. While examples including reports by Chirik, Milstein and other groups employing a π-conjugated system as an non-innocent motif such as aryl-substituted bis(imino)pyridine and pyridine/acridine are fairly well-known, there are relatively few reports in phosphine-based systems. We will report a series of non-innocent activities of an anionic PPP ($PPP^- = P[2\text{-}P^iPr_2\text{-}C_6H_4]_2$) ligand with nickel. Especially, the comparison between tholato and phonolate group transfer mediated by metal-ligand cooperation will be discussed. Recently, we found that the nickel complexes supported by a PPP ligand reveal the reversible transformation between a phosphide-nickel(II) alkoxide and a phosphinite-nickel(0) species via a P-O bond formation/cleavage. In order to expand this unusual metal-ligand cooperation, we are currently studying the group transfer of a sulfur containing moiety to establish the reversible formation of P-S bond with (PPP)NiSPh as an analogue of (PPP)NiOPh. This newly prepared species reveal the migratory behavior as shown in the case of phenoxide resulting in the formation of ($PP^{SPh}P$)NiCO from the reaction with CO(g). In order to examine the potential formation of phosphide-nickel(II) species as a backward reaction, the reactivity of two Ni(0) CO species, ($PP^{OPh}P$)NiCO and ($PP^{SPh}P$)NiCO, toward Lewis acid is currently under investigation.

P^iPr2
P
Ni
SPh
P^iPr2
CO
MeCN
- CO
C6H6
^iPr2P
^iPr2P
Ni
CO
P
SPh

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Synthesis of Silole and Dithienosilole Derivatives and their Copolymerization with Dichlorodisubstitutedsilane

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계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1,3,4-tetraphenylsilole and 4,4-Diphenyl-2,6-bis(trimethylsilyl)dithienosilole as monomer were prepared by the intramolecular cyclization of diphenylbis(phenylethynyl)silane and 3,3'-dibromo-5,5'-bis(trimethylsilyl)-2,2'-bithiophene, respectively. 2,6-Dibromo-4,4-diphenyl-dithienosilole was synthesized by the substitution with bromine at -90 ℃ to 4,4-diphenyl-2,6-bis(trimethylsiltl)dithienosilole. We have synthesized polymeric materials of polycarbosilanes that containing 1,1,3,4-tetraphenyl-2,5-silolene or 4,4-diphenyldithienosilolene and disubstitutedsilylene along the polymer main chain by copolymerization of 2,5-dibromo-1,1,3,4-tetraphenylsilole or 2,6-Dibromo-4,4-diphenyldithienosilole with several dichlorodisubstitutedsilanes using n-butyllithium.

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Interpenetration of Metal-Organic Frameworks with hms topology *via* heat treatment

박정인 나명수*

울산과학기술대학교(UNIST) 화학과

By interpenetrating the structure, the metal-organic frameworks (MOFs) would have advantages in stability and controlling pore sizes. First of all, metal-organic frameworks [Ni(btc)(AP)] having hms topology could be prepared *via* one-pot *de novo* synthesis combining Nickel(Ⅱ) nitrate precursor, btc(btc = trimesic acid) and AP(AP = Azopyridine) in mixed solvent. Then by heat treatment in flowing N_2 gas condition, the MOFs with hms topology would be interpenetrated and we can confirm this status by several analysis methods.

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Postsynthetic ligand exchange of metal organic framework for pillar control

신선영 나명수*

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A 2-MOF, $[Ni_3(BTC)_2(pz)_3(H_2O)_X]$, (where, H_3BTC = 1,3,5-benzenetricarboxylic acid; pz = pyrazine) could not be synthesized *via* one-pot *de novo* solvothermal reaction. The 2-MOF has been achieved *via* postsynthetic ligand exchange. By soaking an 1-MOF, $[Ni_3(BTC)_2(bp)_3(H_2O)_X)]$,(where bp = 4,4’-bipyridine) in a 0.5 M of pz DMF solution, bp pillaring ligands in 1-MOF were exchanged to the shorter pz pillaring ligands completely to form the 2-MOF. The various properties of this MOF will be discussed.

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The Ligand Exchanges of MOFs from Hydroxyl Groups to Methyl Groups for Better Stabilities

원소미 나명수*

울산과학기술대학교(UNIST) 화학과

The series of hollow and non-hollow metal-organic frameworks were developed *via* metal-organic polyhedron single crystals as sacrificial templates. In those series of MOFs, several organic ditopic linkers such as dabco, pz, and bipy (where dabco = 1,4-diazabicyclo[2.2.2]octane; pz = pyrazine; bipy = 4,4’-bipyridine) were used to synthesize the hollow and non-hollow MOF structures using the MOP single crystals of $[Cu_{24}(hip)_{24}S_{24}]$ (where hip = 5-hydroxyisophthalic acid). However, these MOFs are highly unstable at the atmospheric conditions since the building ligand has hydrophilic hydroxyl group attached; therefore, the ligand including those hydroxyl group is exchanged to the ligand with hydrophobic methyl group *via* postsynthetic method to improve the stabilities of those MOF series.

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Single crystalline hollow metal-organic frameworks: a metal-organic polyhedron single crystal as a sacrificial template

김혜현 나명수*

울산과학기술대학교(UNIST) 화학과

While the Zn-MOF [$Zn_{24}(mip)_{24}(dabco)_6(H_2O)_{12}$] (where H_2mip = 5-methylisophthalic acid; dabco = 1,4-diazabicyclo[2.2.2.]octane) based on the cuboctahedral MOP [$Zn_{24}(mip)_{24}(H_2O)_{12}$], as a 12-connected node could only be prepared via one-pot solvothermal reaction, similar attempts to prepare isoreticular Cu-MOFs via conventional one-pot synthetic approach in presence of 5-hydroxylisophthalic acid (H_2hip) and various linkers between the potential MOP intermediate, [$Cu_{24}(hip)_{24}(H_2O)_{12}$], only produced metal-organic polyhedron (MOP), [$Cu_{24}(hip)_{24}(DMF)_8(H_2O)_{16}$]. A series of isostructural and isoreticular Cu-MOFs, [$Cu_{24}(hip)_{24}(L)_6(H_2O)_{12}$] (where L = dabco; pz = pyrazine; bipy = 4,4'-bipyridine), could only be obtained via stepwise reactions using the cuboctahedral MOP, [$Cu_{24}(hip)_{24}(DMF)_8(H_2O)_{16}$], as a molecular precursor. Especially, single crystalline hollow metal-organic frameworks (MOFs) with cavity dimensions in the order of several micrometers and hundreds of micrometers were prepared using a MOP single crystal as a sacrificial hard template. The hollow nature of the MOF crystal was confirmed by scanning electron microscopy of the crystal sliced using a focused ion beam.

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Selective Zinc Sensor Based on Pyrazoles and Quinoline Used to Image Cells

유가림 류가영 박대열 최예원 조태근 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

The synthesis, Zn^{2+} binding, crystal structure, and cell imaging studies of a pyrazole amine quinoline receptor are described. The receptor fluoresces in the presence of Zn^{2+} and not with other metal ions. The receptor forms 1:1 and 1:2 receptor to Zn^{2+} complexes depending on Zn^{2+} concentration and uses all of its nitrogens to coordinate to Zn^{2+}. Upon coordination of Zn^{2+}, the receptor absorbs visible light and fluoresces at 500 nm. The receptor is shown to be a zinc sensor in living cells by fluorescing when excited with visible light.

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Detection of multiple analytes (CN^- and F^-) based on a simple pyrazine-derived chemosensor in aqueous solution: experimental and theoretical approaches

이재준 조태근 박대열 복권희 류가영 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A new colorimetric receptor 1 for the detection of CN^- and F^- has been simply developed. Receptor 1 showed selectively colorimetric responses to CN^- in a near-perfect aqueous solution and F^- in 10% aqueous solution, respectively. An obvious color change of 1 from yellow to colorless was observed for CN^- through a nucleophilic addition mechanism, while F^- was detected through deprotonating mechanism with a distinct color change from yellow to orange. The binding modes of receptor 1 with two analytes ($CN^-$and F^-) were proposed to be 1:1, based on Job plot, ^1H NMR titration, and ESI-mass spectrometry analysis. Moreover, the sensing mechanisms for F^- and CN^- were theoretically supported by DFT and TD-DFT calculation.

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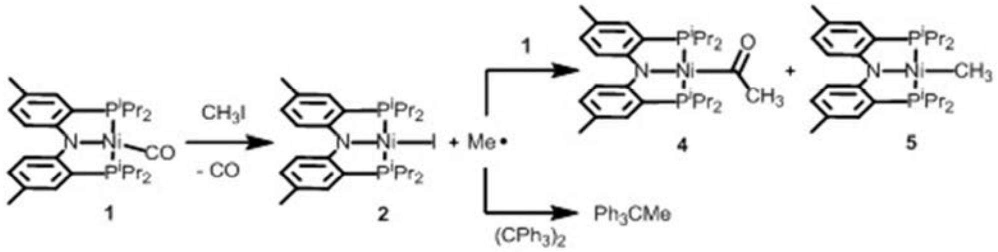
Methyl Transfer Reaction with Nickel(I) Monocarbonyl Species and Its Mechanistic Study

최종훈 이윤호*

한국과학기술원(KAIST) 화학과

Carbon monoxide is widely used in chemical industry as an important C1 source. For example, acetic acid is industrially generated from CO via Monsanto/Cativa process and as a major chemical industry various aldehydes are produced by carbonylation of alkenes; hydroformylation. Since most of industrial CO activation processes are mediated by expensive rare metals, the earth abundant nickel based activation of carbon monoxide is drawing attraction not only because of its economic advantage but also its relevance to biological CO activation in acetyl-CoA synthase (ACS). ACS catalyzes the condensation of CO, methyl and CoA to generate acetyl-CoA. This biological reaction in ACS is evocative to Monsanto process in terms of substrates (CO and methyl) and reaction intermediate (M-acyl). At the active site of ACS, transmethylation of a nickel(I) carbonyl species is proposed in “paramagnetic mechanism.” With inspiration from paramagnetic nickel chemistry of ACS, we are currently developing a new reliable catalyst for the potential CO applications. We recently reported nickel(II/I/0) monocarbonyl species supported by an anionic tridentate PNP ligand and their reactivity toward iodoalkanes. While {(PNP)NiIICO}+ species does not show any reactivity toward MeI, a zerovalent congener {(PNP)Ni0CO}? undergoes a ligand exchange reaction resulting in the formation of a nickel(II) methyl species. Interestingly, (PNP)NiICO reveals unique reactivity to produce a nickel(II) acyl species (Ni-COCH3) via C-C bond coupling. Treatment of Ni(I)-CO with MeOTf results in no product formation, suggesting a radical pathway. A radical trap experiments utilizing Gomberg’s dimer indicates a formation of methyl radical at the initial stage of the reaction. Details of the reaction mechanism will be discussed.


CH$_3$I
- CO
P^{i}Pr$_2$
N
Ni
CO
1
2
+ Me•
1
(CPh$_3$)$_2$
Ph$_3$CMe
CH$_3$
4
+
5

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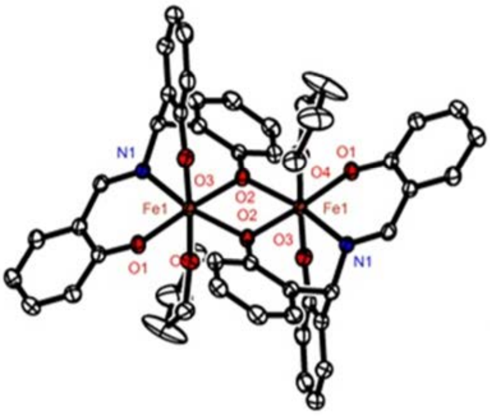
Iron Catalysts for the Selective Formation of Cyclic Carbonates from CO2 and Epoxides

배충만 김현우* 이윤호*

한국과학기술원(KAIST) 화학과

Carbon dioxide conversion to more valuable chemicals has received much attention due to its attractive advantages such as abundance, renewability, and inexpensive resource. Particularly, a coupling reaction of CO2 and epoxides to form polycarbonate or cyclic carbonates can be one of the reliable applications. In this presentation, we will present a new iron catalytic system based on our tetradentate ligands, 2,2'-(((2-hydroxybenzylidene)amino)methylene) diphenol ligand (NO3) and 2,2'-(((2-hydroxy-5-nitrobenzylidene)amino)methylene)diphenol ligand {(5-NO2)NO3}. In order to access pre-organized 6-coordiate intermediate species during catalysis, this newly designed NO3 ligand system is equipped with a planar salicylidene group and a trisubstituted carbon center possessing available cis-binding site in the metal center. Two iron complexes, {(NO3)Fe(THF)}2 (Fe-1a) and {[(5-NO2)NO3]Fe}2 (Fe-1b) were synthesized and characterized by various spectroscopic methods such as IR and UV-Vis spectroscopy as well as X-ray crystallography. X-ray analyses reveal a dimeric nature of both complexes in which two iron centers are bridged by two phenolate oxygen atoms. The catalytic reactions of CO2 with epoxides (terminal or internal epoxide) using Fe-1a and 1b were investigated. The binary FeIII system selectively produces cyclic carbonates from various epoxides in good yield within several hours (2~8 h). Particularly, Fe-1a shows a high catalytic activity (TOF > 650) in propylene carbonate generation. Detailed characterizations and catalytic reactions of CO2 with epoxides will be presented.


N1
O3
O2
O4
O1
Fe1
O2
Fe1
O1
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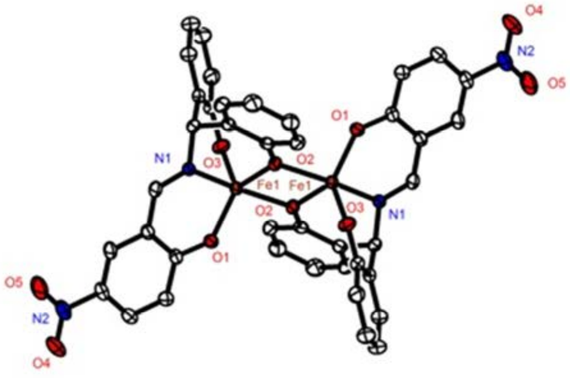
Fe-1a


O4
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Fe-1b

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Two isostructural Co-MOFs containing dipyridylporphyrin linkers with different substituents at 10,20-*meso*-positions

최인환 채승현[1] 허성[*] 이석중[1] 김영미[2]

한국외국어대학교 화학과 [1]고려대학교 화학과 [2]이화여자대학교 나노바이오 기술연구소,화학-나노과학과

Two new isostructural three-dimensional (3D) dipyridylporphyrin-based MOFs, $[Co(DpyDClP)]_6 \cdot 18H_2O$ (I) and $[Co(DpyDCNP)]_6 \cdot 18H_2O$ (II) were prepared and structurally characterized by X-ray crystallography. DpyDClP is 5,15-di(4-pyridyl)-10,20-di(4-chlorophenyl)porphyrin and DpyDCNP is 5,15-di(4-pyridyl)-10,20-di(4-cyanophenyl)porphyrin (DpyDCNP). They displayed exactly same framework structures notwithstanding different substituents at 10,20-*meso*-positions of the dipyridylporphyrin backbones. Both substituents, -Cl for I and -CN for II, are completely exposed toward the open space of solvent-free I and II. Therefore, the two MOFs contain same framework structures with distinct pore functionalities. Solvent-free I and II indicated solvent accessible void volumes of 17.3% and 14.9%, respectively. The thermal properties of I and II are very similar but the gas sorption properties strongly depend on the pore dimensions and functionalities. I exhibited larger uptake of CO_2 compared to II due to the large void volume of I. Especially, CO_2 sorption isotherms at 196 K indicated dramatically different patterns depending on the *meso*-substituents. I showed S-shape isotherms for CO_2 adsorption-desorption at 196 K while II did not show S-shape isotherms. Their gas sorption properties for N_2, H_2, and CH_4 were also investigated.

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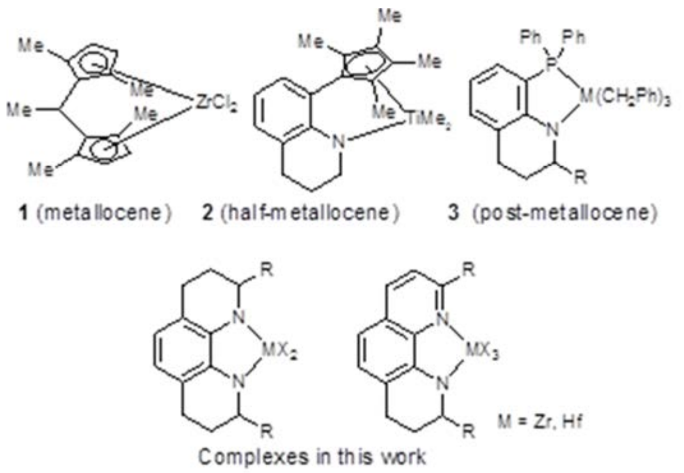
Synthesis of octahydro- and tetrahydro-[1,10]phenanthroline zirconium and hafnium complexes for olefin polymerization

박근호 이분열*

아주대학교 분자과학기술학과

Our group has synthesized a variety of group 4 metal complexes for olefin polymerizations over the last two decades. The initial endeavors focused on the preparation of ansa-zirconocenes, such as 1 (Chart 1), featuring methyl substituents adjacent to the bridge; these complexes exhibit excellent catalytic performance for ethylene/norbornene copolymerization and a-olefin oligomerization. Later, we synthesized ortho-phenylene-bridged CGC analogs, such as 2. The inclusion of a tetrahydroquinoline skeleton resulted in excellent catalytic performance in terms of activity and a-olefin incorporation, enabling the catalyst's use in a commercial process. Recently, we constructed post-metallocenes based on phosphine-amido ligands involving the tetrahydroquinoline skeleton (3). In this work, we report tetrahydro- and octahydro-[1,10]phenanthroline zirconium and hafnium complexes (Chart 1), that also feature the tetrahydroquinoline skeleton. Using 1,2,3,4,7,8,9,10-octahydro[1,10]phenanthroline derivatives, a series of zirconium and hafnium complexes were prepared. Using 1,2,3,4-tetrahydro[1,10]phenanthroline derivatives, a series of zirconium and hafnium complexes, were also synthesized. Reaction of LZrCl2(THF)2 [L = 2,9-H2-C12H12N2 or 2,9-Me2-C12H12N2] with excess Me3Al resulted in the formation of unexpected structures, i.e., L[ZrCl2(Me)][AlMe2] [L = 2,9-H2-C12H12N2 (or 2,9-Me2-C12H12N2], in which the Me2Al unit forms a five-membered ring through binding with the two nitrogen donors while the MeCl2Zr unit undergoes u4-binding with the N?C?C?N fragment. Some are potent catalysts for the production of wax-like low-molecular weight polyethylene (Mn: ~5000), which is widely used in industry.


Me
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ZrCl₂
Me
Me
Me
Me
Me
Me
Me
TiMe₂
N
Ph
Ph
P
M(CH₂Ph)₃
N
R
1 (metallocene)
2 (half-metallocene)
3 (post-metallocene)
R
N
MX₂
N
R
R
N
MX₃
N
R
M = Zr, Hf
Complexes in this work

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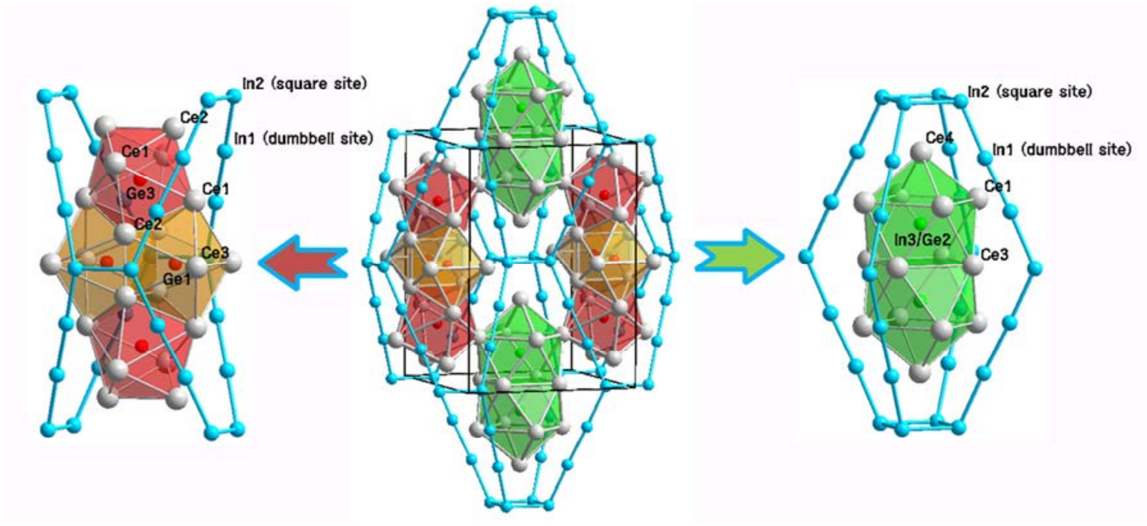
Synthesis, Crystal Structure and Electric Structure of $Ce_{11}Ge_{3.74}In_{6.26}$Indium Excess version of $Sm_{11}Ge_4In_6$

전범용 유태수*

충북대학교 화학과

$Ce_{11}Ge_{3.74(2)}In_{6.26}$ has been synthesized by high temperature reaction method using Nb-tube and characterized by powder and single crystal X-ray diffractions. The title compound crystallized in the tetragonal $Sm_{11}Ge_4In_6$-type structure (space group *I*4/*mmm*, Pearson symbol *tI*84), and Lattice parameters were *a* = 12.0163 Å and *c* = 16.5396 Å. The overall crystal structure can be described as a combination of the cage-shaped 3-dimentional (3*D*) anionic framework and three different types of cationic polyhedra filling the inside of the 3*D* framework. Theoretical investigations using tight-binding linear muffin-tin orbital (TB-LMTO) method were performed to understand overall electric structure as well as chemical bonding of $Ce_{11}Ge_{3.74(2)}In_{6.26}$.Recently, a series of polar intermetallic compounds having a general chemical formula of $A_{11}M_{10}$ (*A* = alkaline-earth metals, rare-earth metals, and *M* = triels, tetrels, pnictogens) adopting the Sm11Ge4In6-type has been widely investigated given its interesting structural and physical characteristics. In particular, two ternary indide systems including the $RE_{11}Ge_8In_2$ (*RE* = Gd-Tm) and the $RE_{11}Tt_4In_6$ (*RE* = Y, La, Gd-Er; *Tt* = Si, Ge) series have been known for their interesting magnetocaloric effects and our group has recently reported two compounds in this series including $La_{11}Ge_4In_{5.00(1)}$ $Li_{1.00}$ and $Ce_{11}Ge_{5.96(3)}$ $In_{4.04}$ with respect to their interesting anisotropic expansion of the anionic framework during the substitution. During our systematic investigation for the anion substitution in the $RE_{11}Ge_{10\text{-}x}In_x$ (*RE* = La, Ce, Gd-Er, Y) system, we previously reported $Ce_{11}Ge_{5.96}In_{4.04}$. Among the known $RE_{11}Ge_{10\text{-}x}In_x$ (*RE* = La, Ce, Gd-Er, Y) series, it has been known that the maximum contents of In substitution for Ge is limited to 6, which indicates the substitution can occurs only at the positions on the framework excluding three isolated Ge sites. However, during our systemic investigation to study the phase-width of the $Ce_{11}Ge_{10\text{-}x}In_x$ phase by varying the ratio between In and Ge, we successfully synthesized $Ce_{11}Ge_{3.74(2)}$ $In_{6.26}$ having the In substitution even at the one of the isolated Ge-site. The site-

preference of the In substitution for Ge follows the size-factor, and the electronic factor seemed to contribute a small influence.



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Synthesis of Palladium(II) complexes containing phosphine and NHC ligands with bulky aryl group and their catalytic activity towards norbornene polymerization

이동진 이익모*

인하대학교 화학과

Pd(II) complexes containing various NHC(N-heterocyclic carbene) ligands have been successfully synthesized by the reaction with phosphines.Treatments of dinuclear NHC-Pd complexes ($[Pd(\mu\text{-}Cl)Cl(NHC)]_2$, (NHCs=IPr,IXy,IMes)) with phosphine such as PPh_3 resulted in new $Pd(NHC)(PPh_3)Cl_2$ complexes and these complexes are characterized by NMR and elemental anaylsis.Moreover, these new palladium complexes showed moderate to good catalytic activities towards norbornene polymerization.

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Preparation, crystal structures and physical properties of supramolecules obtained from the combination of polyazamacrocyclic complexes and tetracyanometallate(II)

서민지 곽지훈[1,*]

순천대학교 화학과 [1]순천대학교 화학교육과

Coordination networks have attracted considerable attention because not only they have an interesting and intrigue architectural pattern but also they are applicable in the field of molecular magnet, sensor, non-linear optics, host-guest chemistry, separation, gas adsorption, etc. We have described some of the supramolecular complexes by using coordination or hydrogen bonding, and the combination of them, and reported interesting multidimensional structures as well as magnetic and photophysical properties from some of obtained supramolecules. Recently, supramolecules from the self-assembly of polyazamacrocyclic complexes and tetracyanometallate(II) were prepared and multi-dimensional structures were characterized. In this presentation, details of the design and preparation of new supramolecules from this work and physical properties of them will be described.

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The Carbon-Coated V_2O_5 Nanoparticles Prepared from MIL-47(V) Metal-Organic Framework as a Cathode Material for Li Rechargeable batteries

김태경 김종식*

동아대학교 화학과

Vanadium pentoxide (V_2O_5) is one of the most promising cathode materials for lithium-ion batteries (LIBs) due to the easy synthesis, abundant sources, and relatively high theoretical capacity (about 294 $mAhg^{-1}$ at 2.1-4.0 V), compared with more commonly used cathode materials such as $LiCoO_2$ (140 mAh g^{-1}) and $LiFePO_4$ (170 mAh g^{-1}). Despite these advantages, the capacity retention of V_2O_5 is relatively worse because of its poor structural stability, low electroconductivity, and sluggish Li ion diffusion. For these reasons, practical applications of V_2O_5 are difficult. In this work, the carbon-coated V_2O_5 nanoparticles are simply synthesized through a controlled thermal decomposition of MIL-47(V) metal-organic framework (MOF) used as a vanadium precursor. MIL-47(V) is built up from infinite chains of corner-sharing VO_6 octahedra interconnected by dicarboxylate groups, which act as a carbon source. The highly crystalline V_2O_5 nanoparticles prepared from MIL-47(V) are coated with a carbon layer of thickness approximately 2-4 nm. The carbon-coated V_2O_5 nanoparticles exhibit an enhanced initial discharge capacity of about 274 mAh g^{-1} in the voltage range of 2.1-4.0 V at 0.1 C rate and good capacity retention of about 85 % after 50 cycles. Even at high current density of 1 C rate, its capacity fading rate is 0.48 % per cycle, which exhibits excellent cycling stability.

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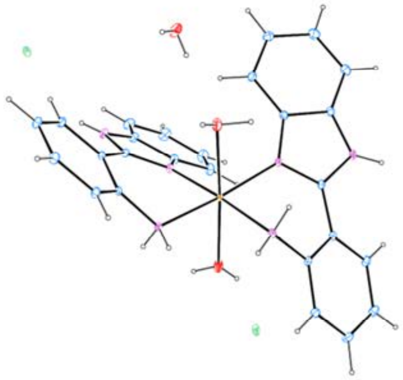
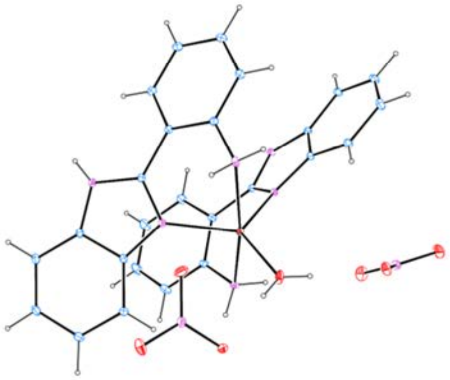
Structures and Spectroscopic Properties of Cu(II) and Zn(II) Complexes with 2-(2-aminophenyl)-1*H*-benzimidazole

김용태 강성권[*]

충남대학교 화학과

The Cu(II) and Zn(II) complexes with 2-(2-aminophenyl)-1*H*-benzimidazole(APBI) were designed and synthesized. The complexes were investigated by IR, UV-Visible spectroscopy and single crystal X-ray crystallography. The APBI ligand is coordinated to the Cu(II) and Zn(II) metals as a bidentate N,N ligand. Geometry around Cu(II) is the distorted octahedral with two N atoms of imidazole, two N atoms of amine and two O atoms from water molecules. And geometry around Zn(II) is the distorted trigonal bipyramidal with two N atoms of imidazole, two N atoms of amine and one O atom from water molecule.





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Solid-state Conversion Chemistry of Multicomponent Nanocrystals Cast in a Hollow Silica Nanosphere: Morphology-controlled Syntheses of Hybrid Nanocrystals

김연준 이인수*

포항공과대학교(POSTECH) 화학과

In the course of investigating the thermal transfor-mation of multicomponent nanocrystals in a silica nanosphere, FeAuPd alloy nanocrystals were found to mi-grate outward, thereby leaving a cavity in the silica me-dium. Through oxidation, these nanocrystals were then converted back into phase-segregated hybrid nanocrys-tals, AuPd@Fe_3O_4, with various morphologies, such as bumpy sphere, dumbbell, three-ball-snowman, and mushroom. The FeAuPd-to-AuPd@Fe_3O_4 transfor-mation was cast by the in situ generated hollow silica mould. Therefore, the morphological parameters of the transformed AuPd@Fe_3O_4were defined by the degree of migration of the FeAuPd in the hollow silica nanoshell. This hollow silica-cast nanocrystal conversion was elu-cidated in order to develop a novel solid-state protocol for producing a range of hybrid nanocrystals and which allows for the systematic and sophisticated control of the resulting morphologies.

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Metal(II) and halogen effects on construction of flexible helical complexes of bis(3-pyridyl)cyclotetramethylenesilane, catalysis, luminescence, and thermolysis

김혜은 정옥상*

부산대학교 화학과

Infinite rectangular-tubular helices, [MX_2L] (M = Zn(II), Hg(II); X^- = Cl^-, Br^-; L = bis(3-pyridyl)cyclotetramethylenesilane), have been efficiently constructed via the combined effects of the potential flexible conformers of L and the tetrahedral geometry of M(II) ions. This helical molecular system affords the racemic mixture of *P*- and *M*-helices in a crystal. The helical pitches (7.8934(4)-8.1560(2) Å) that are sensitive to the natures of M(II) ions and halide anions are attributable to subtle change in the flexible dihedral angles between the two pyridyl groups around Si and the M(II) hinges. Their photoluminescence intensities, correspondingly, are in the order [$ZnCl_2L$] > [$ZnBr_2L$] >> [$HgCl_2L$] > [$HgBr_2L$]. Zinc(II) complexes show recyclable catalytic effect on the transesterification reaction in the order [$ZnCl_2L$] > [$ZnBr_2L$]. Calcination of [$ZnCl_2L$] and [$ZnBr_2L$] at 500 °C produces uniform hexagonal tubular spire crystals of 1.2 × 1.2 × 4.0 μm^3 dimension and spheres, respectively.

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Interfacial Effects of Metallacyclodimers Containing Two Free Quinolinyl Donors on Crystal Organization and Catalysis

김병주 정옥상*

부산대학교 화학과

Reaction of MX_2 (M = Cu(II), Hg(II); X^- = Cl^-, Br^-) with C_3-symmetric tris(6-quinolyl)trimesic ester (L) produces crystals consisting of C_2-symmetric metallacyclodimeric species with two free quinolinyl *N*-donors, $[CuX_2L]_2$. The crystals self-aggregate each other in aqueous media. Furthermore, the reaction with cotton threads and glass-fibers form unique crystal organization on/with cotton threads and glass fibers, respectively. Such crystal aggregation/organization may be ascribed to the hydrogen bonding interactions between the free quinolinyl *N*-donors and the hydroxyl (-OH) groups of water, cotton-threads, or glass-fibers. The composite organization of crystals on/with glass-fiber, $[CuX_2L]_2$@glass, is an effective recyclable heterogeneous catalytic system on catechol oxidation, indicating that the free quinolinyl *N*-donors on the crystal surface play a significant role in the catalysis. The treatment of $[CuX_2L]_2$ crystals with K_2PdCl_4 produces a conceptually advanced composite materials $PdCl_2$@$[CuX_2L]_2$ via Pd(II)-N interaction, which are useful to Suzuki-Miyaura C-C coupling reaction.

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Construction and properties of M_6L_8 octahedron nanocages: indistinguishability and distinguishability depending on the ligand containing amide and ester moieties

이해리 정옥상*

부산대학교 화학과

A series of 25 × 25 × 25 A^3 octahedral coordination cages $[Pd_6(L)_8](NO_3)_{12}$ (L = L^1, 1; L= L^2, 2; L^1 = tris(6-quinolyl)trimesic ester; L^2 = *N*,*N'*,*N"*-tris(6-quinolyl)-1,3,5-benzenetricarboxamide) is reported. L^1 and L^2 are indistinguishable for construction of octahedral nanocages, and thus the desirable mixed ligands nanocage comprising a statistical ligand distribution ($[Pd_1(L^1)_n\ (L^2)_{8-n}](NO_3)_{12}$, 3) can be efficiently constructed. However, the nanocages are distinguishable for functions such as photoluminescence (PL) and catalysis. The PL intensity is in the order 1 >> 3 > 2, wherein 1 shows a blue emission. The nanocages show excellent catalytic activity for the C-C coupling reaction under mild conditions in the order 1 > 3 > 2, presumably owing to the spacer-functional groups.

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Synthesis, Crystal Structures, and Physicochemical Properties of 1D Silver(I) Complexes Containing C_2-Symmetric Tridentate Ligands

김정균 정옥상*

부산대학교 화학과

The unique C_2-symmetric tridentate ligands, 2,6-bis[(2-picolinoyloxy-5-methylphenyl)methyl]-*p*-tolylpicolinate (L^1), 2,6-bis[(2-nicotinoyloxy-5-methylphenyl)methyl]-*p*-tolylnicotinate (L^2), and 2,6-bis[(2-isonicotinoyloxy-5-methylphenyl)methyl]-*p*-tolylisonicotinate (L^3), have been prepared and their silver(I) compounds have been synthesized via self-assembly of silver(I) hexafluorophosphate with the ligands. Single crystal X-ray diffraction measurement reveals that the silver(I) complexes are consisting of 1D coordination polymeric structures of $[Ag(L^1)]PF_6\cdot Me_2CO\cdot 0.5CHCl_3$, $[Ag(L^2)]PF_6\cdot Me_2CO$, and $[Ag_3(L^3)_2](PF_6)_3\cdot 2H_2O\cdot 2C_2H_5OH\cdot 4CH_2Cl_2$, respectively. The present silver(I) compounds are thermally stable up to 270 °C. For $[Ag(L^1)]PF_6\cdot Me_2CO\cdot 0.5CHCl_3$, the solvate molecules can be removed and absorbed reversibly, without the destruction of the skeletal structure and the metallacyclodimeric moieties can incorporate the solvents in the order of acetone > chloroform >> benzene. The present ligands and silver(I) complexes have been investigated via IR, NMR, SEM, and photoluminescence (PL) measurements.

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Synthesis of New Topological 3D Cu(II) Complexes Containing Functional Pores: Catechol Oxidation Catalysis and Solvent Adsorption via Porous Properties

김도언 정옥상*

부산대학교 화학과

The reaction of CuX_2 (X^- = ClO_4^- and BF_4^-) with a new 1,3,5-tris(isonicotinoyloxymethyl)benzene (L) ligand gives rise to 3D coordination networks, $[Cu_3L_4(CH_3CN)_6](X)_6$, with new topology of a Schl?fli point symbol, $\{4{\cdot}8^2\}_4\{4^2{\cdot}8^2{\cdot}10^2\}_2\{8^4{\cdot}12^2\}$. The 3D networks basically have oval-shaped pores with the dimensions of 11.2 × 11.2 × 24.8 Å^3 and 11.1 × 11.1 × 24.4 Å^3 for $[Cu_3L_4(CH_3CN)_6](ClO_4)_6$ and $[Cu_3L_4(CH_3CN)_6](BF_4)_6$, respectively.The 3D porous coordination networks act as good heterogeneous catalysts, which oxidize the catachols in the order of 3,5-DBuCat > 4-BuCat > 4-ClCat. The catalytic effect of $[Cu_3L_4(CH_3CN)_6](BF_4)_6$ is slightly higher than that of $[Cu_3L_4(CH_3CN)_6](ClO_4)_6$. The pores of the 3D networks reversibly adsorb the solvents in the order of $CHCl_3$ > THF > Me_2CO.

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발표분야: 무기화학

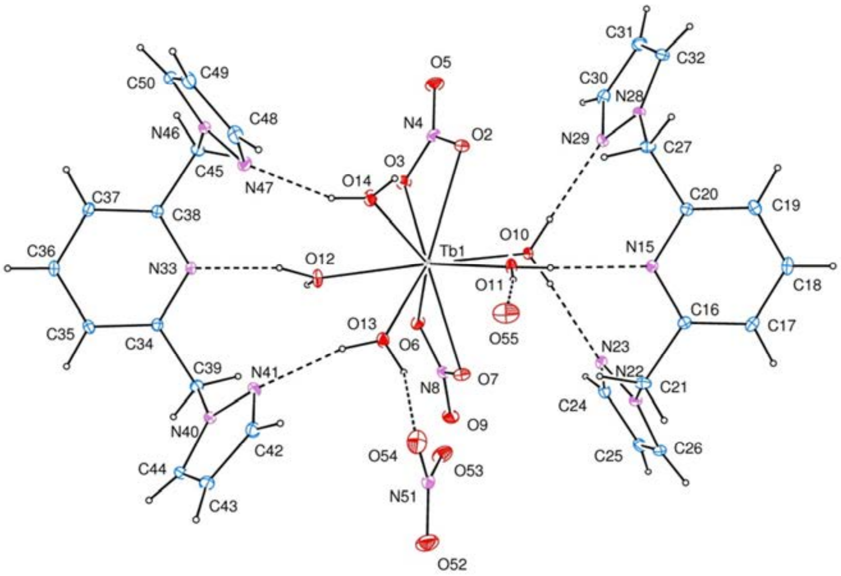
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cocrystallization and Optical Properties of Lanthanide Metals and 2,6-bis((1*H*-pyrazol-1-yl)methyl)pyridine (PMP)

김대영 강성권*

충남대학교 화학과

Tridentate NNN ligand, 2,6-bis((1*H*-pyrazol-1-yl)methyl)pyridine (PMP), were designed and synthesized. Reaction with lanthanide nitrate salts leads to cocrystallization of organic ligand and inorganic salt in one single crystal. The coordination geometry around the europium (III) and terbium (III) ion are distorted tricapped trigonal prism, with the metal nine-coordinated by nitrate O atoms and H_2O. The complexes were investigated by UV, PL spectra and single crystal X-ray crystallography.


C31
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O9
O54
C26
C25
O53
C44
N51
C43
O52

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CO2/epoxide copolymerization catalyzed by Zinc complexes containing alkyl and aryl substituted β-ketoiminate ligands

이병기 이익모*

인하대학교 화학과

Even though aryl-substituted β-diketiminato zinc complexes have been prepared and investigated for the copolymerization of CO2/epoxide, studies with alkyl and aryl substituted β-diketiminato zinc complexes are rare. Recent efficient syntheses of alkyl and aryl substituted β-diketimines make it possible to investigate the electronic and steric effects on the catalytic behaviors of new Zn complexes for CO2/epoxide copolymerization. Preparation and characterization of these new ligands and complexes and catalytic behaviors for CO2/epoxide copolymerization will be presented.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel heteroleptic cobalt complexes

한성호 정택모[1,*] 김창균[2] 박보근[2] 손성욱

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

Cobalt and cobalt oxide have been applied in many fields such as optical gas sensor, catalysts for oxidation reaction, electrochromic devices, high temperature solar selective absorbers, magnetic materials, and negative electrodes for lithium-ion batteries. In particular, noticeable features of the cobalt are high catalytic activity, antiferromagnetism, and electrochromism. We have synthesized novel heteroleptic cobalt complexes with combination of β-diketonate and aminoalkoxide ligands. The complexes were prepared with simple substitution reactions using Co(II) bis(trimethylsilyl)amide as a starting material. All these complexes were characterized by infrared spectra (FT-IR), elemental analyses (EA), thermogravimetric analysis (TGA), mass spectroscopy and single crystal X-ray diffraction. The studies to deposit cobalt thin films using novel heteroleptic cobalt complexes by various deposition techniques are ongoing.

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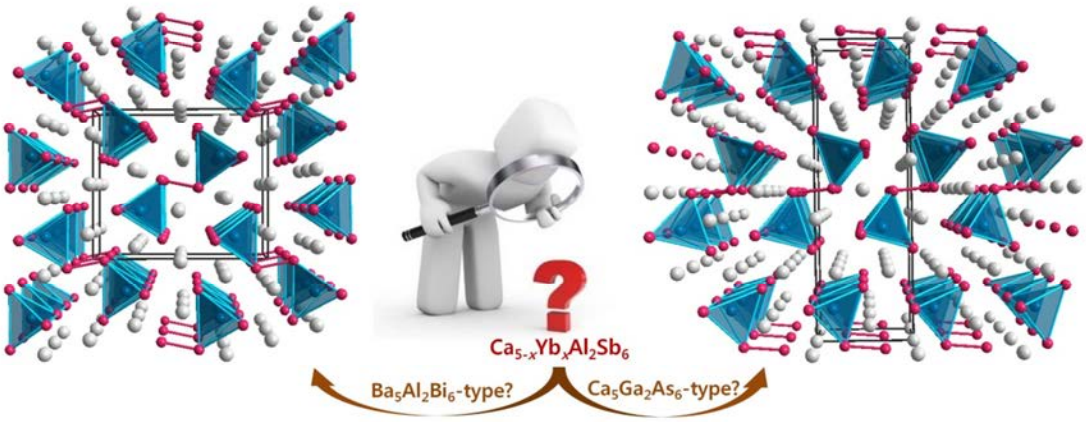
The Correlation between Structural Transformation and Thermoelectric Behavior of the $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1-4) Series

남근우 유태수*

충북대학교 화학과

Four quaternary derivatives of the $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1-4) series have been synthesized by the arc-melting method under an argon filled atmosphere, and the crystal structures have been characterized by powder X-ray diffractions for all compounds and single crystal X-ray diffractions for $Ca_{2.78}Yb_{2.22}Al_2Sb_6$. The $Ca_{2.78}Yb_{2.22}Al_2Sb_6$ crystallized in the orthorhombic $Ca_5Ga_2Sb_6$-type structure (space group *Pbam*, Pearson code *oP*26), and the lattice parameter was a = 12.03, b = 14.02 and c = 4.45 Å. Chemical analysis using energy dispersive X-ray spectroscopy (EDS) was also performed to verify chemical compositions of four title compounds including the ratio between Ca and Yb cations.As the amount of Yb substitution for Ca increased in the $Ca_{5-x}Yb_xAl_2Sb_6$ series, a structural transformation was observed : in two compounds having relatively larger Ca contents (x = 1, 2), the $Ca_{5-x}Yb_xAl_2Sb_6$-type structure was observed; whereas in two compounds with relatively smaller Ca contents (x = 3, 4), the $Ba_5Al_2Bi_6$-type structure (space group *Pbam*, Pearson code *oP*26) was adopted. Two crystal structures share the structural similarities, such as the one-dimensional $[Al_2Sb_6]^{10-}$ double chain composed of the $[AlSb_4]$ tetrahedra and the connecting Sb_2 dimers, and the space filling Yb and Ca atoms. However, a subtle spatial distribution of these structural components differentiates two structure types as well. The site-preference of cationic Yb for available cationic sites was investigated based on the coloring-problem using theoretical calculations. The overall electronic structure and chemical bonding for four title compounds were thoroughly studied using density of states (DOS) and crystal orbital Hamilton population (COHP) curve analyses.


?
$Ca_{5-x}Yb_xAl_2Sb_6$
$Ba_5Al_2Bi_6$-type?
$Ca_5Ga_2As_6$-type?

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Synthesis and Characterization of a Mononuclear Nickel(ll)-Borohydride Complex

탁현우 조재홍*

대구경북과학기술원(DGIST) 신물질과학

Synthetic chemists have long appreciated a huge number of reactions of transition metal hydride complexes, especially in reductions. In this work, nickel(ll)-borohydride complex, [Ni(Me3-tacn)(BH$_4$)]$^{2+}$(Me3-TACN = 1,4,7-Trimethyl-1,4,7-triazacyclononane), was synthesized by the reaction of [Ni(Me3-tacn)(CH3CN)3]2+ with 1 equiv. of NaBH$_4$ under the N$_2$ atmosphere at -20℃. The complex is stable in air after isolation. The nickel(II)-borohydride complex was characterized with various physicochemical methods. The isotope shifts of BH4/BD4 were investigated by ESI-MS and FT-IR. We will discuss about the reactivity of the nickel(II)-borohydride adduct toward external organic substrates.

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A Hollow Assembly and Its Three-Dimensional Network Formation of Single-Crystalline Co3O4 Nanoparticles for Ultrasensitive Formaldehyde Gas Sensors

김진모 송현준*

한국과학기술원(KAIST) 화학과

Formaldehyde is an industrial chemical that is widely used to manufacture building materials and household products. One problem with formaldehyde is, however, its detrimental impact on human health, owing to its potentially carcinogenicity and its capability of forming toxic intermediates. The detection of formaldehyde at a very low concentration is a significant research topic, due to its detrimental impact on human health. In the present study, we fabricated a hierarchical structure by the rational assembly of single-crystalline Co3O4 nanoparticles. A hollow morphology using sacrificial ZnO spheres could form a three-dimensional conducting network in a solid state. The resulting structure was selectively active for formaldehyde sensing, and the detection limit was 50 ppb, which was nearly close to the record-high value among the other semiconducting materials. Such superior properties were attributed to the regular, hierarchically assembled structures with a small crystalline domain size, a thin hollow morphology with a large surface area, and a three-dimensional conductive network with a narrow diameter. We believe that this hierarchical assembly can show great potential as a platform for improving human health through the monitoring of indoor environments.

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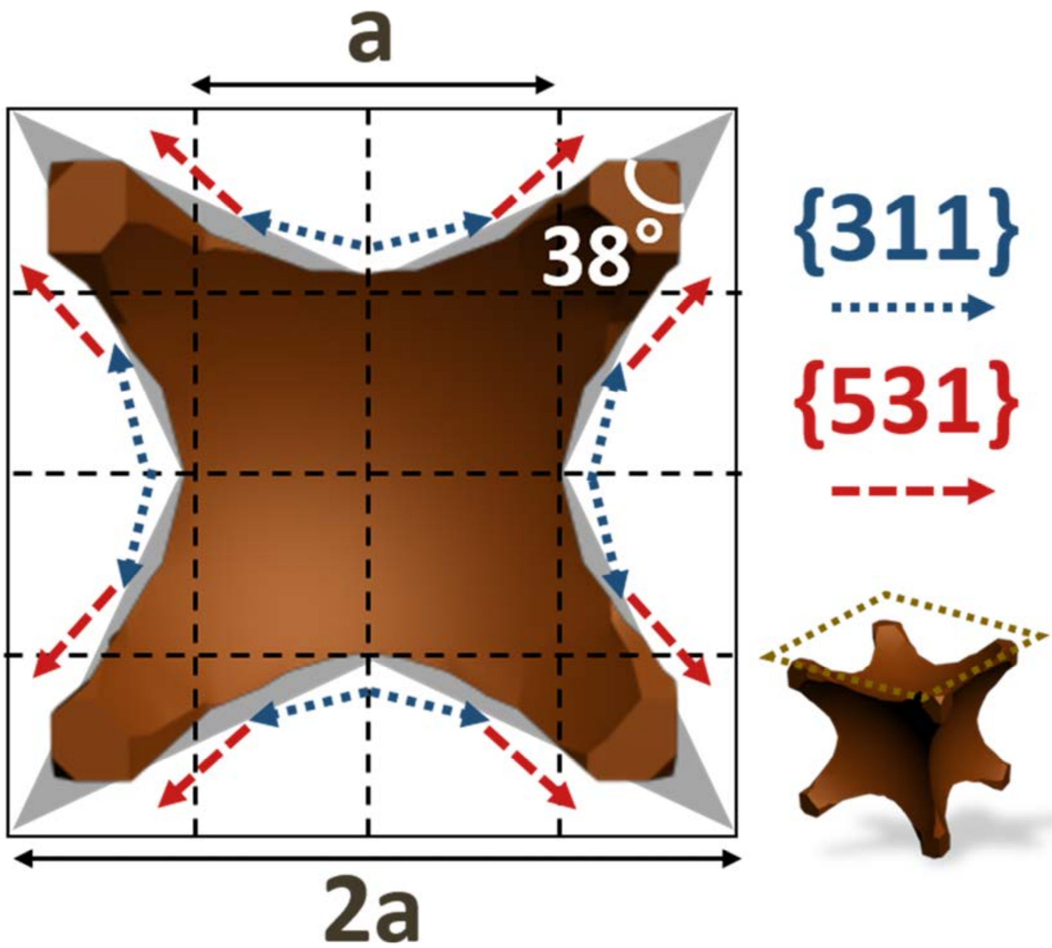
Selective Formation of Regular MnO Nanooctapods Bearing Multiple High-Index Surface Facets

신동우 송현준*

한국과학기술원(KAIST) 화학과

Complex nanostructures with the surface of high-index facet was widely studied for generating catalytic activity in the last year. Among several high-index facet nanostructures, octapod metal nanostructures have been developed for various applications such as changing contrast extension in magnetic resonance images. In our report, we demonstrate the particle synthesis, properties analysis of octapod MnO. The single crystalline octapod MnO nanoparticles were synthesized by thermal decomposing Manganse-Oleate complexes. Oleate was one of the key factors in growth mechanism of ocatapod structures. Oleate ions bound to (100) facets. This particles with a diagonal distance and body width of 47.4±1.7nm and 21.8±2.8nm were easily oxidized to hausmannite Mn_3O_4 in the air condition. Because of their structural uniformity, an ideal three-dimensional model was successfully constructed. The eight arms protruded from the cubic center with the tip angles of 38^o and the surface facets of {311} and {531}. {531} facets were shown at the edge-on of the pods and {311} facets were shown at the edge-on of the body. The ratio of the outer and inner diameter of boundary line was 2: 1 and the edge-on slope was 1/2, and the summation facet could satisfy the x-y atom unit ratio. We can estimate that the edge-on facet composition of octapod was {531}: {311} = 1: 1. Chloride ion was also the growth factor in formatting octapod structure. Adding chloride ions could increase the particle size and maintain the octapod shape at the same time. Chloride ions stabilized the high-index facet of octapod, so the nanoparticle could grow bigger. XPS data showed that chloride ions were binding to MnO.


a
38°
{311}
{531}
2a

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Synthesis of Copolymers Containing 1,1-Diisopropyl-3,4-diphenylsilolene and Disubstitutedsilylene and their Applications to Lithium-ion Battery

정영민 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diisopropyl-3,4-diphenylsilole as monomer was prepared by the intramolecular reductive cyclization of diisopropylbis(phenylethynyl)silane with treatment of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide *in situ*. We have synthesized new polymeric materials (DPS polymers) of polycarbosilanes containing 1,1-diisopropyl-3,4-diphenyl-2,5-silole and disubstituted silane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diisopropyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane using n-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and $CDCl_3$. The prepared materials were characterized by GPC, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular. Characteristically, the DPS polymers have highly stable cycle life and the capacities also increase continually in each C-rate.

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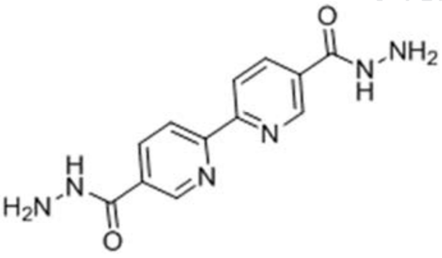
Triple Helix of Bipyridine-Based Gels with Chiral Dopant

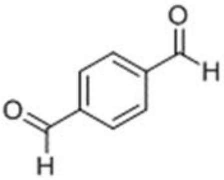
최희경 이지하 정성호 정종화*

경상대학교 화학과

Bipyridine-based compound 1 and 2 were synthesized by hydrazone reaction. Compound 1 and 2 could be gelated in DMSO with and without (1S,2S)-(+)-1,2-cyclohexanediamine by hydrazone reaction. The gel 1 was characterized by SEM, CD, Rheometer. SEM images of gel 1 showed the fiber structure. In particular, CD spectrum of gel 1 with Fe^{2+} exhibited higher than that of without Fe^{2+}. The results indicate that gel 1 with Fe^{2+} forms the triple helical structure. We also observed CD spectra of gel 1 with and without Fe^{2+} by changing temperature. The CD intensity changes of gel 1 with Fe^{2+} were smaller than that of without Fe^{2+}. In this conference, we will present on triple helix of bypyridine gel 1 with Fe^{2+}.



Compound **1**



Compound **2**

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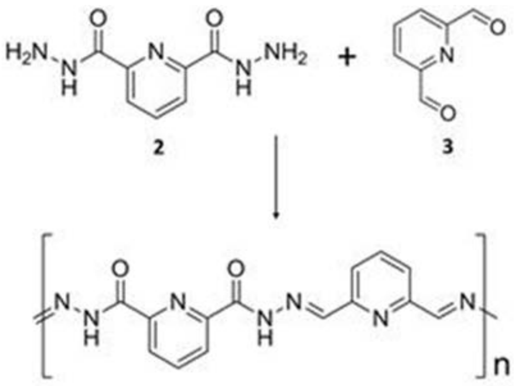
Pyridine- Based Supramolecular Gel Induced by Hydrazone Bond

최연원 정종화*

경상대학교 화학과

A pyridine-based hydrazine moiety possessing compound (2) was synthesized in one step and the compound 2 was reacted with compound 3 which contains aldehyde group at terminal in dimethylsulfoxide with various concentrations of hydrochloric acid to afford supramolecular gels via formation of hydrazone bond in several minutes. Chemical and physical properties of the supramolecular gels were studied by rheological analysis, differential scanning calorimetry, fluorometric analysis, and the formation of hydrazone bond between 2 and 3 was confirmed by IR and NMR spectroscopy. Interestingly, the gel could exchange containing solvent, dimethylsulfoxide for water by putting the gel in aqueous media. The hydrogel produced by solvent exchange showed higher viscosity and elasticity than dimethylsulfoxide containing gel. The supramolecular gel prepared by facile and fast process is expected to be a contributable material for design and development of supramolecular hydrogels.



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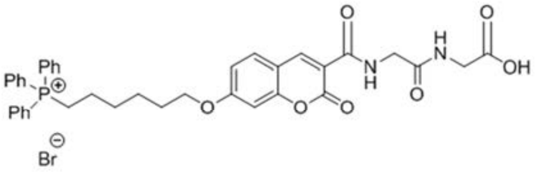
미토콘드리아를 타겟으로 하는 트리페닐포스페이트 유도체 합성

백영은 정성호 정종화*

경상대학교 화학과

본 연구에서는 미토콘드리아를 타겟으로 하는 트리페닐포스페이트와 형광 유도체인 쿠마린을 도입한 화합물 1 을 합성하였고, 미토콘트리아에 도달하여 항암제로 작용하는 doxorubicin 과 hydrazone 결합을 유도하여 약물운반체인 화합물 7 을 합성하였다. 화합물 1 과 화합물 7 을 섞은 후 PH=7 에서 적당한 열을 가하여 마이셀을 제조하였다. 마이셀의 크기는 입도분석기와 SEM 을 이용하여 분석하였다. 그 결과 대략 50~200 nm 정도의 구형모양을 가지고 있었다. 그리고 마이셀의 형광 특성을 형광분광기로 연구하였다.



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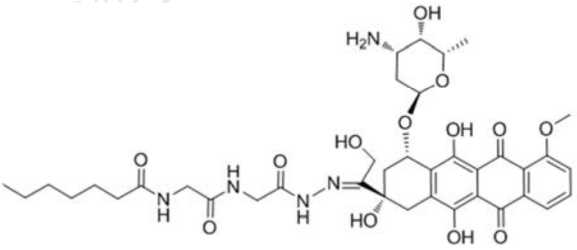

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C3대칭 리간드를 이용한 배위고분자 입자의 제조

차유빈 정성호 정종화*

경상대학교 화학과

금속이온과 여러자리 결합을 할 수 있는 작용기와 카이랄 센터를 동시에 가지고 있는 C3-대칭리간드를 이용하여 아연이온의 존재 하에서의 다양한 조건변화를 통해 MOF(Metal-Organic Frameworks)형 CPPs(Coordination Polymer Patricles)제조 및 모폴로지의 제어를 연구하였다. L-TMTAH3(L-TrimesoylTriAlanine) 리간드가 DMF 용매에서 아연이온과의 반응으로 구형의 속 빈 모폴로지가 생성 되었다. 아연 이온의 농도 변화에 따라 모폴로지 변화를 주는 것을 확인 하였다. 또한, Zn-TA-DMF(Zinc-Terephthalic Aicd-Dimethyl Formamide)시스템에서의 L-TMTAH3 리간드가 아연이온이 2.0Equiv. 일 경우에 속 빈 사각큐브의 형태를 형성하였다. 그 결과 조건의 변화에 따라 모폴로지의 형태를 제어할 수 있었으며, 모폴로지 제어를 통한 형태제어 및 응용방안을 연구하였다.

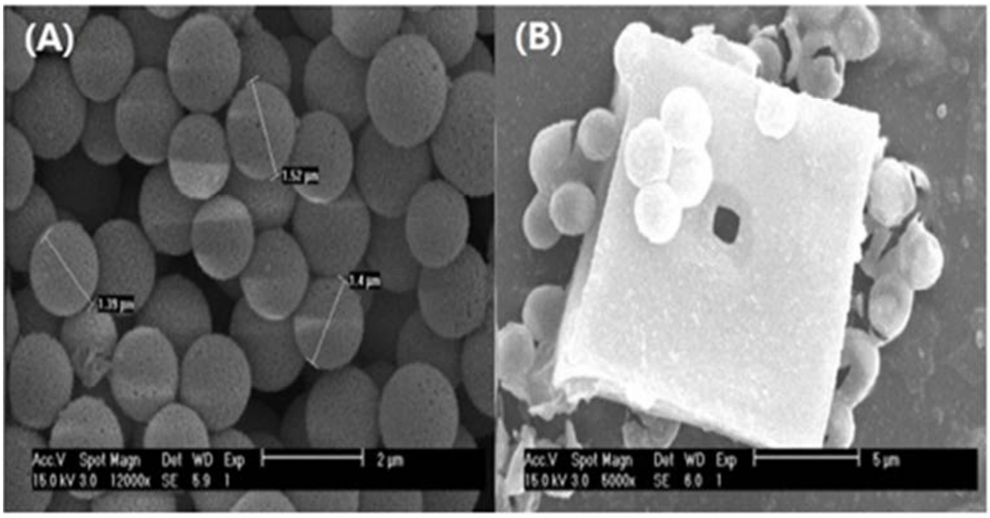

Figure 1 (A) L-TMTAH$_3$와 Terephthalic Acid 리간드를 이용한 Zn(NO$_3$)$_2$의 MOF의 SEM 이미지 (B) Zn(NO$_3$)$_2$의 당량 변화(2equiv.)로 인한 모폴로지의 변화

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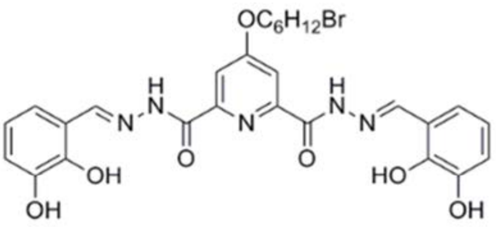
고감도 및 고선택성 세슘 이온에 대한 형광센서

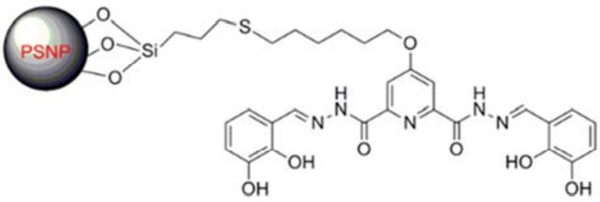
박정수* 정성호 정종화*

경상대학교 화학과

본 연구에서는 Cs^+를 검출하는데 있어서 선택성이 기대되는 리간드를 합성하고 이 리간드를 이용한 유기-무기 하이브리드 센서 개발을 목적으로 화합물 4 (Rigand 2)를 합성하였다. 기존에 발표 되었던 세슘 이온을 선택적으로 검출 할 수 있는 리간드에 실리카와 합성하여 센서물질로 만들기 위해 알킬사슬을 붙여 새로운 리간드를 합성하여 이 리간드도 Cs^+에 선택적으로 검출 할 것으로 예상하여 이 리간드를 설계 하였습니다.마찬가지로 기존에 발표되었던 리간드와 세슘 이온이 결합한 complex 가 형성 되면서 광 유발 전자전이로 인해 형광이 나타나므로 화합물 4 (Rigand 2)도 세슘 이온과 결합하여 complex 가 형성 되면서 광 유발 전자 전이로 형광이 나타날 것으로 예상한다. 따라서 화합물 1 (Rigand 1)이 세슘 이온의 검출에 다양한 용도로 사용될 수 있을 것으로 판단된다.



화합물 4



화합물 1

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발표종류: 포스터, 발표일시: 수 16:00~19:00

코발트 금속 이온의 당량에 따른 초분자 구조 제어

박혜송 이지하 정종화*

경상대학교 화학과

본 연구는 터피리딘 유도체와 코발트 금속 이온이 배위 고분자 젤을 형성하면서 코발트 금속 이온의 당량에 따라 발생하는 초분자의 구조 제어에 대한 것이다.먼저 터피리딘 유도체의 구조 분석을 NMR, MS 등으로 확인하였다. 터피리딘 유도체는 코발트 금속 이온이 0 당량에서 1 당량 존재할 때 초분자 젤이 제조되었다. 이 때 코발트 착물의 구조 변환을 CD 와 UV 로 측정하고 특정 당량에서 나선방향의 반전이 일어나는 것을 확인하였다. 또한 나선 방향의 반전을 AFM, SEM 을 통한 분자이미지 관찰을 하였다.따라서 본 학회에서는 터피리딘 유도체와 코발트 이온과의 착물에 의한 초분자 젤의 구조 제어에 대해서 발표할 것이다.

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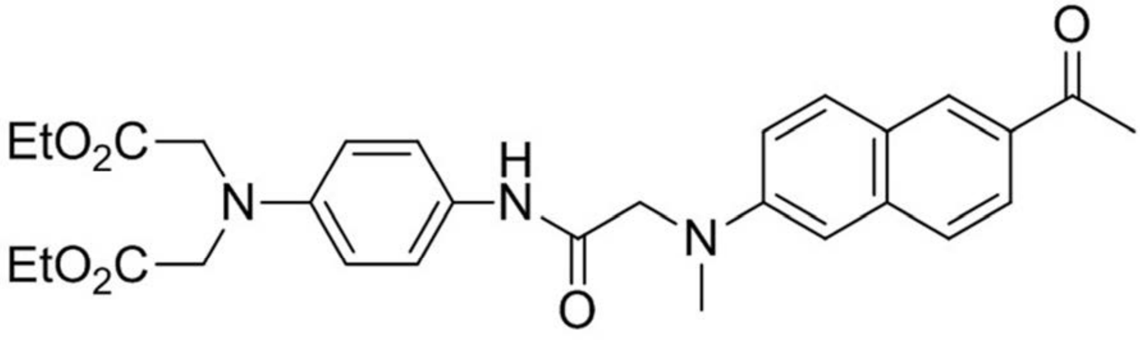
나프탈렌기를 기본으로 한 아연 센서 및 바이오 이미징

문규리 정성호 정종화[*]

경상대학교 화학과

화합물 1 은 나프탈렌과 아닐린에 이미노다이아세테이트를 도입하여 합성하였다. 화합물 1 의 최대 흡수 및 방출 파장 세기는 UV 및 형광 분광기를 사용하여 확인하였다. 화합물 1 은 경쟁 금속 이온의 존재 하에서 아연 이온을 첨가함에 따라 강한 형광을 나타내었다. 화합물 1 의 pH 효과는 다양한 pH 조건에서 형광 분광기를 이용하여 최적의 pH 범위를 찾아내었다. 이 결과를 바탕으로, 화합물 1 은 세포 내에서 아연 이온을 감지하였다. 공초점 형광 현미경으로 관찰한 결과, 화합물 1 은 아연 이온이 존재하는 세포 내에서 강한 형광을 나타내었다. 따라서, 화합물 1 의 소수성기는 지질 이중층으로 이루어진 세포막을 비교적 용이하게 통과하는 것으로 판단된다.



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Arabidopsis thaliana SPL14전사인자에 결합 가능한 DNA duplex가 도입된 금 나노입자 응집체를 이용한 단백질 검출 기술

안준호 이준화 정종화*

경상대학교 화학과

DNA 가 도입된 금 나노입자는 말단에 싸이올 기를 지니는 상보적 DNA 를 각 금 나노입자 표면에 salt aging 방법으로 도입하여 제조 하였고, 이는 IR 분광기를 통해 확인하였다. DNA 간의 수소결합으로 형성되는 금 나노입자 응집체의 분석은 UV-Vis 분광기, 입도분포 측정기, TEM 을 이용하였으며, 약 2 nm 정도의 입자간 거리를 두고 금 나노입자 응집체를 형성하는 것을 확인할 수 있었다. 이중나선을 형성한 채 응집된 금 나노입자는 SPL12 의 첨가로 UV-Visible 영역 내에서 파장의 이동이 관찰되었다. 관찰된 파장의 이동은 UV-Vis 분광기, 투과전자현미경, 입자크기분포를 통해 단백질-DNA 의 결합을 이루어 유발된 것임을 확인하였다. 첨가되는 단백질 양에 따라 파장이동의 변화를 UV-VIS 분광기로 확인 하였으며, 대조군 단백질로 BSA(Bovine serum albumin)을 사용하여 단백질-DNA 간의 선택적 결합이 이루어진다는 것을 UV-Vis 분광기와 입자크기분포 분석을 통해 증명하였다. Wild type DNA duplex 의 Imino peak 영역대의 1D NMR 분석을 통하여 SPL12 가 DNA duplex 와 상호작용 함으로써 입자간 응집 특성에 관여한다는 것을 확인할 수 있었다. 이를 통해 DNA 가 도입된 금 나노입자가 SPL12 결합성 염기서열이 포함된 DNA duplex 을 형성하며 응집되면 SPL12 단백질로 인해 더욱 응집이 심화된 입자를 형성하는 것을 확인하고 DNA duplex 와 SPL12 단백질 상호작용에 기인한 것이라는 것을 증명하였다.

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Selective Formation of Ru-Ag Heterometallic Supramolecules via Stoichiometrically Controlled Coordination-Driven Self-Assembly

박유진 류지연 이민형[1,*] 이준승[*]

전남대학교 화학과 [1]울산대학교 화학과

Organometallic Ruthenium half-sandwich complexes and 5?(2-hydroxyphenyl)?1H?tetrazole(LH_2), a linker for (*p*-cymene)Ru half sandwiches, have been used to construct supramolecular cages AgOTf was used for the purpose of the abstraction of chloride ions by producing AgCl precipitate as well as electron acceptor units to form supramolecular assembly. The reaction of (*p*-cymene)Ru and LH_2 in a ratio of 1:1 and 6:4 produced Ru complex bridging Cl and *L*H and rectangular supramolecule containing ruthenocene, respectively. The addition of AgOTf resulted in the formation of unique supramolecules which are cylindrical structure formed by Six Ru, six Ag, six *L* and double cone shape formed by six Ru, eight silver, six *L* selectively. They were characterized by ^{1}H-NMR, IR, ESI-MASS and their solid state structures were confirmed by X-ray crystallography.

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Temperature-Dependent Surface Migration of Au alloy on Si Nanowires

박이슬 이진석*

숙명여자대학교 화학과

Si nanowires (SiNWs) have been identified as useful building blocks including field-effect transistors, catalysts, solar cells, and biological applications, especially. It is important to accurately control their diameter, length, conductivity, and contamination for successful applications. In general, SiNWs can be synthesized by various methods, such as laser ablation, molecular bean epitaxy, and chemical vapor deposition (CVD) via vapor-liquid-solid (VLS) mechanism assisted by a Au catalyst. For this reason, one of the most important problems is contamination by Au catalysts, due to rapidly diffusion and migration of Au into the Si. Therefore, it is important to understand the behavior of Au migration in SiNWs for application in electronic devices. In this study, we report the effect of Au alloy migration on the vertically aligned SiNW arrays during cooling with different cooling rate after VLS growth. There are interesting phenomenon in regard to Au migration between fast and slow cooling owing to different Au migration kinetics, which are influenced by temperature. Furthermore, Au migration depends on the diameter of Au alloy on the top of SiNW, which can be controlled by synthesizing from thin- or thick-Au film as a metal catalyst. The Au migration mechanism are studied in detail on the basis of obtained results by characterizing vertically aligned SiNWs with different experimental conditions.

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Polarized Microscopic Raman Spectroscopy for Graphene Domain Grown on Copper using a Liquid Benzene Precursor

강청 정희경 이진석*

숙명여자대학교 화학과

Graphene is a two-dimensional allotrope of carbon comprising of a one-atom-thick planar sheet of sp2-bonded carbon atoms densely packed in a honeycomb crystal lattice. It has been attracting great interest because of its excellent structural and electrical properties. Moreover, the high electron mobility and tunable band gap of graphene makes it a potential material for electronics and sensing applications. Of the various synthetic approaches of the graphene for electronic applications, it has been well-known that metal assisted chemical vapor deposition (CVD) is the most reasonable and proper method to produce large-scale and low-defect graphene films.In this article, we report the first successful attempt of atmospheric pressure CVD graphene growth on Cu foil using liquid benzene as a precursor and hydrogen as a carrier gas. We analyzed the varied reaction parameter, such as precursor temperature and H2 gas flow rate, effects on the number of graphene layers. Also, we investigated the role of the H2 gas, Ar gas, and benzene vapor pressure on the formation of graphene layers by comparing the size of the graphene domains using scanning electron microscopy (SEM) and micro-Raman spectroscopy.

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Cyclic tetramers of five-membered palladacycle based on head-to-tail-linked isocyanate dimer: synthesis, structure and cyclotrimerization of isocyanates

김용주* 최준환 김건우 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Reactions of [Pd(styrene)(PR3)2],generated from trans-[PdEt2(PR3)2]and styrene,with 2 equiv. of benzyl isocyanate in THF at room-temperature afforded unusual cyclic Pd-tetramers of five-membered rings consisting of organic isocyanate dimers and palladium, [Pd(PR3){-C(O)N(R)C(O)N(R)-}]4(PR3 = PMe3; PR3 = PMe2Ph) as well as a cyclic trimer, (RNCO)3 (R = benzyl) as a catalytic product. One of the isolated complexe was characterized by spectroscopicanalyses and X-ray diffraction study. Treatment of the cyclic tetramer (1) with 4 equiv. of chelated phosphine, such as (1,2-bis(diethylphosphino)ethane) (DEPE) or (1,2-bis(dimethylphosphino)ethane) (DMPE), readily caused conversion to a metallacyclic cis-form, [Pd{N(R)C(O)N(R)C(O)}(P~P)] (P~P = DEPE; P~P = DMPE) in quantitative yields. In contrast, reactions of Pd(0)-PR3 with 2 equiv.of Ar-NCO (Ar=Ph,p-Tolyl, p-ClC6H4)afforded metallacycliccomplexes having a dimericisocyanato moiety, cis-[Pd{C(O)N(Ar)-C(O)N(Ar)}(PR3)2](PR3 = PMe3 Ar=C6H5; p-MeC6H4; p-Cl-C6H4; PR3= PMe2Ph, Ar=p-Cl-C6H4). Treatment of the palladacyclic complex with an equimolar amount of chelated phosphine such as DEPE readily caused conversion to a palladacyclic cis-form, [Pd{N(Ar)C(O)N(Ar)C(O)}(DEPE)] in quantitative yield. The catalytic cyclotrimerization of benzyl isocyanate to [Pd(styrene)(PMe3)2] was achieved by varying the molar ratio of R-NCO (R = benzyl). Experimental detail will be discussed.

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Supramolecular gels with unprecedented strength and elasticity by tuning of calix[4]arene-derived networks

이지하 정종화*

경상대학교 화학과

Supramolecular gels comprised of low-molecular weight gelators are generally regarded as mechanically weak and unable to support formation of free-standing structures, hence their practical use with applied loads has been limited. Here, we reveal a technique for in situ generation of high tensile strength supramolecular hydrogels derived from low-molecular weight gelators. By controlling the concentration of HCl during hydrazone formation between calix-[4]arene-based gelator precursors, we were able to tune the mechanical and elastic properties of the resulting gel. Organogels formed without HCl exhibited impressive tensile strengths, higher than 40 MPa, which is the strongest among self-assembled gels. Hydrogels, prepared by solvent exchange of organogels in water, showed 7,000~10,000 fold enhanced mechanical properties due to further hydrazone formation. This unique method of molding also allowed the gels to retain shape after processing, and furthermore, we found organogels when prepared as gel electrolytes for lithium battery applications to have good ionic conductivity.

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Synthesis and chemical reactivites of cyclic tetramers of five-membered metallacycle involving isocyante dimer and Pd or Pt atom

김용주* 최준환 김남수 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Metallacyclic Pd(II) or Pt(II) complexes having a dimeric isocyanato moiety, cis-[M{C(O)N(Ar)-C(O)N(Ar)}(PR3)2](PR3= PMe3 Ar= p-MeC6H4,1; p-Cl-C6H4, 2; PR3= PMe2Ph, Ar= p-Cl-C6H4, 3) were reacted with excess elemental sulfur to afford cyclic tetramers of five-membered palladacycle or platinacycle. Treatment of the cyclic tetramers with t-butyl isocyanide caused novel M(II) complexes having t-butyl isociande and dimeric isocyanoto ring. Experimental detail wiil be discussed.

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Synthesis and characterization of Pd(II) complexes *N*, *N'*, *X*-tridentate ligands containing *N*-coordinated pyrrole group

안승현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The reaction of [Pd(CH$_3$)$_2$Cl$_2$] and *N*, *N'*, *X*-tridentate ligands, HL$_n$ (HL$_1$ = *N* ^{1}-((1H-pyrrol-2-yl)methylene)-*N* ^{3}-methyl-*N* ^{3}-phenylpropane-1,3-diamine, HL$_2$ = *N*-((1H-pyrrol-2-yl)methylene)-3-methoxypropan-1-amine, HL$_3$ = *N* ^{1}-((1H-pyrrol-2-yl)methylene)-*N* ^{3},*N* ^{3}-dimethylpropane-1,3-diamine, HL$_4$ = *N*-((1H-pyrrol-2-yl)methylene)-3-(methylthio)propan-1-amine) in ethanol, yielded neutral monomeric complexes, [PdLnCl] by deprotonation of pyrrole group, respectively. In [PdLnCl] complexes, each Pd(II) ions adopts distorted square planar geometry. In addition, these complexes were used as a catalyst for the MMA polymerization.

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Cooling Rates Dependent Growth of Graphene Domain via Chemical Vapor Deposition Method

정희경 강청 이진석*

숙명여자대학교 화학과

Graphene is a two-dimensional carbon material that has attracted great scientific and technological interest due to its intriguing physical properties and enormous potential for various applications. To overcome the disadvantage of small-scale production of graphene using mechanical exfoliation of highly orientated polymeric graphite, chemical vapor deposition (CVD) of large-area single-layer graphene on metal films has been explored from various aspects. In general, the electric properties and device performance are strongly dependent on the size, shape, crystallinity, layer numbers, and edge structures of pristine graphene. Controlling these parameters of graphene in synthesis or post-synthesis manipulation is thus critical to achieve tunable properties and optimized device performance.In this paper, we demonstrate the synthesis of graphene to control its size at atmospheric pressure. Here we present the main reaction details for each growth process and a proposed growth mechanism as a function of the partial pressure of the H2 and CH4 gas during the cooling process by CVD method. Furthermore, we found that controlled size and defect density (continuous) of graphene by changing experimental parameters such as cooling rates, flow rates during cooling. Moreover, we compared to the size and quality of graphene domains using scanning electron microscopy (SEM) and micro-Raman spectroscopy. This focused on the partial pressure (H2 and CH4 gases) and cooling rates during the cooling of CVD method.

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High-water content hydrogel by mixing clay and calix[4]arene derivate

김채린 이지하 정종화*

경상대학교 화학과

본 연구는 Guanidinium Ion 과 clay nano sheets (CNSs)와의 정전기적 상호작용을 통해 젤을 제조였다. 특히 calix[4]arene 유도체 및 나노 크래이 시트의 농도변화에 따라 다양한 종류의 젤을 제조하고 레올로지를 통해 점성과 탄성을 측정하였다. CNSs 나 calix[4]arene 유도체에 대해서 제조된 하이드로 젤은 삼차원 네트워크 형성에 의해서 좋은 물성을 나타내었다. 이는 CNSs 에서 1.3-calix[4]arene 유도체가 분자 접착제 역할을 하기 때문이다. 따라서 본 학회에서는 clay 와 calix[4]arene 유도체에 의해서 제조된 하이드로 젤에 대해 발표할 것이다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel star-shaped hole transporting meterials with a triazine unit introducing fused shape

조현준 도광석[1] 최혜주[1] 박소진[1] 이혜정 심장근[2] 김기동 고재중[1,*]

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New types of hole transporting materials with donor?p?acceptor (D?A) systems by incorporating an electron-deficient 1,3,5-triazine core and an electron-rich diphenylamino unit. We already sythesized Triazine-Th-OMeTPA, Triazine-Ph-OMeTPA before. Herein, we institute fused shape ligand for increasing planarity. It was demonstrated that the introduction of these compounds increased crystallizability by packing themselves, which changed their morphology. In conclusion, we confirmed the power conversion efficiency increased more than our previous work, showing competitive photovoltaic performance with the widely used spiro-OMeTAD based solar cell.

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Efficient hole transporting materials with dimethylfluorenylamino moiety for perovskite solar cells

최혜주 도광석 박소진 조현준[1] 이혜정[1] 고재중*

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Novel star-shaped hole transporting materials (HTMs) with dimethylfluorenylamino moiety have been synthesized and evaluated for the high performance perovskite solar cell applications. Maximum power conversion efficiency of 14.21% has been achieved using the HTM with a fused TPA core and the long-term stability was also shown to be comparable with that of spiro-OMeTAD.

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Efficient hole transporting materials with a silole unit for perovskite solar cells

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Dye-sensitized solar cells (DSSCs) have been considered a promising alternative to the silicon-based solar cells due to their low-cost production and simple device fabrication. DSSCs using liquid electrolytes of Co^{II}/Co^{III} redox couples have shown efficiencies surpassing 12%. However, the stability issues of the DSSCs devices arise from leakage and evaporation of liquid electrolyte. Many efforts have been made to replace liquid electrolytes with quasi-solid-stateelectrolytes or solid-state hole conductors to alleviate the stability issues. However, the photovoltaic power conversion efficiency of solid-state DSSCs (ssDSSCs) remains significantly below that of liquid electrolyte-based devices. Recently, the organometal halide perovskites ($CH_3NH_3PbX_3$, X = Cl, Br, I) have attracted great attention due to their direct band gap, large optical absorption and high mobility. An impressive photovoltaic performance was achieved over 15% power conversion efficiency using 2,2′,7,7′-tetrakis[N,N-di(4-methoxyphenyl)amino]-9,9′-spirobifluorene (spiro-OMeTAD) as a hole transporting material (HTM). The most effective HTM for the hybrid solar cells is spiro-OMeTAD, even though another small molecule HTMs such as 3,4-ethylenedioxythiophene-, pyrene-, linear π-conjugated structure, butadiene-, and swivel-cruciform thiophene- based HTMs gave high conversion efficiencies of 10~13%. However, the high synthetic cost of spiro-OMeTAD gives another problem for the commercialization. Therefore, the development of cost-effective HTMs with high efficiency and long stability is very important. We report new types of hole transporting materials with donor-π-acceptor (D-A) systems by incorporating silole derivate core and an electron-rich diphenylamino unit.

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Novel hole transporting materials based on dihydro-indenoindene derivatives and dihydro-indoloindole core for high efficiency perovskite solar cells

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A series of novel hole transporting materials(HTMs) with planar core units have been designed and synthesized for perovskite solar cells. Perovskite solar cells based on π-delocalized conjugated structure have attracted considerable interest due to their high mobility of electrons. Here, we introduce two type of hole transporting materials. One is 5,10-Dihydroindolo[3,2-b]indole (DINI) core based HTM, which represents a highly π-conjugated, electron rich, and planar aromatic polycyclic fuse structure. The other is dihydro-indenoindene (DINE) with bulky phenyl rings core based HTM, which shows excellent hole mobility.

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Synthesis of New Manganese Oxide Precursors for MOCVD/ALD

이선주 성명모* 박보근[1] 정택모[2] 김창균[1]

한양대학교 화학과 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학소재연구단

Manganese is an important component in several classes of materials such as solid electrolytes in Li-based batteries, magnetoresistive oxide (La1-xAxMnO3-α and Pr1-xCaxMnO3), multiferroic (BiMnO3), and catalyst. Manganese oxide thin films have been deposited by several methods including liquid-phase electrochemical methods, physical vapor deposition (PVD), metal organic chemical vapor deposition (MOCVD), and atomic layer deposition (ALD). MOCVD and ALD processes are useful to form large area thin films of good uniformity using metal precursors. The manganese-containing thin films have been used to Mn(tmhd)3, MnCp2, Mn(EtCp)2, Mn(hfa)2?tmeda, and Mn(N,N'-di-isopropylpentylamidinato)2. However, development of new manganese precursors require due to thermal instability, low shelf life, and low vapor pressures of the used precursors.In this study, we report the synthesis of new heteroleptic precursors containing aminoalkoxide for thin films containing manganese, and characterization by IR, thermogravimetric analyses (TGA), and microanalyses, as well as single-crystal X-ray diffraction study.

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Synthesis of Perovskite Solar Cells beased on Characteristic Cores and Effect of Their Chemical Structures on Physical Properties

박소진 도광석 최혜주 조현준[1] 이혜정[1] 고재중[*]

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과

Perovskite solar cells in combination with organic hole transport materials have attracted attention due to their high power conversion efficiencies. Now that these high efficiencies have been reached it is important to address fundamental questions regarding the requirements of the material properties. Here we set up to three hole transporting material (HTMs). N4-(4'-(bis(4-methoxyphenyl)amino)biphenyl-4-yl)-N4',N4'-bis(4-methoxyphenyl)biphenyl-4,4'-diamine (BPAOMe-DA) is a class of such compounds which is conventionally prepared from triphenylamine (TPA) derivatives. In order to investigate the structural and morphological effect on physical properties, the optical and electrical properties were measured and compared among the three materials containing biphenyl, 3,4-ethylenedioxythiophene (EDOT) or 2,1,3-benzothiadiazole (BTD) as the core.

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Synthesis and Characterization of Co(II) Complexe with H_2pmidp ligand (H_2pmidp= *N*-(2-pyridylmethyl)iminodiisopropanol)

박지혜 민길식[1,*]

경북대학교 화학교육과 [1]경북대학교 사범대학 화학교육과

N-(2-pyridylmethyl)iminodiisopropanol (H_2pmidp) ligand is considered to have the potential to form interesting metal complexes with transition metals. Recently, dinuclear cobalt(II) complex, $[Co_2(H_2pmidp)_2Cl_2]CoCl_4$(1) has been synthesized using H_2pmidp and $CoCl_2$?$6H_2O$. The cobalt(II) ion is coordinated with two nitrogens, two oxygens from H_2pmidp as well as two Cl ions from $CoCl_2$?$6H_2O$. That is, an $[Co_2(H_2pmidp)_2Cl_2]CoCl_4$ unit result from the bridging of two cobalt(II) ion through two Cl of the $CoCl_2$?$6H_2O$. This compound is blue in the solid state at room temperature. However, the color changes depending on the solvent, due to the $CoCl_4$ anions. In this poster, we will present the synthesis of 1 and the characterization by elemental analysis, IR, UV-Vis, magnetism and single X-ray diffraction.

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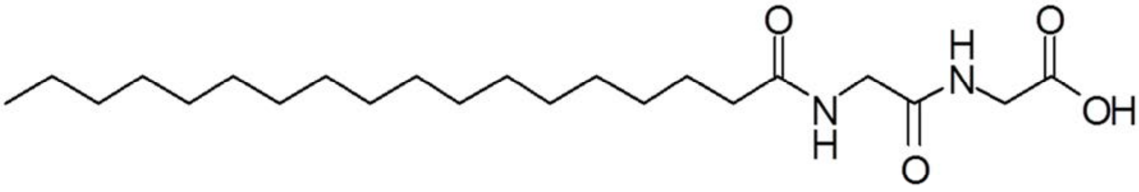
펩타이드 하이드로 젤의 제조

정민진 정성호 정종화*

경상대학교 화학과

본 연구에서는 글리신-글리신으로 구성된 양친매성 gelator 를 3 단계로 합성하였다. Gly-Gly-OEt 와 stearoyl chloride 를 반응시켜 최종 화합물 1 을 합성하였다. 이렇게 합성된 화합물 1 은 물을 이용하여 하이드로 젤을 제조하였다. 그리고 하이드로 젤 1 의 특성을 전자현미경, 자외선-가시광선 분광기 등을 이용하여 분석하였다. 본 학회에서는 하이드로 젤 1 에 대해서 자세히 소개 할 예정이다.



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Pulsed EPR Spectroscopy of Cu-Amyloid Peptide Relevant to Alzheimer's Disease

김동훈 김선희*

한국기초과학지원연구원 서울서부센터

Copper ion has been proposed to play an important role in aggregation of the A*b*(amyloid *b*) peptide via oxidative stress. Thus, the elucidation of the structural details of Cu-A*b* is essential in understanding Cu-A*b* fibrillization. In addition to Cu-*h*A*b*, the investigations Cu-*m*A*b* is required for a better understanding of Cu-A*b* fibrillization because a murine does not suffer from AD. We use multi-frequency, multi-technique pulsed EPR spectroscopy such as 33 GHz ENDOR (Electron Nuclear Double Resonance), 9 GHz ESEEM (Electron Spin Echo Envelope Modulation) and 9 GHz HYSCORE (Hyperfine Sublevel Correlation) to characterize Cu-*h*A*b* as well as Cu-*m*A*b* in a conjunction with isotope labeling. Our results provide detailed structure of Cu-A*b*.

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Multi-frequency CW and Pulsed EPR studies on transition metal complexes: Oxidation states, geometries and electronic structures

김유정 김선희*

한국기초과학지원연구원 서울서부센터

EPR spectroscopy has been proven to be a powerful tool to study transition metal complexes. EPR can provide information about oxidation states of metal ions and geometrical structures of metal complexes. We will present the examples of multifrequency and multi-technique EPR on transition metal complexes provided by our collaborators. Electronic structures and the coordination environment of different metal complezes will be discussed based on the 9/34 GHz multi technique EPR such as ENDOR(Electron Nuclear Double Resonance), ESEEM(Electron Spin Echo Envelop Modulation) and HYSCORE(HYperfine Sub-level CORrElation).

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Design and preparation of macrocyclic complexes covalently linked with Ru(II)-polyphyridyl moiety

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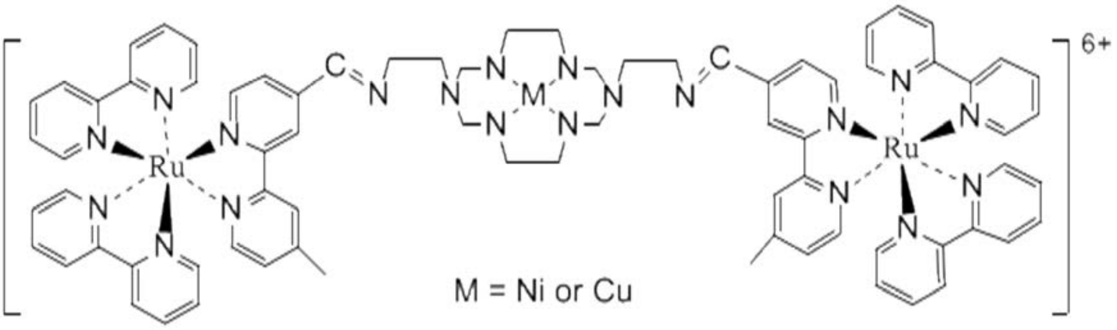
순천대학교 화학과 [1]순천대학교 약학대학 약학과 [2]순천대학교 화학교육과

Ru(II)-polypyridyl derivatives have been attracted much attention because they play a distinctive role of photosensitizer, or antenna. In recent years the luminescent excited state of tris(2,2'-bipyridine)ruthenium(II) (*Ru(bpy)3 2+) has attracted considerable attention because of its promise as a mediator in solar energy conversion. This excited state, a very strong reductant, rapidly reduces even mild oxidant, for example Co(II) complex and is thermodynamically capable of reducing water to hydrogen through electron-transfer from excited Ru(II) to Co(II). Also, it has been reported the photochemical reduction of carbon dioxide, which is concerned one of the important recent issues of the fixation and activation of carbon dioxide using covalently linked Ru(II)-Ni(II) system. However, the systems available in the photo induced catalytic reaction of hydrogen evolution or carbon dioxide activation is extremely limited and their efficiencies are very low. Now, we designed a new covalently linked Ru(II)-M(II) (M = Ni or Cu) system which is applicable to the hydrogen evolution or carbon dioxide activation. In this presentation, the characterization and properties of some organic and inorganic species which obtained from the attempted preparation of A will be described.



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New Layered Pd polyselenide, $[Pd(Se_7)_2]^{2-}$

WANGDI 김강우*

인천대학교 화학과

Layered Pd polyselenides, $[Pd(Se_7)_2]^{2-}$ stabilized with $EtMe_3N+$ and Et_2Me_2N+ organic cations, have been successfully synthesized by the solvothermal method using methanol as a solvent. Crystal structures of $(EtMe_3N)_2[Pd(Se_7)_2]$ and $(Et_2Me_2N)_2[Pd(Se_7)_2]$ compounds were determined by the single crystal X-ray diffraction study. Reddish black polyhedral crystals of $(EtMe_3N)_2[Pd(Se_7)_2]$ crystallize in the monoclinic space group P21/c (no. 14) with a = 9.415(1) Å, b = 14.345(1) Å, c = 12.473(1) Å, β = 113.403(2)°, Z = 4, V = 1545.9(2) Å3. Reddish black block crystals of $(Et_2Me_2N)_2[Pd(Se_7)_2]$ crystallize in the monoclinic space group P21/n (no. 14) with a = 9.224(1) Å, b = 15.150(1) Å, c = 12.220(1) Å, β = 109.683(2)°, Z = 4, V = 1607.8(5) Å3. 2D layered $[Pd(Se_7)_2]^{2-}$ is composed of square planar Pd metal centers interconnected by heptaselenide(Se_7^{2-}) ligands. To be noteworthy, the heptaselenide ligand is the longest polyselenide ligand to form complexes with Group 10 metals. Details of synthetic condition and physical properties for $(EtMe_3N)_2[Pd(Se_7)_2]$ and $(Et_2Me_2N)_2[Pd(Se_7)_2]$ will be presented.

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Reversible Chiral Information of Achiral Solid State through Helical Rearrangement

정성호 정종화*

경상대학교 화학과

Although there are numerous examples of helical and spiral conformations in nature, including plant tendrils, snail shells, and even collagen, the occurrence of supramolecular systems that are able to reversibly undergo solid-to-solid helical transformation based on environmental chiral triggers is rare. In this work, we present the use of a supramolecular, non-helical nanofiber which will carry out a distinct helical rearrangement in the presence of specific diamines and monoamines, such as cyclohexanediamines, alanine, lysine, and phenylalanine, depending on the molecular chirality of surrounding analytes. A detailed investigation of the structural organization of the nanofibers using SEM and CD spectra analysis confirmed the repeatable and reversible nature of this amplification of chiral information. Further preparation of an electrospun nanofiber film demonstrated the ability to discern chiral diamines and monoamines in solution by film immersion and CD analysis, which is the first example of amplification of chiral information in solid-state using electrospun nanofiber films. With this system, we could demonstrate a reusable means for detecting molecular chirality, which also provided a unique example of reversibly controlling a solid state rearrangement in supramolecular helicity.

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Synthesis of efficient and recyclable mesoporous silica spheres embedded with FeCo/graphitic shell nanocrystals for propargylic substitution reactions

김진우 박강현*

부산대학교 화학과

The magnetic nanoparticles which embedded in mesoporous silica sphere (MSS) have been mostly developed to achieve a recyclability. Most of magnetic nanoparticles in MSS have been considered as Fe-containing metal oxide. However, in order to apply as catalyst support, Fe-containing metal oxides are still necessary to improve the stability as a priority.Heteropoly acids have been the focus of extensive research in organic synthesis due to their high catalytic activity and low cost. Among the various heteropoly acids, phosphomolybdic acid (PMA) is one of the least expensive commercially available solid acids. PMA enhances the activity of selected catalysts and shows self-catalytic activity in various organic reactions. FeCo has superiormagnetic properties of the highest saturation magnetization and a high superparamagnetic limit above 20 nm, but it has yet to be explored because its easy oxidation and potential toxicity. Recently, one-step chemical vapor deposition (CVD) method has afford a way to solve these problems through synthesis of FeCo/graphitic carbon shell (FeCo/GC) nanocrystals.We have successfully prepared highly stable and magnetically recyclable MSS embedded with FeCo-graphitic carbon shell nanocrystals (FeCo/GC@MSS) by a simple one-step CVD method. This superparamagnetic FeCo/GC@MSS showed high saturation magnetization and superior chemical stability against acid etching and oxidation. Furthermore, FeCo/GC@MSS was loaded with phosphomolybdic acid(PMA), which have been used as acid catalyst for various organic reactions. The resulted PMA-loaded FeCo/GC@MSS was used as a green catalyst for propargylic substitution reactions of various aromatic compounds with 1,3-diphenylprop-2-yn-1-ol.

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Metal-Organic Frameworks로부터 유래된 계층적 다공성 탄소 나노 소재의 제조

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다공성 탄소 소재는 높은 표면적 및 공극률과 함께 열적/화학적 안정성을 지닌 물질로 기체의 저장과 분리, 촉매 작용, 에너지 저장과 전환 등의 다양한 분야에 걸쳐 응용되고 있다. 이 소재는 제올라이트나 실리카 메조포러스를 고체 주형으로 사용하여 정렬된 나노 혹은 메조 탄소 세공체를 합성하는 이른바 nanocasting 방법을 사용하여 합성되고 있다. 최근 금속-유기 골격체(Metal-Organic Framework, MOF)를 템플릿 또는 전구체로 이용하여 다공성 탄소 소재를 합성하는 연구가 시도되어 왔다. MOF 는 금속 이온 또는 금속 클러스터가 유기 리간드에 의해 연결되어 3 차원 골격 구조를 형성한 다공성 물질로 표면적과 기공 부피가 크고 화학적 특성을 조절할 수 있다는 장점을 지닌다. 특히 MOF 의 특성 중 하나인 규칙적으로 정렬된 내부 구조와 풍부한 유기 리간드는 정렬된 구조를 가지는 다공성 탄소 소재를 형성시키기에 적합하다. 이러한 특성으로 인해 템플릿 또는 전구체로써 MOF 를 열분해시켜 다공성 탄소 소재를 형성시키는 방법이 연구되어 왔다. 하지만 MOF 는 열적 불안정성에 의해 열분해 과정 동안에 기공 구조가 무너지기 쉽고 따라서 정렬된 다공성 탄소 구조를 필요로 하는 응용이 제한된다. 따라서 정렬된 구조의 다공성 탄소 소재를 형성시키기 위해서는 MOF 의 적절한 열분해 조건 및 carbon source 에 대한 연구가 필요하다.본 연구에서는 열분해 조건 및 carbon source 가 다공성 탄소 소재의 기공 구조와 특성에 미치는 영향을 알아보았다. 전구체로 이용하는 MOF-177 의 열 중량 분석(Thermogravimetric analysis)결과를 바탕으로 결정된 서로 다른 온도에서 열분해 과정을 수행하였다. 또한 열분해 과정 중에 기공 구조를 유지시키기 위해 carbon source 를 기공에 담지 후 열분해를 진행하였다. 생성된 물질의 비교 분석 결과 열분해 온도와 carbon source 의 첨가에 따라 표면적과 기공의 크기 및 탄소 소재의 특성이 달라지는 것을 확인하였다.AcknowledgmentsThis research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

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The geometry control of secondary building units (SBU) depend on solvent exchange in Zn-MOF

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울산과학기술대학교(UNIST) 화학과

The tuning of status of SBU is one of the challenges for proper target properties in coordination chemistry. The reaction of Zn^{2+} ion and carboxylate generate $Zn_4O(COO)_6$ SBU frequently. Here we examined reactions of $Zn(NO_3)_3 \bullet 6H_2O$ and H_3BTB ligand in DMF and obtained 2-fold interpenetrated structure composed of 3-c BTB ligand and 6-c $Zn_4O(COO)_6$ metal cluster, thereby, it is 3,6-c ant net. It is tuned that coordination geometry of $Zn_4O(COO)_6$ SBU on synthesized metal-organic frameworks (MOFs) depend on exchanging solvents. We will be discussed analysis of MOFs based on solvent exchange.

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Green Phosporescent Iridium(III) Complexes with Carbene Derivatives as Ancillary Ligands for Organic Light?Emitting Diodes (OLEDs)

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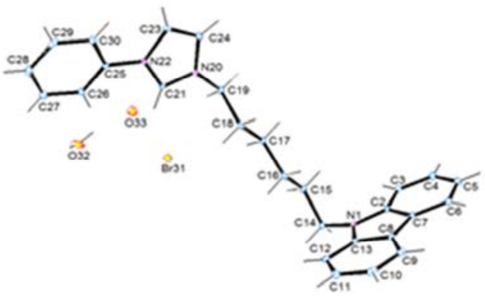
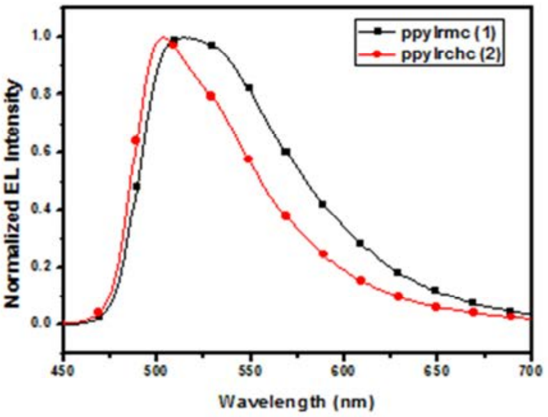
The heavy transition-metal complexes as Ir(III), Pt(II) have attracted intensive attention for application of organic light-emitting diodes (OLEDs) because of their high performance in the devices and easy control of color tuning. In this research, we designed and synthesized two cyclometalated Ir(III) complexes containing carbene derivatives as C^C ancillary ligands ; ppyIrmc (1), ppyIrchc (2), (ppy = 2-phenylpyridine ; mc = 1-phenyl-3-methylimidazolin-2-ylidene and chc = 1-phenyl-3-hexylcarbazolylimidazolin-2-ylidene). The ancillary carbene ligands, mc and chc were synthesized through Ullmann reaction with imidazole using bromobenzene, bromomethane and bromohexylcabazole, respectively. In addition, the photophysical, electrophysical properties and devices performance of complex (1) and (2) were investigated.Two complexes showed band gap of green region as 2.68, 2.67 eV for (1) and (2), respectively. The complex (1), (2) showed green phosphorescent emissions at 510, 509 nm in PL spectra and exhibited good quantum yields of 49, 43 % in dichloromethane solution, respectively.


C29
C30
C28
C25
C27
C26
C23
C24
N22
N20
C21
C19
O33
C18
O32
Br31
C17
C16
C15
C3
C4
C5
C2
C6
C14
N1
C8
C7
C12
C13
C9
C10
C11


ppy Irmc (1)
ppy Irchc (2)
Normalized EL Intensity
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
450
500
550
600
650
700

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Sky-blue Heteroleptic Iridium(III) Complex Containing 1-((2,4-difluorophenyl)-3-hexylcarbazolylimidazolin-2-ylidene and Photoluminescence Propertiy

송영광 최지혜[1] 김영인[1,*]

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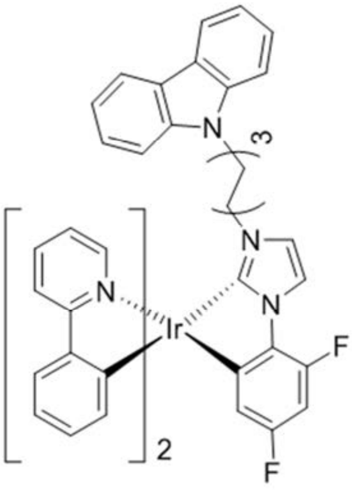
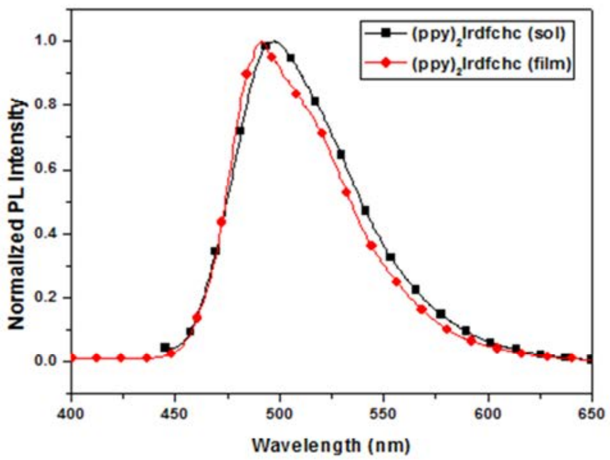
The heavy metals such as Ir (III) lead the florescence and phosphorescence, using both the singlet and the triplet energy state achieved theoretically 100% emission efficiency. The pioneers have been studied to increase luminescent properties for applied organic light emitting diodes(OLED). In this study, we designed and characterized carbene derivative ancillary ligand ; dfchc. We also synthesized cyclometalated Ir(III) complex containing this carbene ligand ; Ir(ppy)2(dfchc) (ppy = 2-phenylpyridine ; dfchc = 1-((2,4-difluorophenyl)-3-hexylcarbazolylimidazolin-2-ylidene). In addition, the photophysical, electrophysical properties of this complex were investigated.The Ir(ppy)2(dfchc) showed sky-blue phosphorescent emission at 497 nm in PL spectra and exhibited good quantum yields of 34 % in dichloromethane solution. The Ir(ppy)2(dfchc) showed band gap of sky-blue region as 2.84 eV


N
3
N
N
N
Ir
N
F
F
2


(ppy)$_2$Irdfchc (sol)
(ppy)$_2$Irdfchc (film)
Normalized PL Intensity
1.0
0.8
0.6
0.4
0.2
0.0
400
450
500
550
600
650
Wavelength (nm)

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Metal-Organic Frameworks(MOFs)의 열분해를 통한 Alcohol Oxidation반응 촉매제조 및 반응조건 최적화

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인천대학교 에너지화학공학과 [1]인천대학교 화학과 [2]인천대학교 에너지 화학공학과

MOFs(Metal-Organic Frameworks)는 금속 클러스터와 유기 리간드가 자기조립을 통해 형성된 결정성 물질로 다공성을 가지며 비표면적이 높아 다양한 분야에 적용되고 있다. 특히 촉매 분야에서의 MOFs 는 비표면적이 클 뿐만 아니라 촉매활성자리의 밀도가 높고 균일하여 불균일 촉매로서 주목 받고 있는 물질이다. 하지만 MOF 는 화학적 안정성 및 수분 안정성이 떨어져 실제적으로 산업에 응용하기에 어려움이 있으며 나노 크기의 동공 크기는 다양한 기질에 적용되기엔 한계가 있다. 본 연구에서는 MOFs 의 한 종류이자 Cu 가 포함된 HKUST-1 을 열분해 하여 화학물질 혹은 수분에 안정한 새로운 MOFs 기반 촉매를 제조하였다. 합성된 촉매(HKUST-1-py)는 BET, XRD, SEM 등을 이용하여 그 특성을 확인하였으며, 제도된 촉매로 산업적으로 매우 중요한 알코올 산화 반응을 수행하였다. 반응 종료 후 NMR 분석을 통해 합성된 촉매의 반응에 대한 활성과 반응온도, 반응시간, 반응환경, 조촉매 등이 알코올 산화반응의 전환율, 수율에 미치는 영향을 알아보고 반응조건을 최적화 하였다.AcknowledgmentsThis research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

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Synthesis of monodisperse and nitrogen-doped carbonaceous materials using dopamine precursor and its CO2 adsorption study

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한양대학교 응용화학과

Among carbon dioxide (CO2) capture materials, carbonaceous materials have been of great interest due to low cost, high chemical and thermal stability, and low sensitivity to moisture. In attempt to increase adsorption capacity for CO2 using carbonaceous materials, increase of ultramicropore (less than 1 nm) and incorporation of basic moiety (e.g., nitrogen doping) into the carbon frameworks have been proved as the most important factors. Herein, we report how monodisperse melanin polymer spheres with size ranged from 100 to 1000 nm can be synthesized using dopamine precursor that contains nitrogen in the backbone. As-prepared and N-enriched melanin polymer spheres were then carbonized to provide N-dopedcarbonaceous materials with a good monodispersity and its nitrogen content was as high as 7 wt%. In addition, activation process that increases the specific surface areas of N-doped carbon was applied and a gradual increase of surface areas were controlled up to around 2300 m2/g. Highly activated and N-doped carbon was then tested for identifying the capability for CO2 capture application. The details for the relationships between structural information (i.e., porosity and surface area), dopant degrees in the carbon frameworks and CO2 uptake properties were investigated through gas sorption measurements (N2 and CO2), electron microscopy investigations (SEM and TEM), IR, XPS, XRD, Raman and elementary analysis.

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Crystal Structure of a Metal-Organic Framework Exhibiting Abnormal Bond Geometry of Fluorobenzene Moiety

홍지수 장유나 임나래 우경택 김자헌*

숭실대학교 화학과

UHM-32 is a known MOF prepared from copper nitrate and H_3Fbtc (2-fluoro-1,3,5-benzenetricarboxylic acid) in DMA at 100 ^{o}C. Its formula is Cu_2(Fbtc)(DMA)(μ_3-OH)?DMA and has a tetranuclear Cu cluster held by two hydroxo and six carboxylate groups. When a same reaction was conducted now with a potassium salt of H_3Fbtc, the produced MOF revealed a same framework structure as that of UHM-32 but showed a partial structural disorder not observed in UHM-32. Moreover, crystal structure refinement with a carefully applied disorder model indicated that the F atom bonded to the ligand benzene ring adopted abnormal bond geometry; the covalently bonded F atom is located significantly above the benzene molecular plane. A possible reason will be discussed.

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Various Photophysical and Theoretical Interpretation of Carborane-Containing Iridium Complexes

최태섭 한원식[1] 손호진* 강상욱*

고려대학교 소재화학과 [1]서울여자대학교 화학과

본 연구에서는 대표적인 인광발광재료인 polypyridyl 이리듐 착물에 최근 활발한 연구가 시작된 새로운 광물리적 특성을 보여주는 카보란 (Carborane) 유도체의 도입을 통하여 이리듐(Iridium)-카보란(carborane) 착화합물들이 준비되었다. 화합물의 광물리적, 전기화학적 특성이 및 이론적 계산에 대한 연구를 진행되었으며 카보란 위치에 페닐이 치환된 화합물들이 기준물질로 사용되어 비교되었다

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Water Sorption Properties of Al-based Metal-Organic Frameworks

최판규 김태민 유래경 김자헌*

숭실대학교 화학과

Metal-Organic Frameworks (MOFs) are considered as promising water sorbent materials applicable for thermally driven adsorption chillers (TDC). The water vapor adsorption-desorption by MOFs mediate heat transformation, leading to producing cooling water. The efficiency of this process is largely dependent on the working capacity of MOFs at a desired relative pressure range, $0.1 < P/P_0 < 0.3$ as demonstrated some MOFs including Al-fumarate. In this presentation, the water vapor sorption behaviors of various Al-MOFs such as CAU-8, CAU-10, and MIL-53(Al) will be discussed in comparison with that of Al-fumarate. The optimized synthetic procedure for Al-fumarate will be also presented.

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Carbon Dioxide Capture Using Amine-embedded Porous Materials

심재웅 노경규 오유진 김자헌*

숭실대학교 화학과

In order to develop efficient carbon dioxide absorbing materials, we have prepared a series of composite materials via simple inclusion of various amines in porous host solids. PEI-800/MIL-101(Cr) as a reference compound was subject to repeated TGA measurements under the flow of a mixed gas with CO_2/N_2 = 15/85% in v/v : absorption at 40 ^{o}C and desoprtion at 70 ? 120 ^{o}C. The employed amines were linear polyamines (TEPA and DETA) and five different PEIs with difference molecular weights. The porous carbon hosts were prepared by heating MOF-5 under nitrogen stream or by treating the obtained carbon with KOH. The carbon dioxide absorption capacities of the various amine/host composites will be presented and discussed in terms of host porosity and the types of amines.

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Development of Bis-Triazolyl-Silanes based Electron Transporting Material for Good Charge Balancing in Deep-Blue Phosphorescent OLEDs: Their Opto-Electronic Alteration to facilitate facile electron injection via Structural Modification

김진형 한원식[1] 강상욱* 손호진*

고려대학교 소재화학과 [1]서울여자대학교 화학과

A series of four triazol-containing compounds for the type of dimethylbis(4-(4-phenyl-5-(4-(X)phenyl)-4H-1,2,4-triazol-3-yl)phenyl)silane (ST) derivative have been tested as electron-transport material for deep blue phosphorescent OLEDs. A systematic change in the electronic structures is achieved in these compounds by incorporating electron-withdrawing (EW) and -donating (ED) groups (X = $-CF_3$, -Me, -^{t}Bu, and -OMe) at the 4-position of the phenyltriazole group. From their electrochemical properties obtained from cyclic voltammetric measurement, we observed that the LUMO level was significantly affected by different substituents. Overally, all prepared compounds have relatively high triplet energy levels, which is compatible with the energy level of blue phosphorescent emitting layer in blue OLED device. TDDFT calculations were also performed to figure out their frontier orbital distributions and their transition states. Using current-voltage (I-V) and IS measurement of electron only devices (EOD) and OLED, we have obtained values for the Richardson factor, the barrier height, trap density, density of states (DOS) and carrier mobility of ST derivatives and interfaces as device parameters.

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Molecular engineering of efficient organic sensitizer incorporating o-carborane moiety linker unit for dye-sensitized solar cells

조민지 김소연 한원식[1] 강상욱[*] 손호진[*]

고려대학교 소재화학과 [1]서울여자대학교 화학과

카보란 뭉치 화합물을 염료 감응형 태양 전지에 적용하기 위해, Electron donating group 인 Triphenylamine 과 Carbazole 과 Electron withdrawing group 인 cyanoacetic acid 를 카보란에 치환하여 합성하였다. Thiophene 을 linker 로 사용하여 HOMO 와 LUMO energy level 이 조정되었으며, 이 화합물의 흡수 스펙트럼과 발광 스펙트럼을 분석을 통하여 이 화합물의 광 물리적 특성을 확인되었다. 또한 Cyclic voltammetry 측정을 통해 결정된 전기 화학적 특성을 바탕으로한 HOMO-LUMO 준위가 결정되었다. 끝으로 염료 감응형 태양 전지소자제작을 통하여 o-carborane 의 치환효과를 확인되었다.

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Significance of hydrophilic characters of Organic dyes in photocatalytic CO_2 reduction catalytic system based on Dye/TiO_2/ReC triad

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이전 연구에서 가시광을 이용하여 CO_2 환원을 시키기 위해 TiO_2 반도체에 흡광체로 유기염료(DMOM)와 CO_2 환원촉매로 Re(I) complex 를 접합시킨 triad 구조가 제시되었다. 가시광 영역인 ≥420 nm 빛을 조사하였을 때, 유기염료가 광자를 흡수하여 들뜬 전자들은 TiO_2 의 conduction band 로 이동되고 그 전자들은 최종적으로 Re(I) complex 위치로 이동하여 CO_2 가 CO 로 환원되는 촉매 메커니즘을 가진다. 또한 전자를 건네 준 염료는 SDN 에 의해 전자를 제공받아 재생되는 catalytic cycle 을 가진다. 본 연구에서는 이전에 보고된 유기염료(DMOM)를 기반으로 Hydrophilic 한 그룹을 치환시키는 것을 통하여 앞서 제시한 triad 시스템을 최적화하는 것에 초점을 맞추었다. Hydrophilic group 이 치환된 OD-NO (R^1 = morpholine-CH_2)와 OD-NN (R^1 = 4-methylpiperazine-CH_2) 염료들이 성공적으로 준비되었으며 좀더 넓은 가시광선영역의 빛을 흡수하기 위한 방법으로 ethylene 그룹이 첨가하여 확장된 conjugation 을 가지는 염료들이 또한 준비되었다. 광반응장치를 통하여 신규 염료들이 흡착된 광촉매시스템의 전환효율이 평가 및 비교되었으며 정확한 메커니즘 분석을 위한 광물리적 그리고 전기화학적 특성이 분석되었다.

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Understanding CO2 adsorption in metal-organic frameworks with cofacial metal centers

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Metal-Organic Frameworks are outstanding materials in energy science with potential applications, ranging from catalysis, sensors, to CO2 capture and separations. The advantages of these new class of materials include remarkable tunable nature of organic building blocks and metal nodes.An interesting series of metal-organic frameworks is the one with cofacial metal centers, acting as molecular traps embedded in the solid state. In this work, we focus on a rht structure type that has cofacial metal centers, derived from four types of polyhedral cages (small and big rhombicuboctahedron, cuboctahedron, and square prism). The chemical environment of such metal centers is extremely important in controlling CO2 gas seperation, including high CO2 binding energy.

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Homogeneous Electrochemical CO_2 Reduction by Half-Metallocene Complexes of Group 9 Metals

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9 족 전이금속 Half-Metallocene Complexes 는 열적 안정성, 물에 대한 높은 용해도, 그리고 우수한 촉매활성특성으로 인하여 다양한 화학변환촉매분야에서 활용되고 있다. 최근에는 Homogeneous Electrochemical CO_2 reduction 분야로의 적용 사례가 보고되었다. 하지만 과거 연구사례들의 경우, Photo-induced hydride transfer 능력이 큰 Catalytic intermediate 효과에 대한 고려 없이 진행되었기 때문에 정확한 메커니즘 분석이 확인되지 못하였다. 이에 본 연구에서는 빛이 없는 조건 하에서 Homogeneous Electrochemical CO_2 reduction 실험을 진행하여 9 족 전이금속 Half-Metallocene Complexes 촉매공정의 메커니즘을 연구하였으며 세부적으로 Ligand 의 electronic density 및 3 종의 전이금속 (Ir, Rh, Co) 조절을 통하여 변화효율과 생성물인 수소와 Formic acid 의 상대적인 비율을 분석하여 비교하였다.

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High-turnover Photoreduction of CO_2 by a Re(I) complex stabilized on dye-sensitized TiO_2 with visible light radiation

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근래 화학계에서는 탄소 자원의 고갈, 지구 온난화 그리고 인공광합성에서 CO_2 환원 반쪽반응(half cycle)의 완성을 위해 광촉매를 이용한 CO_2 환원을 중요하게 생각하였다. Rhenium 과 Ruthenium 기반의 금속 착물 중 CO_2 를 높은 선택성과 광자 효율로 CO 나 HCOOH 로 환원시키는 광촉매들이 알려졌었다. 그러나 기존 분자 기반의 homogeneous 광촉매는 약한 환원제인 물 속에서 산화 능력의 급격한 감소와 재사용이 제한적이라는 문제점이 있다. 본 연구에서는 가시광을 이용하여 CO_2 환원을 시키기 위해 TiO_2 반도체에 흡광체로 유기염료(DMOM, Squaraine dye, and porphyrin dye) 와 CO_2 환원촉매로 Re(I) complex 를 접합시킨 구조를 제시하였다. 광전환 시스템에서 전자주개(SD)로는 SDN 을 사용하였다. 본 연구에서 가시광 영역인 ≥420 nm 빛을 조사하였을 때, 유기염료가 광자를 흡수하여 들뜬 전자를 TiO_2 의 conduction band 로 넘겨주고 이 전자는 Re(I) complex 로 이동하여 CO_2 가 CO 로 전환되는 메커니즘을 제시하였다. 이때 전자를 건네 준 염료는 SDN 에 의해 전자를 제공받아 재생되는 구조를 이루고 있다. TiO_2 는 3 그룹으로 나뉘어 실험이 진행되었으며 결정형의 [001] facet (S-TiO_2)와 분말형태의 Hombikat UV-10 (H-TiO_2), [001] nanotube (T-TiO_2)를 이용하였으며 S-TiO_2 를 사용하였을 때 가장 높은 광전환 효율을 보였다. 또한 다양한 첨가물을 통한 효율적인 CO 전환, H_2 발생을 보았다. Acetic acid 의 처리를 통한 TiO_2 의 표면상태, Particle size 변화를 예측하고 이를 광반응에 적용시켜 높은 CO 전환 효율을 보았다. 유기 흡광체가 TiO_2 primary particle 과 결합한 형태로 분해되는 것을 관찰하고, ALD(Atomic Layer Deposition)을 통한 유기 흡광체의 안정화를 확인하였다.

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Study of Ion-Paired Iridium Complexes (Soft Salts) and Their Application in Molecular Photoelectrocatalysts for Visible Light-Driven Hydrogen Evolution from Neutral Water

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Iridium 을 기반으로 한 cation 과 anion 을 접합시킨 상태의 Ion-paired Ir complexes(soft salts)는 Neutral 형태의 물질들과는 다른 charge localization 을 가진다. Soft salts 층의 정공이 positive polaron 일 때 확실하게 positive 하지 않은 상태를 유지하고, soft salts 의 격자 구조 전체에 positive charge 가 delocalization 된다. 따라서 일반적으로 anion 과 cation 간 Ionic paired complex 조합은 필요한 anion 의 수 보다 더 많은 cation 이 주변에 위치하게되며 이러한 특성 때문에 기존 물질보다 빠른 charge mobility 가 기대된다. 이에 본 연구에서는 cation 은 광촉매로, anion 은 light harvesting 물질로 사용하여 새로운 형태의 광촉매 시스템을 구현하는 것에 초점을 맞추었다. 세부적으로, 동일한 cationic 광촉매에 흡수 영역 대가 서로 다른 anionic light harvester 들이 치환 됨에 따라 광물리적 그리고 전기화학적 특성이 크게 변화되는 것이 관측되었으며 cation 의 방출 영역 대와 anion 의 흡수 영역 대의 겹침정도에 따라 다른 분자 내 에너지 전달 효율이 관찰되었다.

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A Combined Computational and Experimental Study of Blue Emitting Cyclometalated Platinum Complexes to develop an efficient, long-lasting blue PHOLED emitter

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Cyclometalated platinum complexes have been the focus of considerable research, driven in large part by their potential use as sensitizers, photocatalysts, and chemosensors. Platinum complexes have also attracted strong interest as luminescent materials for use in organic light emitting diode (OLED) based display and lighting applications due to their ability to harvest both electro-generated singlet and triplet excitons, resulting in a theoretical 100% electron-to-photon conversion efficiency. Despite the dominance of iridium at present, platinum remains an exciting field of study. If the intrinsic electroluminescent properties of phosphorescent platinum complexes can be unmasked and optimized, these complexes can provide a viable alternative to existing iridium emitters and spur further growth in this emerging field. planar platinum complexes possess excellent structural flexibility, with the ability to employ various cyclometalating ligands. New platinum complexes were synthesized and characterized. These Platinum complexes are highly luminescent, emitting blue to green light in solution. Finally, developed Pt-complexes were tested as dopants in prototype phosphorescent organic light-emitting diode devices and found to show deep blue electroluminescence with high emission efficiency and color purity.

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Morphology-Preserved Transformation of Metal-Organic Framework to Metal/Metal Oxide Nanoparticles Inside Nanoporous Carbon Matrix: Control of the Particle Size and Porosity

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Utilization of metal-organic frameworks (MOFs) as a precursor (or template) to synthesize metal or metal oxide via thermal treatments has been of great interest for heterogeneous catalysis and electrochemical applications. However, the morphology of produced metal or metal oxide is usually collapsed due to loss of organic moieties during heat treatments. Here, we report a facile method for morphology-preserved transformations of MOFs (here, HKUST-1) to metal/metal oxide@carbon (M/MO@C) composites. Catalytic-site specific polymerization occurs on the metal centers of MOFs via a gas-phase polymerization of phenol and formaldehyde (PF). The produced PF@MOF shows the same morphology and crystallinity as the MOF used. Upon careful choice of carbonization process, morphology-preserved M@C or MO@C composites can be synthesized. The crystal size and the porosity of the composites can also be controlled by carbonization time and the amount of polymer deposited inside MOFs, respectively.

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Synthesis of New Tungsten Precursors for Thin Film Applications

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In the present scenario where the electronic devices becomes smaller and smaller the importance of tungsten materials gaining much interest. Firstly because of the employment of tungsten as a current-carrying material for metallization of ICs. As the electronic devices become smaller, this material continues to withstand progressively greater current densities. Despite the fact that a tungsten layer has higher electrical resistance than an aluminum layer, the tungsten films are to a smaller degree prone to electromigration, and they differ but little in their thermal-expansion coefficient from silicon and silica, which are most often used in technology. Secondly, Tungsten nitride is a promising barrier material for copper metallization because of its refractory nature and excellent thermal, chemical (acid-resistant), and mechanical properties. Compared to the other transition metal nitrides, WN has the lowest electrical resistivity (single crystal). Copper forms no known compounds with tungsten nitride, indicating its stability as a barrier.For both of these applications it is important to have good tungsten precursors with good volatility and stability. In this work, we designed tungsten complexes with imido and amido ligands to achieve the desired properties.The complexes was prepared by substitution reactions from tungstenhexachloride using corresponding ligands. The complexes were characterized by FTIR, FTNMR, EA and thermogravimetric analyses.

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Synthesis, structural characterization, and physical properties of a 3-D dysprosium(III) compound

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고려대학교 화학과

A new dysprosium(III) complex, [Dy(oxalate)$_{1.5}$(formate)](H$_3$O) (1) has been produced by solvothermal reaction method. Complex 1 was characterized by elemental analysis, TG analysis, and single crystal X-ray diffraction. The Dy(III) ion adopts a square anti-prism geometry and the local symmetry is close to D_{4d}. The dynamic magnetic properties of 1 exhibit weak frequency-dependent out-of-phase (χm'') signals of ac magnetic susceptibilities under zero external field. The activated 1 shows the gas uptake of CO_2, whereas N_2 is not adsorbed. Detailed structure, sorption and magnetic properties will be given in the presentation.

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Zn(II) metal-organic frameworks showing nitrobenzene sensing and structural conversion

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We prepared 5-interpenetrating zinc based MOFs [Zn(ethoxy-L)(bpy)](1) and [Zn(propoxy-L)(bpy)](2) using ethoxy and propoxy-H_2L ligand (H_2L=biphenyl-4,4'-dicarboxylic acid). Each Zn center is coordinated by four ligands. Irreversible structural transformation occurs between two complexes. It is probably associated with their thermodynamic stability. These compounds exhibit significant quenching of NB (nitrobenzene). Notably, the fluorescence intensities were almost quenched even at 1 ppm (NB).

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Structural and CO_2 adsorption properties in M_2(dondc)

<u>김남우</u> 임광수 송정화 홍창섭*

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Open metal sites of metal-organic frameworks have been attracted much attention for use in gas separations. To elucidate correlation between CO_2 binding affinity and structural parameters, a series of extended MOF-74 M_2(dondc) (M = Mg^{2+}, Mn^{2+}, Ni^{2+}, Co^{2+}; $dondc^{4-}$ = 1,4-dioxido-2,6-naphthalendicarboxylate) was prepared by a microwave reaction. These compounds were characterized by elemental analysis, infrared spectroscopy and powder X-ray diffraction. Detailed structural and CO_2 adsorption properties will be given in the presentation.

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The effect of solid solution on proton conductivity of UiO-66 partially functionalized with sulfonic acid

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We have investigated the controlled proton conductivities of $Zr_6O_4(OH)_4(DSBDC)_x(BDC)_{1-x}$, ($DSBDC^{2-}$ =2,5-disulfo-1,4-benzenedicarboxylate), where X was 0, 0.2, 0.4, 0.6, 0.8 and 1. Sulfonic acid functionalized UiO-66 was synthesized by oxidizing the thiol-substituted UiO-66 material which was $Zr_6O_4(OH)_4(DMBDC)_x(BDC)_{1-x}$ ($DMBDC^{2-}$=2,5-dimercapto-1,4-benzenedicarboxylate). The above thiol-substituted UiO-66 was prepared by microwave-assisted reaction with $ZrCl_4$ as a metal ion and different molar ratios of H_2BDC (1,4-benzenedicarboxylic acid) and H_2DMBDC(2,5-dimercapto-1,4-benzenedicarboxylic acid) as organic linkers. As varing the number of ligand-based proton donor, we were able to observe the dependence of proton density toward proton conductivity. Detailed structures and other measurements will be given in the presentation.

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Effect of Lewis acidity at the open metal sites of expanded MOF-74 on CO_2 capture

조현아 박소라 홍창섭*

고려대학교 화학과

M_2(dobpdc) (M = Mn, Co, Ni, Zn; dobpdc^{4-} = 4,4'-dioxido-3,3'-biphenyldicarboxylate) containing high-density open metal site with hexagonal one-dimensional channels were synthesized via solvothermal and microwave methods. To investigate Lewis acidity at the open metal sites, acetone was chosen as a probe guest. In the IR spectra, C=O stretching vibrations of acetone showed the order of Lewis acidity, indicating its correlation with CO_2 adsorption enthalpy. Among these frameworks, Ni_2(dobpdc) was stable to refluxing water conditions as well as to acidic or basic solutions.

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A highly porous metal-organic framework: synthesis, structure and sorption property

박소라 권소라 홍창섭*

고려대학교 화학과

Metal-organic frameworks(MOFs) known as porous coordination polymers are an emerging class of porous materials constructed from metal-containing nodes and organic linkers and have applications in gas sorption, storage and separation because of high surface area. We synthesized a highly porous framework using extended carboxylates, which exhibits large surface area. We will present the detailed structure and sorption properties of MOF.

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Synthesis, structure and sorption properties of a metal-organic framework with high porosity

권소라 조현아 홍창섭*

고려대학교 화학과

Metal-organic frameworks (MOFs) are high porous materials that have attracted extensive research interest due to tunable porosity and various application in gas sorption, storage and separation. We have designed a large pore spaces of metal-organic frameworks (MOFs) by adopting more long linker in order to enhance carbon dioxide capture abilities. We designed a new ligand, H_4L [= 4,4’-Dihydroxy-(1,1’-triphenyl)-3,3’-dicarboxylic Acid]. The reaction of H_4L and Mg(Ⅱ) allows the formation of an expanded MOF-74 structure type via microwave method. We will present the detailed structure and sorption properties.

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Synthesis and Physical Properties of Multi-Redox-Centered Ligand and Its Porous Coordination Network

하주연 **Masaki Kawano***

포항공과대학교(POSTECH) 첨단재료과학부

In the field of porous coordination networks, signi?cant progresses have been achieved to find unique functions such as gas sorption ability, catalytic activity, molecular separation, and so on. Especially, porous coordination networks which can realize mixed-valence state are promising as novel effective porous electrical conducting materials useful for electrode of batteries, fuel cell, capacitors. However, to the best of our knowledge, there is no report of multi-redox-centered ligands which realize mixed-valence state in networks. In this presentation, we will report the preparation and properties of the a porous coordination network composed of Cd(Ⅱ) ions and multi-interactive ligand 5,5',8,8'-tetra(4-pyridyl)-2,2'-(1,4-phenylene)bis-1H-perimidine (TPP) based on diazaphenalene (DAP) moieties.

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Rational Design of Dicyanobenzene Derivatives for Effective TADF Characteristics

김효정 김준열 이석중*

고려대학교 화학과

It has been proposed that the thermally activated delayed fluorescence (TADF) system as next generation-luminescent material may provide a solution for the electroluminescence devices such as OLEDs. And it has attracted much interest as alternatives for fluorescence and phosphorescence based OLEDs due to an effective use of not only singlet but triplet excitons for fluorescence using efficient charge transfer from the triplet excited state (T1) to the singlet excited state (S1) with reverse intersystem charge crossing (RISC). With appropriate molecular design, such as a twisted structure between donor and acceptor, the restricted HOMO-LUMO overlap can be achieved. Therefore, with elegant molecular design, efficient charge transfer allows for TADF to yields over 90% of internal quantum efficiency. As such, TADF have been considered one of the most promising alternatives to achieve high efficient emission in wide range of colors. In this regard, we carefully designed dicyanobenzene derivatives with distorted geometry to induce a small band gap between HOMO and LUMO in order to obtain effective emitting materials with TADF mechanism. As a result, DCN series were synthesized and evaluated their performances as potential OLED dopants. Here, we like to present their performances in OLED devices based on the dicyanobenzene derivatives.

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Semiconducting π-Extended Porphyrin Dimer and its Characteristics in OFET and OPVC

채승현 이석중*

고려대학교 화학과

In recent years, studies of soluble π-conjugated porphyrins have produced considerably interesting results for their applications in organic thin film transistors (OTFTs) and organic photovoltaic cells (OPVCs). The π-conjugated molecules may provide the successful electrical charge transport with effective aggregations of π-orbitals. In this regard, we report here on the design and synthesis of new solution processable semiconducting π-extended porphyrin dimer (PD-1), and its OFET and OPVC characteristics. Due to strong π-π interactions, PD-1 showed high crystallinity in film state which displayed excellent electrical characteristics with high hole mobility of 0.026 cm2/Vs and high current on-off ratio of >105, when the device was fabricated in the mixed solvents of toluene and THF. This mobility is 1000 times better than that of a device fabricated from a solution either THF or toluene alone. Considerably high packing density of J-aggregated arrays has been generated in the mixed solvents of toluene and THF verified by PXRD result showing high crystallinity. Furthermore, the photovoltaic performance of PD-1 device shows a PCE of 0.58 %.

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Synthesis and X-ray Structure of Copper Complexes Bearing Methylfuryal and Methylthiophene Derivatives of (*R*,*R*)-1,2-diaminocyclohexane

함지혜 정종화*

경북대학교 화학과

Chiral secondary *vic*-diamines, specifically those derived from enantiomerically pure (*R*,*R*)-1,2-diaminocyclohexane are particularly attractive ligands for many metal catalyzed asymmetric transformations. Novel series of four dichloro copper complex ligated by the enantiopure bidentate ligands, L^1 ? L^4, where L^1 is (1*R*,2*R*)-N^1,N^2-dimethyl-N^1,N^2-bis((thiophen-2-yl)methyl)cyclohexane-1,2-diamine, L^2 is (1*R*,2*R*)-N^1,N^2-dimethyl-N^1,N^2-bis((5-methylthiophen-2-yl)methyl)cyclohexane-1,2-diamine, L^3 is (1*R*,2*R*)-N^1,N^2-bis((furan-2-yl)methyl)-N^1,N^2-dimethylcyclohexane-1,2-diamine, and L^4 is (1*R*,2*R*)-N^1,N^2-dimethyl-N^1,N^2-bis((5-methylfuran-2-yl)methyl)cyclohexane-1,2-diamine, have been synthesized in high yield and purity. The crystal structures of the complexes were determined by X-ray crystallography. These complexes are found to be monomeric and exist in distorted square planner geometries. The complexation of the metal to ligand framework resulted in five membered heterocyclic ring that blocks the nitrogen and induces chirality in them. O_{furyl}-Cu interactions exit in CuL^3Cl_2 and CuL^4Cl_2 that lead to the disappearance of original C_2-symmetry of the ligands, L^3 and L^4.

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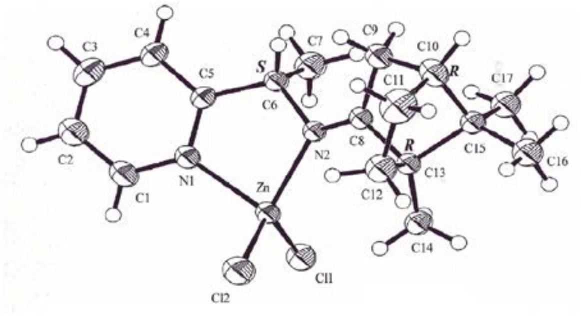
Synthesis and X-ray Structures of Zinc and Copper Complexes supported by Camphor Based Imino-pyridine Ligand

권경섭 정종화*

경북대학교 화학과

Chiral imino-pyridine ligands, specifically those derived from *(1R)*-(+)-camphor is particularly attractive ligands for many metal catalyzed asymmetric transformations. The condensation of (±)-1-(pyridin-2-yl)ethanamine with *(1R)*-(+)-camphor resulted in two diastereomers of L^1, where L^1 is N-(1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene)-1-(pyridin-2-yl)ethanamine. The resultant diastereomers were unable to be separated by column chromatography. Dichloro Zn(II) and Cu(II) complexes were synthesized by treating the corresponding metal precursors with crude ligand L^1 (containing both diastereomers) in EtOH. In case of Zn(II) only one diastereomer selectively coordinated to Zn centre in *S-R-R* configuration, while in case of Cu(II) both distereomeric complexes co-crystallized in *R-R-R* and *S-R-R* configurations which are confirmed by X-ray diffraction studies. The geometry around the Zn(II) centre was found to be distorted tetrahedral, while that for Cu(II) is distorted square planner.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Cl2
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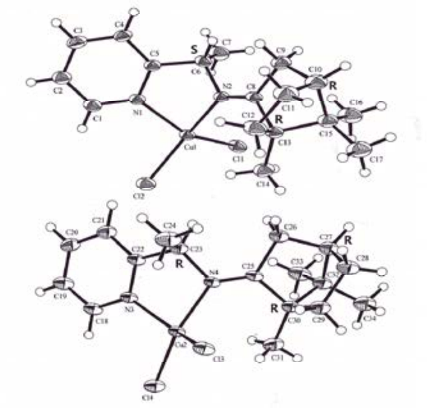
C3
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C12
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Cu1
Cl1
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C14
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C27
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Cu2
Cl3
C31
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Development of efficient photocatalytic system (Dye/TiO_2/ReC) for CO_2 reduction using Ni-Cyclam derivatives as a reduction catalyst (ReC)

정원조 원동일 손호진* 강상욱*

고려대학교 소재화학과

화석연료의 사용량 증가로 인한 CO_2 발생량의 폭발적인 증가로 인하여 지구온난화와 기후변화로 기인된 자연폐해가 가속화 됨에 따라 전세계적으로 CO_2 저감 및 활용을 위한 연구개발에 많은 투자가 이루어지고 있는 상황이다. 많은 관련 기술 중 가시광을 이용 CO_2 환원반응을 유도를 위한 방법으로 태양빛을 이용한 청정공정연구가 각광받고 있는 상황이며 이에 본 연구에서는 TiO_2 에 유기염료인 DMOM 과 Ni-Cyclam 유도체를 접합시킨 새로운 Triad-hybrid 구조(Dye/TiO_2/ReC)를 통하여 효율적인 공정시스템을 구현하고자 하였다. 우선적으로 효과적인 환원촉매인 Ni-Cyclam 을 TiO_2 에 anchoring 하기 위한 방법으로서 -PO_3H_2 그룹이 치환된 화합물이 고안되었으며 합성 간 NMR 과 ESI Mass 분석을 통해 신규 Ni-cyclam 유도체의 합성여부가 확인되었다. 또한 Cyclic voltammetry 측정을 통하여 전기화학적 거동이 확인되었으며 광화학반응을 통한 CO_2 에서 CO 로의 전환효율이 측정 비교되었다.

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Gas sensing Device Fabrication Using Redox Active Porous Coordination Networks

김재준 **Masaki Kawano***

포항공과대학교(POSTECH) 첨단재료과학부

Porous coordination network (PCN) has attracted considerable attention as one of the promising candidates for sensing application because it has porosity with large surface area which enables signal amplification. Conventional studies about PCN-based sensing materials exhibit fluorescence as a dominant indicator for signal transduction which is induced by guest encapsulation. On the other hand, it is not trivial to use other physical property like conductivity as a signal indicator. In this presentation, we report humidity sensing devices on the basis of selectively-prepared two kinds of PCNs using redox active 2,5,8-tris(4-pyridyl)diizaphenalene (TPDAP). The target materials were prepared by the formation of PCN with TPDAP and Cd(NO3)2 on the Si substrate with the solution casting method. The obtained PCN film kept crystallinity and showed clear electron conductivity switching behavior with high sensitivity depending on outer humidity. X-ray diffraction analysis revealed that the electron current ON/OFF property was induced by structure changes in PCNs. These results allow us to reveal the mechanism on the basis of structural information and open the way for the practical use of redox active PCN as electrical sensors.

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SERS Hot Spot Formation with Thiol Functionalized Cucurbit[6]uril and Single Molecule Detection

황우습 김남훈[1] 김기문[*] 백강균[2] 윤경원[2] 김지홍

포항공과대학교(POSTECH) 화학과 [1]한국화학연구원 나노바이오융합연구단 [2]기초과학연구원 복잡계자기조립연구단

Surface-enhanced Raman scattering (SERS), which can provide unique molecular fingerprint information with a single-molecule sensitivity in a non-destructive manner, has attracted considerable interest as a powerful spectroscopic tool in a wide range of applications. Herein, we developed a new strategy for the generation of SERS hot spots by attaching a silver nanoparticle to a bulk silver substrate with a thiol functionalized cucurbit[6]uril (thiol-CB[6]), which allows securing a single spermine-tagged molecule in close proximity to the SERS hot spot through the strong host-guest interaction between CB[6] and spermine. FT-IR and X-ray photoelectron spectroscopy (XPS) studies confirmed the vertical geometry of thiol-CB[6] on silver substrate suggesting that the CB[6] pore is open for guest binding. Using the polarization dependent SERS mapping technique, the single molecular behaviors of the spermine-tagged dye molecules were investigated. The details of this work will be presented.

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Structure and Surface Transformation of High Conducting Multi-interactive Molecule by Hydration

이길령 **Masaki Kawano***

포항공과대학교(POSTECH) 첨단재료과학부

Structure determination of efficient ion conducting system is one of the most attractive fields in the material chemistry. Although still there are many problems to be solved, recent efforts from various fields have been overcoming them. Especially, it is technically very difficult to analyze accurate structure using X-Ray diffraction under high humid conditions. Recently, we have successfully revealed the structure of efficient conduction state with nano-meter size water layer formed by multi-interactive molecule, tris(4-pyridyl)hexaazaphenalene (TPHAP) by ab initio XRPD analysis. The potassium salt of TPHAP showed high ion conductivity up to 3.4 x 10?3 S/cm by hydration. This conductivity was realized by the large water layer formation which was stabilized by multi-interactivity of TPHAP. Furthermore, we observed the surface transformation of KTPHAP single crystal depending on hydration process. Our material can be a good example for understanding the water-mediated conduction mechanism which is difficult to solve by soft materials.

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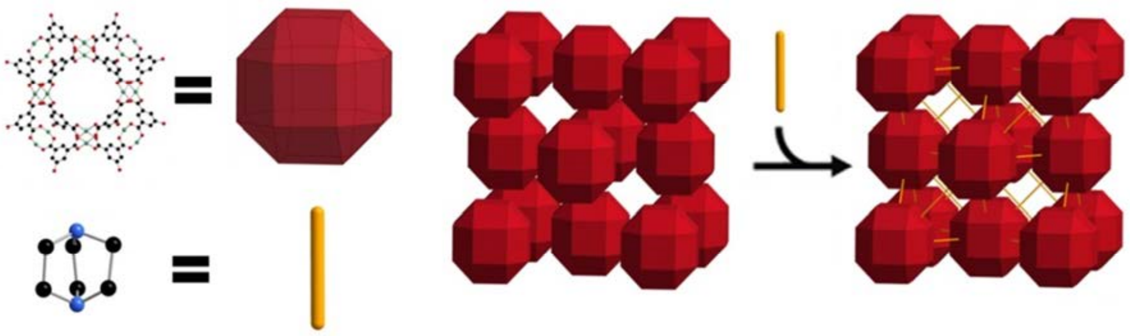
Single-crystal to single-crystal transformation from Metal Organic Polyhedra(MOPs) to Metal Organic Frameworks (MOFs)

이지영 최원영*

울산과학기술대학교(UNIST) 화학과

Metal organic Frameworks (MOFs) and Metal Organic Polyhedra (MOPs) are hybrid porous crystalline materials which consist of metal nodes and organic linkers. There are structural similarities between 0D MOPs and 3D MOFs. In this work, we focus on the rhombicuboctahedron MOPs and face-centered cubic (fcu) net MOFs. The rhombicuboctahedron MOPs are often constructed from copper paddlewheel metal node and dicarboxylic linkers, consisting of 8 triangle faces and two types of 16 square faces, and can be classified as body-centered cubic or face-centered cubic patterns. An interesting way to synthesize the face-centered cubic (fcu) net is that connect the axial position of 12 copper paddle-wheels of rhombicuboctahedron cages acting as supramolecular building blocks. In this poster, we demonstrate the single-crystal to single-crystal transformation from MOPs to MOFs, together with possible application in nanoscience.



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Synthesis and Reactivity Studies of copper complexes with a new N3O Ligand

문건우 이동헌* 유아람별

전북대학교 화학과

The reactivity studies of O2-transition metal with oxygens are inspired by biological metalloenzyme. The transition metal ion in active site of metalloenzyme is an important portion in biological catalysis. Oxidation of organic substrates using molecular oxygen can be critical in green environment and industry. In this study we investigated dioxygen reactivity with a newly synthesized mononuclear copper complex with a pyridyl chelate. The new ligand (6-((methyl(pyridin-2-ylmethyl)amino)methyl)pyridin-2-yl)methanol is tetradentate and has a primary alcohol moity. We have synthesized copper complex 1 [Cu()](ClO4)2, the solid state structure of a copper complex 1 [Cu(1)](ClO4)2 determined by single crystal X-ray diffraction studies. The molecular structure showes a distorted octahedral geometry around the Cu(II) ion. Exposure of copper(I) and to air at 25 ℃ yielded in a product in which the primary alcohol functional group converted to an aldehyde group. Additional experimentals show that the oxidation was achieved by the atmospheric oxygen. Further investigation is needed to gain more insight on the reaction mechanism for the oxidation.

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Water Sorption Properties of Al-based Metal-Organic Frameworks

최판규 김태민 유래경 김자헌*

숭실대학교 화학과

Metal-Organic Frameworks (MOFs) are considered as promising water sorbent materials applicable for thermally driven adsorption chillers (TDC). The water vapor adsorption-desorption by MOFs mediate heat transformation, leading to producing cooling water. The efficiency of this process is largely dependent on the working capacity of MOFs at a desired relative pressure range, $0.1 < P/P_0 < 0.3$ as demonstrated some MOFs including Al-fumarate. In this presentation, the water vapor sorption behaviors of various Al-MOFs such as CAU-8, CAU-10, and MIL-53(Al) will be discussed in comparison with that of Al-fumarate. The optimized synthetic procedure for Al-fumarate will be also presented.

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Synthesis and Structural studies of Metal complexes of N,N'-Disalicylidene-2,2'-(ethylenedioxy)bis(ethylamine)

임종완

심인고등학교 화학

Two manganese complexes [Mn(L)Cl], [Mn(L)(CH3COO)] [L=N,N'-Disalicylidene-2,2'-(ethylenedioxy)bis(ethylamine)] and nickel complex have been prepared and characterized by X-ray diffraction measurements. The crystallographic analysis of the complex revealed that the two Mangneses compexes are mononuclear structure. On the other hand Ni complex is polynuclear structure.

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알루미늄 촉매계를 이용한 cyclic carbonate 합성 연구

황상구 김영조*

충북대학교 화학과

CO2 와 다양한 에폭사이드를 사용하여 지방족 cyclic carbonate 를 합성할 수 있는 촉매계에 대한 많은 연구가 수행되어 왔다. 특히 cyclic carbonate 합성용 알루미늄 촉매계는 대부분 알루미늄에 배위되는 방향족 리간드의 변형에 치우쳐져서 연구가 진행되어왔다. 이에 비해 지방족 리간드가 배위된 알루미늄 화합물을 촉매로 이용한 경우는 상대적으로 덜 알려졌다. 본 연구에서는 새로운 형태의 세자리 또는 네자리 지방족 리간드를 고안/합성한 후, 알루미늄에 배위시켜 단핵, 이핵 촉매계를 합성하였으며 이를 cyclic carbonate 합성용 촉매로 사용한 결과를 발표하고자 한다.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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금속카보닐 촉매계를 이용한 효율적 CO_2 고리화 첨가 반응

조우리 김영조*

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에폭사이드와 CO_2 로부터 생성되는 aliphatic cyclic carbonate 에 대한 연구는 최근 수 년 동안 꾸준하게 수행되어 왔다. aliphatic cyclic carbonate 이 생ㅅ형되기 위해서는 적절한 촉매와 조촉매가 사용되어야 하고, 일반적으로 높은 온도와 높은 CO_2 압력이 필요하다. 본 연구에서는 기존에 cyclic carbonate 촉매로 전혀 사용되지 않은 새로운 카보닐계 금속 화합물을 이용하여 cyclic carbonate 의 합성에 대한 보고를 하고자한다. 더 나아가 금속에 배위되는 특정 리간드의 촉매 활성에 미치는 영향에 대해 살펴보았다.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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Oxidative Decomposition of Weak-Link Approach Supramolecular Complexes

장현재 문현경 윤효재*

고려대학교 화학과

The research for air-sensitivity of supramolecular coordination complexes is a challenging issue in various scientific fields. This presentation describes the air-sensitivity of weak-link approach (WLA)supramolecular constructs formed by d^8 transition metal (Rh(Ⅰ), Pt(Ⅱ)) and hemilabile phosphine-thioether ligands ($Ph_2PCH_2CH_2SR$). We investigate water- and oxygen-tolerance of WLA supramolecular complexes by changing the following experimental conditions: solvent, d^8 transition metal, and molar ratio between metal and ligand. ^{31}P NMR spectroscopy was used to monitor the decomposition process of WLA supramolecular complexes under various conditions. This study shows that the air-sensitivity of Rh(Ⅰ)-based WLA system results from the oxidation of tertiary phosphine moiety of hemilabile ligand, and establishes that the oxidation reaction is catalyzed by Rh(Ⅰ) metal center.

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신규 이핵 알루미늄 촉매계를 사용한 폴리락타이드 합성 연구

안지윤 김영조*

충북대학교 화학과

현재 상용화되고 있는 고분자는 낮은 분해성으로 인하여 환경 오염 문제가 대두되고 있기 때문에 생분해성 고분자인 폴리락타이드에 대한 연구가 활발히 이뤄지고 있다. 본 연구에서는 기존에 알려지지 않은 헤테로아로마틱 리간드를 새로 디자인하고 알루미늄을 중심금속으로 사용하여 배위시킨 금속화합물을 합성하였다. 본 연구에서는 헤테로아로마틱 리간드를 함유한 이핵 알루미늄 화합물의 합성, X-ray 단결정 구조 및 폴리락타이드 합성용 촉매로서의 응용성에 대해 발표하고자 한다.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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폴리락타이드 합성용 유기촉매계에 대한 연구

김혜진 이정훈 김영조*

충북대학교 화학과

락타이드 단량체의 고리열림중합에 의해 만들어지는 폴리락타이드 합성용 금속 촉매는 매우 다양하다. 이러한 폴리락타이드 합성용 금속 촉매들은 중합 후에도 고분자에 소량 남아있기 때문에 생체적합성이 좋지 않다는 문제점이 알려져 있다. 이러한 문제점을 해결하기 위한 노력으로 N,N-dimethylaminopyridine(DMAP)과 같이 금속을 함유하지 않는 유기 촉매계가 최근 문헌에 보고되었다. 본 연구에서는 DMAP 과는 다른 새로운 형태의 유기 촉매계를 체계적으로 고안/합성하고 이들을 폴리락타이드 합성용 촉매로 사용한 결과를 발표하고자 한다.

Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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Synthesis and Optical Characterization of Germafluorene for Blue OLED and Sensor Application

엄성용 손홍래*

조선대학교 화학과

Various functionalized germaflourenes have been synthesized and their optical properties were investigated. Germaflourene compounds were synthesized from the reaction of 2,2'-dibromobisfluorene with germanium tetrachloride in THF at room temperature. Germafluorenes were characterized by 1H-NMR, UV-Vis absorption, and photoluminescence spectroscopy. The optical absorption spectra showed an absorption edge at 280 nm and photoluminescence at 350 nm. These compounds are used as light emissive layers, as they possess relatively low LUMO energy levels while maintaining high HOMO-LUMO optical gaps. Differential scanning calorimetry measurements indicate that germafluorene compounds shows a remarkable thermal stability up to 350 oC. Organic light-emitting diode device has been fabricated using thermal evaporation technique. Germaflourene compounds emit blue light with an excellent diode behavior under the forward bias. This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Aggregation Induced Emission Enhancement Properties of Bis(silacyclopentadiene) and Oxybis(silacyclopentadiene): The Effect of Oxygen between AIE Fluorephores

신보미나 손홍래*

조선대학교 화학과

The aggregation of highly emissive organics into a solid state causes an emission-quenching effect, since the aggregation of molecules forms less emissive species such as excimers. In contrast, few results on aggregation-induced emission (AIE) properties have been reported. For possible applications, they used as chemo-sensor to detect nitro-aromatic compounds, such as 2,4,6-trinitrotoluene (TNT). A linear Stern-Volmer relationship was observed for the analytes. The mechanism of quenching is attributed to electron transfer from the conduction band of Silole to the LUMO of the analytes.1-Chloro-1-methyl-2,3,4,5,-tetraphenyl-1Silacyclopentadiene (1) was reacted with sodium to give 1,1-bis(1-Methyl-2,3,4,5-tetraphenyl-1-Silacyclopentadiene). 1-Chloro-1-methyl-2,3,4,5,-tetraphenyl-1silacyclopentadiene (2) was reacted with H2O to give 1,1'-oxybis(1-methyl-2,3,4,5-tetraphenyl 1-silacyclopentadiene). The resulting products characterized by UV-vis and IR spectroscopy as well as X-ray single crystallography. Optical properties and aggregation behavior will be discussed. This research was supported by Agency for Defense Development.

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High Refractive Polysiloxane Hybrimer Based on Dendrimer-Type Siloxane for LED Encapsulant Application

김종준 손홍래*

조선대학교 화학과

Phenyl-vinyl-oligosiloxane (PVO) has been was synthesized by nonhydrolytic sol-gel condensation process from the reaction of vinyltrimethoxysilane (VTMS) and diphenylsilanediol (DPSD). Barium hydroxide monohydrate was used as a catalyst and promotes the direct condensation reaction between the methoxy radical of VTMS and diol radical of DPSD from siloxane bonds. The 1,3,5-tris(dimethylhydrosilyl)benzene (TDMSB), crosslinking agent, was synthesized through in situ Grignard reactions of 1,3,5-tribromobenzene with chlorodimethylsilane. The synthesized PVO were thermal cured with a cross-linker, TDMSB, through a hydrosilylation reaction under a Pt catalyst, Platinum cyclovinylmethyl-siloxane complex (Pt0?[CH2=Ch(Me)SiO]4). The resulting polysiloxane-based hybrimer has a high refractive index of 1.57 and good transmittance of 97 ~ 98 % at 460 nm, after thermal curing at 180℃ for 2 h, which is the most important optical properties for the photo-extraction efficiency of LED encapsulantThis work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Optical and Structural Characterization ofSilafluorenes Containing Triptycene Moiety for Explosive Sensing Application

이성기 손홍래*

조선대학교 화학과

The synthesis, spectroscopic characterization, and fluorescence quenching efficiencies of silafluorene were reported. The synthesized compounds were characterized by 1H and 13C NMR spectroscopy. Absorption and emission spectra for these compounds were obtained by using UV-Visible and fluorescence spectroscopy in solution. Their emission behaviors and quantum yield for these compounds were investigated both in the solid and colloid state. Our results indicated that both compounds were used as the chemo-sensor to detect various type of explosives such as nitro-amines (1,3,5-trinitroperhydro-1,3,5-triazine, RDX), nitro-aromatics (1,3,5-trinitrotoluene, TNT), and nitrate esters (PETN). The results of detection efficiencies showed that both compounds could be used as an excellent chemo-sensor and other silafluorene derivatives were synthesized and their photonic behaviors were investigated. This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)This research was supported by Agency for Defense Development.

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Aggregation Induced Emission Enhancement of Poly(tetraphenylsilole) Siloxane Nanoaggregates and Their Sensing Applications

이성기 손홍래*

조선대학교 화학과

New photoluminescent and nanoscale poly(tetraphenylsilole) siloxane nanoaggregates for the detection of 2,4,6-trinitrotoluene (TNT) were developed by using aggregation-induced emission property. Poly(tetraphenylsilole) siloxane nanoaggregates exhibited that photoluminescence (PL) intensity was increased when the water fraction was increased to 90% by volume. Relative PL efficiency of poly(tetraphenylsilole) siloxane nanoaggregates was exponentially increased to the percent of water fraction and particle diameter was dependent on solvent composition. Particle size of poly(tetraphenylsilole) siloxane nanoaggregates was tuned by controlling the water fraction by volume. Poly(tetraphenylsilole) siloxane nanoaggregates showed neither further aggregation nor degradation. Detection of TNT was achieved from the measuring of quenching PL of poly(tetraphenylsilole) siloxane nanoaggregates by adding the TNT. A linear Stern?Volmer relationship was observed for the detection of TNT.This research was supported by Agency for Defense Development..

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1D coordination polymers with amino acid formed by in situ double Michael addition of ethylenediamine to *(E,E)*-muconic acid

강재은 강종욱 도정환* 박용선*

건국대학교 화학과

A new 1D nickel coordination polymer, Ni(*rac*-piperazine-trans-2,3-diacetate)(H_2O)$_2$, has been synthesized and characterized by single-crystal X-ray diffraction techniques. Under mild hydrothermal conditions, Michael addition of ethylenediamine to *(E,E)*-muconic acid led to the formation of racemic mixtures of *rac*-piperazine-2,3-diacetate anion. The structure consists of 1D chain in which nickel atoms are alternatively bridged by racemic piperazine-2,3-diacetate anions and two additional water molecules bonded to nickel atoms complete the Ni(*rac*-piperazine-2,3-diacetate)(H_2O)$_2$ chains. The chains are further connected by hydrogen bonds to form a framework structure.

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Electrochemical Behaviors of (diphosphine)M(1,2-dithiolene) Complexes where M = Ni(II) and Pt(II)

이윤경 노동윤*

서울여자대학교 화학과

The (diphosphine)M(1,2-dithiolene) complexes where the diphosphine is 1,2-bis(diphenylphosphino)ethane (dppe) or 1,1'-bis(diphenylphosphino)ferrocene (dppf), were synthesized using (diphosphine)MCl_2 and the dithiolene ligands such as 1,3-dithiole-2-thione-4,5-dithiolate (dmit) and maleonitriledithiolate (mnt). X-ray structural analysis for Ni(II) complexes show that the P_2NiS_2 cores are more distorted square planar than those of Pt(II) analogues. Electrochemical properties of Ni(II) and Pt(II) complexes were confirmed through cyclic voltammetry. The Ni(II) and Pt(II) complexes are variously compared depending on diphosphine and dithiolene ligand. Cyclic voltammograms of (dppx)$NiCl_2$ complexes show irreversible reduction peak of reduction of Ni(II) and (dppx)Ni(dithiolene) complexes show redox cycle of reduction of Ni(II) at a cathodic region. The electrochemical behaviors for Ni(II) complexes seem to be closely related to their molecular structures, their co-operative behaviors are discussed. For detailed description of electrochemical properties, DFT calculation (B3LYP/LanL2DZ method) was performed the complexes. (NRF 2010-0011478)

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Synthesis and Properties of Multi-metallic Complexes with [Fe(II)-Pt(II)-Pt(II)-Fe(II)]-Ni(II) System

박태정 노동윤*

서울여자대학교 화학과

The asymmetric and symmetric [(dppx)Pt(SEtOH)$_2$Pt(dppf)][ClO$_4$]$_2$ complexes where dppx is 1,2-bis(diphenylphosphino)ethane or dppe (1) and 1,1'-bis(diphenyl-phosphino)ferrocene or dppf (2), were synthesized and characterized. Cyclic voltammograms of the complexes show one redox cycle due to Fc/Fc$^+$ in dppf ligand. The current intensity for the redox cycle of complex (2) is almost twice that of complex (1), indicating the complex (1) has an asymmetric structure. A multi-metallic complex, [(dppf)Pt$_2$(SEtOH)$_2$(dppf)][Ni(dmit)$_2$] (3), is obtained through the metathesis of complex (2) and [TBA]$_2$[Ni(dmit)$_2$] where dmit = 1,3-dithiol-2-thione-4,5-dithiolate. The properties of complex (3) are investigated and to be presented. (NRF 2010-0011478)

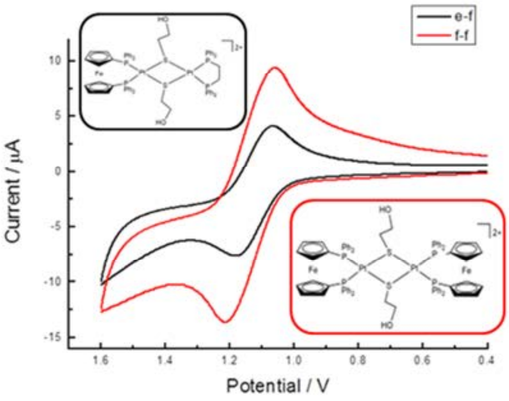

Fig. 1 The cyclic voltammogram of [(dppe)Pt(μ-SEtOH)$_2$Pt(dppf)]$^{2+}$ (**1**) and [(dppf)Pt(μ-SEtOH)$_2$Pt(dppf)]$^{2+}$ (**2**) measured in CH$_2$Cl$_2$ (Fc/Fc$^+$ = 0.540 V vs Ag/AgCl).

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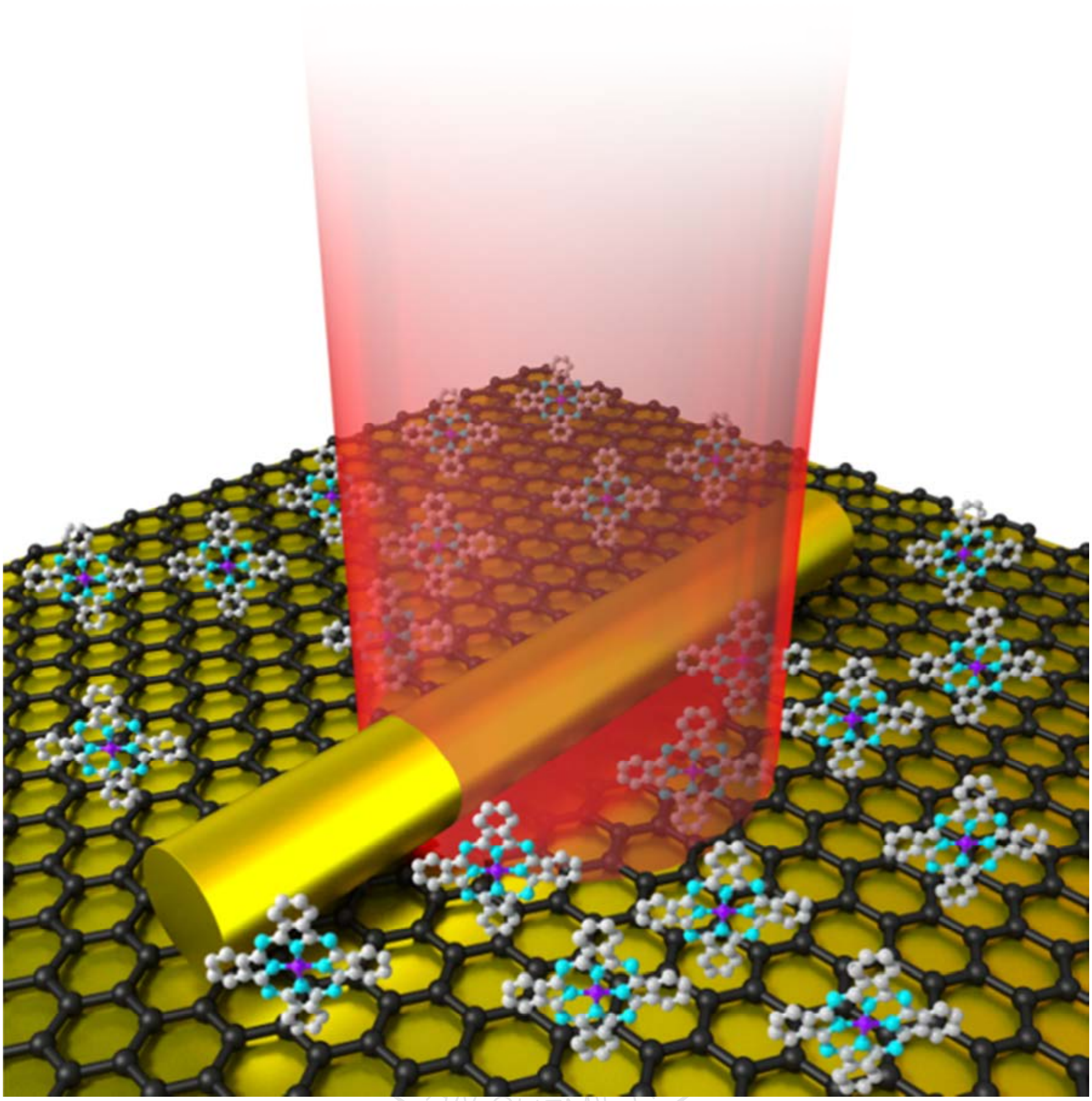
Single Nanowire on Graphene for Efficient Surface-enhanced Raman Scattering Platform

김홍기 김봉수[1,*]

한국과학기술원(KAIST) 화학 [1]한국과학기술원(KAIST) 화학과

Surface enhanced Raman scattering (SERS) is an attractive analytical technique, which can detect the analytes at single molecule level, but poor reproducibility and stability of SERS hinder quantitative analysis in various practical situations. Recently, graphene-mediated surface enhanced Raman scattering (G-SERS) have attention as an advanced SERS platform among diverse promising nanostructure. However, conventional G-SERS substrates reported thus far have been based on the nanoparticles-on-graphene platform, which often caused inevitable inter-particle aggregation and uncontrollable particle size distribution, resulting in degradation on signal uniformity. In this work, we proposed novel single nanowire on a graphene (SNOG) structure for efficient SERS template. Well-aligned continuous nano gap is placed between the atomically uniform Au nanowire and monolayer graphene underlying Au film, leading to uniform line shaped hot-spot profile. We identified unique polar dependence of SNOG template and demonstrate experimentally and theoretically the hot-spot profile along the nanowire which results in extra-high hot-spot uniformity. In addition, we confirmed that SNOG template enhanced photostability and reproducibility of Raman spectra. The combination of atomically uniform single crystalline Au nanowire and single-layer CVD-grown graphene was expected to serve as an excellent SERS platform for practical sensing application.



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Ultrasmall mixed (Mn/Dy) oxide nanoparticles as MRI contrast agent

Badrul Alam Bony 이강호*

경북대학교 화학과

We accomplished a novel and an efficient one-pot synthesis of biocompatible D-glucuronic acid coated ultrasmall Mn/Dy oxide nanoparticles. Aqueous suspensions of the prepared nanoparticles were found to possess enhanced r_2 relaxivities and their in vitro studies indicated significant dose-dependent contrast enhancements in T_2 map images indicating as a potential T_2 MRI contrast agent. Remarkable features like high magnetic moment and relaxivities of Mn/Dy oxide nanoparticles were observed. Moreover, the toxicity of the prepared nanoparticles was also minimized compared to MnO/ Mn_2O_3 or Dy_2O_3 nanoparticles. The efficiency of D-glucuronic acid coated ultrasmall Mn/Dy oxide nanoparticles as T_2 MRI contrast agent was proved through in vivo T_2 MR Images of a mouse.

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Laser-induced fabrication of Ag@SiO_2@Ag sandwich nanostructures

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서울대학교 화학부

Nanoscale noble-metals have attracted attention from researchers in various fields of study because of their unusual optical properties as well as novel chemical properties. It is well-known that gold and silver nanoparticles show strong absorption bands in the visible region due to their surface-plasmon oscillation modes of conductive electrons. Silver nanoparticles stand out from various types of noble-metal nanostructures due to their superior performance in a range of applications involving localized surface plasmon resonances, catalysis, surface-enhanced Raman scattering, and biosensing. Thus, extensive efforts have been devoted to the investigation of silver-based nanocomposites to achieve high catalytic performances and utilization efficiencies. Recently, Ag@SiO_2@Ag sandwich nanostructures have shown good catalytic performances compared with Ag@SiO_2 due to the large surface-to-volume value and the activity of Ag particles on the surface of silica. Furthermore, as Ag@SiO_2 nanoparticles are irradiated by laser pulses, silver clusters attached on the surface of silica have been found to grow to particles, enhancing catalytic performances. In other words, the laser-induced fabrication of Ag@SiO_2@Ag sandwich nanostructures has been found to catalyze the degradation of rhodamine B efficiently in the presence of $NaBH_4$. Moreover, as silver nanoparticles on the surface of silica get larger, their absorption band shifts to the red, enabling Ag@SiO_2@Ag sandwich nanostructures to be applied in the fields of drug delivery, photo-diagnosis, and photothermal therapy.

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Photo-Deposition of Noble Metals (Au, Pt) on Wurtzite ZnS Nanobelts

함수호 김연호 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. Thus, we have synthesized ZnS nanobelts which possess high photo-catalytic efficiency via a one-pot hydrothermal method. To get higher visible light response and to increase the lifetime of photo carriers, we have doped gold and platinum on the surface of the ZnS via a photo-deposition method by using a Xenon lamp. Deposition of noble metals on semiconductor surfaces forms barrier which promotes charge separation. The properties of as-formed samples have been affected by reaction factors such as duration, irradiation power, and the amount of dopants, and hole scavengers like ethanol. We have tested the photo-catalytic efficiency of each sample via the degradation test of rhodamine B under UV and visible-light irradiation. The photo-catalytic performance of 4% platinum-doped ZnS nanobelts has increased by 50% compared to pristine ZnS nanobelts.

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Fabrication and Characterization of Hybrid J-Aggregate Nanofibers Consisting of Poly(3-hexylthiophene)-Coated Gold Nanoparticles

이동기 김준기 장두전*

서울대학교 화학부

Hybrid nanocomposites of conjugated polymers and inorganic materials have received intense attention for applications in optoelectronic devices such as light-emitting diodes, biosensors, and photovoltaic cells. The comprehensive investigation and understanding of the fundamental photophysical dynamics of conjugated polymers such as poly(3-hexylthiophene) (P3HT), which is most commonly used in optoelectronic devices, are critical research points for the development of new materials. In particular, understanding the influence of conformation and packing on the electronic properties of P3HT remains as a long-standing challenge to optimize the performance of this material for optoelectronic applications. Thus, we have fabricated hybrid nanofibers (NFs) consisting of poly(3-hexylthiophene)-coated gold nanoparticles (Au@P3HT NPs) via a self-assembly approach in poor solvents, and compared them with non-aggregated Au@P3HT NPs to investigate the dynamics of photo-generated exciton relaxation using time-resolved transient-absorption and emission spectroscopy. The spectroscopic data of fabricated hybrid NFs show multiple vibronic peaks that appear to be associated with the existence of both H- and J-type aggregates. The emission decay kinetic profile of hybrid NFs monitored at 650 nm has been deconvoluted into two decay components of 340 ps (80%) and 1800 ps (20%), suggesting that high intrachain J-aggregate character exists within hybrid nanofibers.

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Cation Exchange of CdS Quantum Dots to Control Optical Properties

최다연 김연호 장두전*

서울대학교 화학부

Three different types of water-soluble$Cd_{1-x}Zn_xS$ quantum dots (QDs) having nearly identical sizes and compositions have been synthesized via simple and low-cost methods to understand the effect of internal structures on the optical properties of QDs. Compared with the other two types: CdS@ZnS core-shell $Cd_{1-x}Zn_xS$ QDs and alloy $Cd_{1-x}Zn_xS$ QDs, composition-gradient CdS@ZnS core-shell $Cd_{1-x}Zn_xS$ (G-$Cd_{1-x}Zn_xS$) QDs, which have been prepared by exchanging the Cd^{2+} ions of CdS QDs partially with Zn^{2+} ions with conserving the shapes and sizes, have shown the longest lifetime and the highest quantum yield of photoluminescence due to the smallest nonradiative and the largest radiative decay constants of photogenerated charge carriers. The composition-gradient ZnS shells, which passivate the CdS cores optimally with alleviating the lattice strain caused by the lattice mismatches between the CdS cores and the ZnS shells, have been considered to be the main reason for the enhanced optical properties of G?$Cd_{1-x}Zn_xS$ QDs. Among our prepared G-$Cd_{1-x}Zn_xS$ QDs, the quantum yield and the lifetime of photoluminescence are the highest (22%) and the longest (290 ns), respectively, due to the smallest nonradiative dacay constant when about half of Cd^{2+} ions in CdS QDs are replaced by Zn^{2+} ions with composition gradients from their surfaces, where it was hard for Zn^{2+} ions to diffuse into the central parts of CdS QDs, suggesting that internal structures play an important role on the relaxation dynamics of photoexcited charge carriers.

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Facile Fabrication and Time-Resolved Emission Study of Poly(3-hexylthiopene)-Grafted Gold Nanorods

이동기 정수경 장두전*

서울대학교 화학부

Hybrid nanocomposites of conjugated polymers and inorganic nanocrystals have received intense attention for applications in optoelectronic devices such as light-emitting diodes, biosensors, and photovoltaic cells. Since the enhancement of power-conversion efficiency in organic solar cells is an important challenge, the comprehensive investigation and understanding of the fundamental photophysical dynamics of conjugated polymers such as poly(3-hexylthiopene) (P3HT), most commonly used in the active layer of an organic solar-cell device, are critical research points for the development of new materials used for the active layer. Poly(3-hexylthiopene)-coated gold nanoparticles having surface-plasmon resonances (SPR) have been investigated to understand the interaction between the photo-generated excitons of P3HT and SPR. For a better understanding on the effect of SPR of inorganic nanocrystals on the dynamics of exciton relaxation of P3HT, we have incorporated gold nanorods (NRs) having two distinctive, transverse and longitudinal, SPR modes, and compared them with pristine P3HT to investigate the dynamics of the exciton relaxation and decay using time-resolved transient-absorption and emission spectroscopy. The stable morphology of P3HT-grafted gold NRs has been studied by transmission electron microscopy. The dynamics of photo-generated excitons in P3HT-grafted gold NRs has also been investigated in comparison with that in pristine P3HT using time-resolved emission spectroscopy, revealing that the first-excited singlet-state decay of P3HT-grafted gold NRs is found to be slower than that of pristine P3HT due to the conformational effects of P3HT.

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Microwave-Assisted Morphological Variation of Anatase TiO_2 Crystals via Forming Titanium Glycerolate Precursors

김형배 김솔네 장두전[*]

서울대학교 화학부

The development of the facile and rapid synthetic methods of nanostructures with functional properties has become increasingly important. Particularly, the syntheses of metal oxide nanomaterials having controllable shapes and sizes have been extensively explored because of their wide applications. Without using any additional surfactants or ionic additives, we have controlled the morphologies of anatase TiO_2 crystals from rod-like structures to various hedgehog-like hierarchical structures via forming titanium glycerolate precursors as sacrificial templates. The morphologies of the precursors have been controlled readily under microwave irradiation by adjusting the relative solvent volumes of isopropanol and glycerol; whereas rod-like titanium glycerolate structures have been prepared in the absence of isopropanol, hierarchical titanium glycerolate structures have been synthesized at high solvent-volume fractions of isopropanol. The simple hydrolysis of as-prepared titanium glycerolate precursors for 10 min under microwave irradiation has yielded intrinsic morphology-retained anatase TiO_2 nanostructures, although smooth surfaces of the precursors have been turned into rough surfaces of anatase TiO_2 crystals during the hydrolysis. It has been found that the variation of the relative volume fractions of isopropanol and glycerol having significantly different boiling points and viscosity values has changed the nucleation and growth kinetics to control the morphologies as well as the sizes of titanium glycerolate precursors. Our presenting method is suggested to contribute considerably to the development of a new synthetic strategy for the morphology-controlled fabrication of inorganic nanomaterials under microwave irradiation.

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Preparation of Anatase TiO_2 Nanotube Arrays Dominated with Highly Energetic {001} Facets via Anodization

이혜리 장두전*

서울대학교 화학부

The preparation of anatase TiO_2 nanomaterials with dominant {001} facets has been a hot research topic because their surfaces are normally more reactive than energetically favorable {101} facets. However, the tailored synthesis of anatase TiO_2 nanotube arrays dominated with highly energetic {001} facets still remains as a challenge. To study the synergistic effects of highly ordered one-dimensional structures and exposed {001} active facets, anatase TiO_2 nanotube arrays have been synthesized by anodization in ethylene glycol electrolytes containing ammonium fluoride and water. The morphology of as-formed nanotubes has been found to depend on the duration of anodization, applied voltage, and the concentration of ammonium fluoride. The photocatalytic activity of as-prepared anatase TiO_2 nanotube arrays, evaluated by the photodegradation of rhodamine B, has been found to increase with exposed {001} facets. Thus, the exposure of high-energy {001} facets is suggested to make anatase TiO_2 nanotube arrays a promising material for environmental and energy-related applications.

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Correlation of the Rates of Solvolysis of Phenyl p-Methoxy Phenoxy Thiophosphinyl Chloride Using an Extended Grunwald-Winstein Equation

고한중

전주교육대학교 과학교육과

The extended Grunwald-Winstein equation can be expressed as in equation (1) ; k and ko represent the specific rates of solvolysis of a substrate RX in a given solvent and in the standard solvent (80% ethanol), respectively; l is the sensitivity of the solvolysis towards changes in solvent nucleophilicity (NT); m is the sensitivity of the solvolysis towards changes in solvent ionizing power (YX, for a leaving group X); and c is a constant (residual) term. log (k/ko) = l NT ＋ m YX ＋ c (1)In this work, we investigated the solvolyses of phenyl 4-methylphenoxy thiophosphinyl chloride (1) in pure solvents and mixed binary solvents to obtain an exact kinetic information in various solvents at 55.0 oC, equation. The solvolysis of 1, where bond making (l = 1.08) is more progressed than bond breaking (m = 0.53), and the values are still in the range of SN2 mechanism, reflecting on the degree of the nucleophilic assistance based on the measure of solvent nucleophile.

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Estimating thermal effects in the CO photolabilities of Ru complexes coordinated by 2-phenylazopyridine using experimental rate constants and variational transition state theory

장효원* 허경식

순천대학교 화학과

The CO dissocation reactions initiated by UV/vis irradiation of the corresponding Ru complexes are modeled as thermal reactions on the ground potential energy surface. The experimentally determined reaction constants are combined with variational transition state theory calculations to produce the equilibrium temperatures substantially higher than 298K, which is the temperature of the bulk reaction mixtures. Therfore, we conjecture that the corresponding CO photolabilities occur via light absorption followed by thermal degradation and local heating processes.

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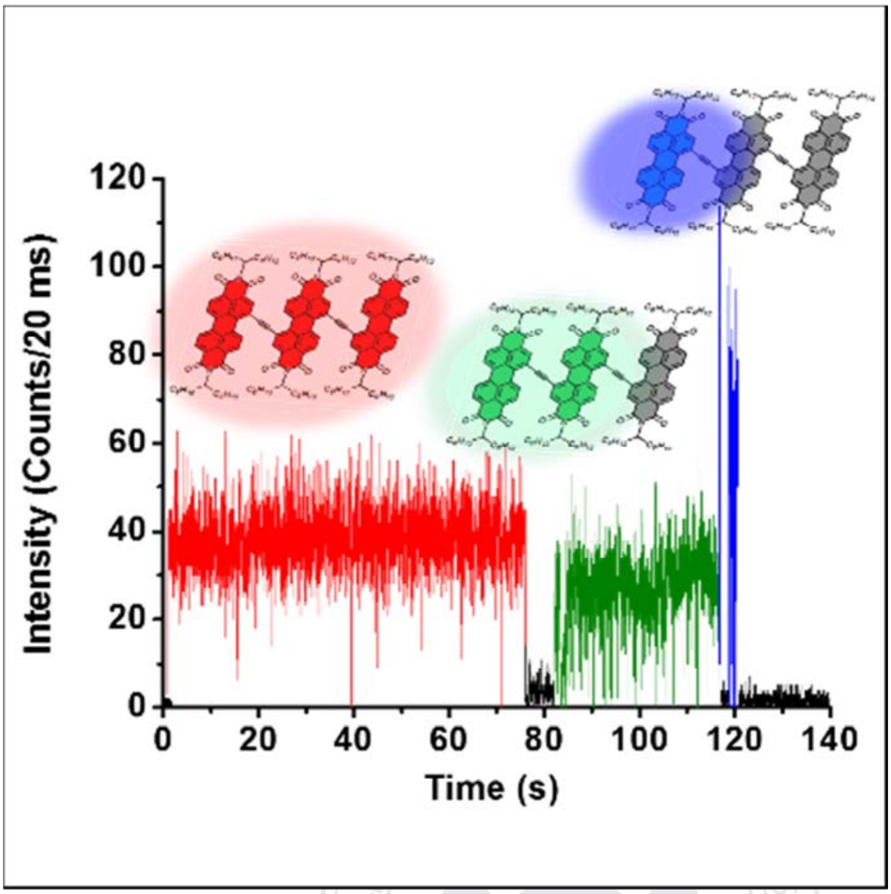
Intramolecular Interactions of Highly π-Conjugated Perylenediimide Oligomers Probed by Single-Molecule Spectroscopy

조재원 김동호*

연세대학교 화학과

Highly π-conjugated perylenediimide (PDI) oligomers are promising low band gap organic materials for various applications in optoelectronics. In this work, individual fluorescence dynamics of ethynylene- and butadiynylene-bridged dimeric and trimeric PDIs (PEP, PBP, and PEPEP) were monitored and analyzed by single-molecule fluorescence spectroscopy to gain information on the degree of extension of π-conjugation through the acetylene bridge in PDI multichromophores. The simultaneous measurements of fluorescence intensity, lifetime, and spectrum indicate a sequential decrease in π-conjugation upon photobleaching of PDI monomer units. Furthermore, Huang-Rhys (HR) factors, S, are obtained to evaluate the degree of electronic coupling in view of π-conjugation and overall rigidity between the PDI units in PDI oligomers at the single-molecule level. In addition, butadiynylene-bridged dimeric PDI (PBP) reveals conformational heterogeneity due to the long butadiynylene linker. These results suggest a new way to control the photophysical properties of the PDI multichromophoric system by expansion of π-conjugation and modification with different linker groups.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Time (s)
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Structure-property relationship of two-dimensionally extended benzoporphyrin arrays probed by single-molecule fluorescence spectroscopy

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Multiporphyrin assemblies have attracted great attention because of their potential application in molecular scale photonic devices such as light-harvesting arrays, molecular wires, photovoltaic cells, and nonlinear optics. In this work, individual fluorescence dynamics of two-dimensionally extended benzoporphyrin arrays have been investigated by single-molecule fluorescence detection techniques to gain information on the degree of extension of π-conjugation. The simultaneous measurements of fluorescence intensity, lifetime, and spectrum indicate a sequential decrease in π-conjugation upon photobleaching of porphyrin monomer units. Furthermore, structural information of benzoporphyrin arrays were monitored and analyzed by defocused wide-field imaging techniques. Our studies will provide further information on the structure-property relationship of single molecules in the solid state.

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Nanoscale Uniformity-Enhanced Adhesion Property on Catechol-Immobilized Ultraflat Single-crystalline Gold Nanoplates

이미연 김봉수*

한국과학기술원(KAIST) 화학과

We report the characterization and formation of catechol-terminated molecules immobilization using N-(3,4-dihydroxyphenethyl)-2-mercaptoacetamide (Cat-EAA-SH) on ultraclan, ultraflat, single-crystalline gold nanoplates (Au NPLs). Au NPLs are synthesized using chemical vapor transport (CVT) method by one-step process, constructing coherently linked between molecule and substrates because Au NPLs make it possible to highly well-ordered and closely packed Cat-EAA-SH molecules immobilization network onto large-scaled surface. We carried out characterization as topography of atomic force microscopy (AFM) in order to verify the how well of catechol-terminated self-assembled molecules immobilization on other kinds of gold substrates. When compared to topography and local force-distance curves, our Au NPLs show not only uniformly and densely immobilize regular-oriented immobilization, but overall higher adhesion than others Au substrates.

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A theoretical study on CO_2 absorption mechanism in amine solvents and enhancement of CO_2 absorption in blended amine solvents

김선경 조대흠 SHIHU 남연식 이진용[*]

성균관대학교 화학과

Carbon dioxide is one of the greenhouse gases that cause the global warming. Amines have been used as efficient solvent for CO_2 capture from exhaust gas. However, the reaction mechanism is unclear though it is well known that a carbamate is formed during the CO_2 capturing reaction. Herein, reaction mechanism for CO_2 absorption in amine solvent was investigated by DFT and *ab initio* calculations. The reactants were CO_2 and six amines (MEA, DEA, PZ, AMP, AEEA, and DETA), and the reactions were designed with or without additional water or amine molecule. Additional water and amine molecules increased intermolecular interaction between reactants and play a role as proton accepter that withdraw proton from amino group of amine. The carbamate formation reaction mechanism that involves additional amines as a base was confirmed to be more reasonable than the other mechanisms. This model can describe the zwitterion mechanism. While previous studies suggest that zwitterion formation step is rate-determining step, the activation energies of zwitterion formation step and proton transfer step were not much different. Moreover, the additional amine process can be applied to understand the enhancement effect of CO_2 absorption in blended amine solvents. We report a new attempt that describes reaction mechanism in blended amine solvent by applying additional amine base. Among various blended amine combination, MEA+PZ, MEA+AEEA, and MEA+DETA could improve the CO_2 capturing capability compared with single MEA solvent. Our result is in excellent agreement with previous experiment studies. Our work should be useful in choosing a proper blended amine solvent for better CO_2 absorption.

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Effect of Hartree-Fock Exact Exchange on the Evaluation of Intramolecular Magnetic Coupling Constants of Organic Diradicals

조대흠 김선경 SHIHU 남연식 이진용*

성균관대학교 화학과

The intramolecular magnetic coupling constant (J) of diradical systems linked with five- or six-membered aromatic rings were calculated to investigate the scale factor (experimental J / calculated J ratio) for various DFT functionals. Scale factors of Group A (PBE, TPSSh, B3LYP, B97-1, X3LYP, PBE0, and BH&HLYP) and B (M06-L, M06, M06-2X, and M06-HF) were shown to decrease as the amount of Hartree-Fock exact exchange (HFx) increases, in other words, overestimation of calculated J becomes more severe as the HFx increases. We further investigated the effect of HFx fraction of DFT functional on J value, spin contamination, and spin density distributions by comparing the B3LYP analogues containing different amount of HFx. It was revealed that spin contamination and spin densities at each atom increases as the HFx increases. Above all, newly developed BLYP-5 functional, which have 5 % of HFx, was found to have the scaling factor of 1.029, indicating that calculated J values are very close to that of experimental values without scaling. BLYP-5 has potential to be utilized for accurate evaluation of intramolecular magnetic coupling constant (J) of diradicals linked by five- or six-membered aromatic ring couplers.

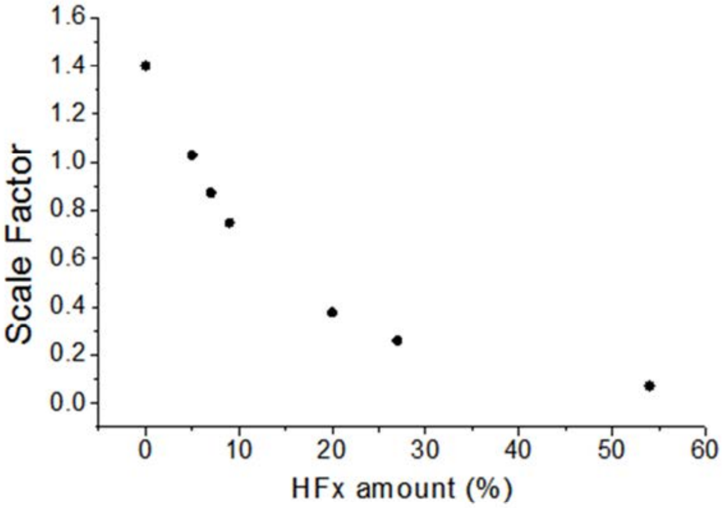

Figure 1 Correlation between scale factor for B3LYP analogues and HFx.

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Effect of Deprotonation State of Histidine in Amyloid β-peptide (1-40) on Structure and Aggregation Properties

SHIHU 조대흠 김선경 남연식 이진용*

성균관대학교 화학과

As a result of pH effect, different deprotonated states of histidine including Hie and Hid were considered as an important factor promoting amyloid β-peptide (Aβ peptide) aggregation, which has been associated with the pathogenesis of Alzheimer’s disease (AD). In present study, replica exchange molecular dynamics simulations were implemented to elucidate the changes of structure and aggregation properties upon different His states (Hie or Hid). Our results show that the different deprotonated combination states on Aβ(1-40) monomer can strongly influence the structural properties. In details, DDE (Hid6-Hid13-Hie14) and DDD prefer sheet structure, while EEE, EDE, and DED are prone to disorder structure. The further results show that representative structure of DDD prefer to expose the K16, E22, and D23 charge residues, as well as LVFFA region, indicating that Aβ(1-40) monomers can easier contact each other by electrostatic interactions, and then promoting hydrophobic interactions of LVFFA region, which are benefit for Aβ(1-40) monomers aggregation. This work is helpful to understand the fundamental role of deprotonated state of His in aggregation, which could be useful for further development of new drugs to inhibit Aβ(1-40) aggregation.

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Reactivity and Regioselevtivity for NO2 Substitution of Monosubstituted Benzene Ring: An Ab Initio Study

남연식 김선경 조대흠 SHIHU 이진용*

성균관대학교 화학과

Reactivity and regioselectivity for NO2 substitution of monosubsituted benzene ring were investigated by means of Becke’s Three-parameter, Lee-Yang-Parr Theory (B3LYP) calculations [B3lyp/6-31+G(d,p)]. Previous studies explain reactivity and regioselectivity by comparing inductive effect through σ bonding and resonance effect through π bonding. 7 well-known substituents were selected to invetigate electron population by Natural Bonding Oribtal (NBO) calculation. It was found that σ population of benzene ring decreased regardless of substituents. In contrast, π population of benzene ring, which is substituted with π donor group, was increased while that of benzene ring, which is substituted with π withdrawing group, was decreased. All of π electron donor substituents were ortho, para directing and all of π electron withdrawal substituent were meta directing. Further, reactivity of each monosubstituted benzene ring was compared through nucleophilicity. It was compared by calculating Highest Occupied Molecular Orbital (HOMO) energy of each monosubstituted benzene which acts as nucleophile. As a result, it was found that all of benzene rings, which has higher HOMO energy level than benzene, is more reactive than benzene while benzene ring, which has lower HOMO energy, shows less reactivity. In conclusion investigation of π population and HOMO energy of substituted benzene ring can be used to predict reactivity and regioselectivity of substituted benzene ring for electrophilic aromatic substitution.

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Photophysical Study of Ethyne-Bridged Porphyrin Arrays by Single-Molecule Fluorescence Spectroscopy

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Single-molecule spectroscopy technique can provide insight into the fundamental photophysical properties of molecular systems. By using the single-molecule spectroscopy, we have studied the ethyne linked porphyrin dimers Z2E, trimer Z3E, pentamer which have star-shape structure Z5E. Fluorescence Intensity trajectories(FITs), fluorescence lifetimes, fluorescence spectra, changes in polarization and changes in defocused image were measured to investigate the single-molecule photophysical properties of these porphyrin arrays. One step photobleaching behaviors of Z2E, Z3E and Z5E demonstrate that ethyne-bridged arrays act as one quantum system due to strong interporphyrin conjugation. Our study provides detailed information on the respective role of electronic couplings in the excited state dynamics of porphyrin arrays at the single molecule level, which will be a guideline for future applications as solid-state molecular devices.

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Efficiency roll-off in doped phosphorescent organic light-emitting diodes

강주연 배소현 민경석[1] 김경우[2] 권장혁[2] 김성근[*]

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Applications of organic light-emitting diodes (OLEDs) in display devices and solid state lighting require achievement of high brightness. In terms of efficiency, OLEDs can compete with highly efficient conventional light sources but their efficiency typically decreases at high brightness levels, an effect known as “efficiency roll-off”. In recent years, much effort has been undertaken to understand the underlying processes but detailed mechanism at the molecular scale is yet to be unraveled. We carried out time-resolved photoluminescence measurements to investigate the excitonic mechanism for the efficiency roll-off phenomenon. We found that exciton quenching is largely at play, including triplet?triplet annihilation or quenching by polarons.

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Study of OLED Degradation Study by Combined Optical Imaging System

배소현 강주연 민경석[1] 김경우[2] 권장혁[2] 김성근[*]

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Extended operation of organic light-emitting diode (OLED) results in materials degradation. To investigate the degradation mechanism, many analytical methods have been introduced such as HPLC-MS or MALDI-TOF, which are mostly destructive techniques. Here we demonstrate a non-destructive, in-situ analytical technique based on optical microscopic imaging. We show that wavelength-dependent lateral imaging of luminescence intensity can pinpoint a specific degradation layer. Furthermore, we show that lifetime imaging of photoluminescence provides additional information about energy transfer efficiency between the host and dopant materials.

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Covalently Functionalized Graphene Composites: Mechanistic Study of Interfacial Fluorescence Quenching and Recovery Processes

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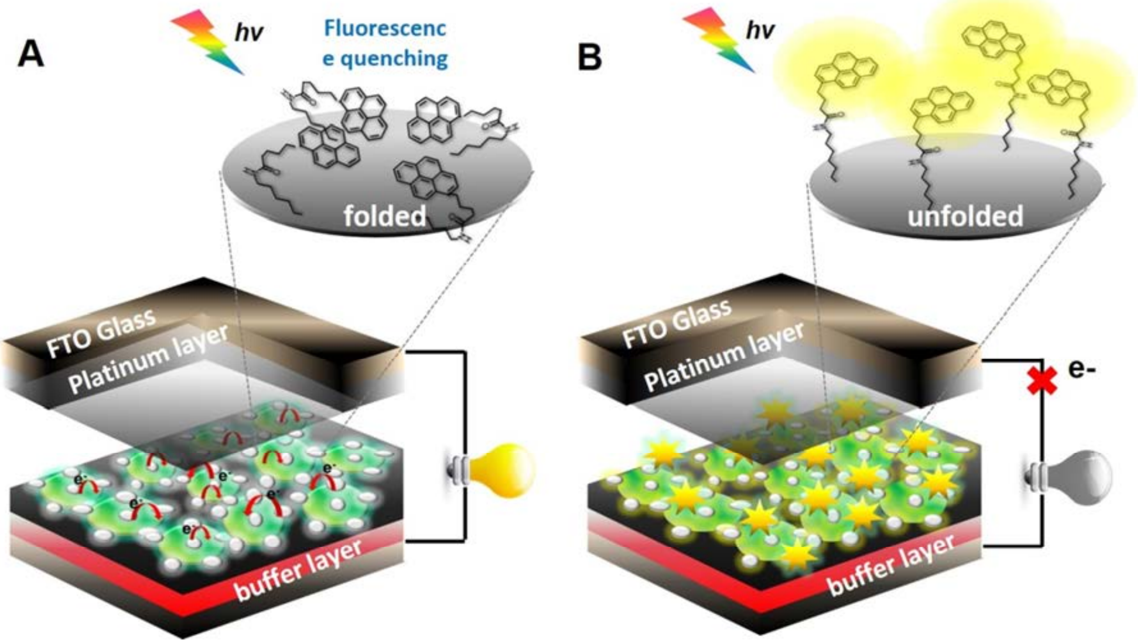
Functionalized graphene-oxide nanosheets (GON) have received a great deal of attention in various fields of applications from optoelectronic devices to biological sensors. Although fluorescence study is one of the most powerful techniques for obtaining information about the conformational or dynamic changes, the mechanism of fluorescence quenching in complex functionalized carbon systems has not been clearly understood due to strong interactions/quenching between chromophore and carbon material. Therefore, the strategic method to overcome the strong interaction and restore its fluorescence should be considered. In this study, we report here a new mechanistic study of interfacial quenching and recovery processes of covalently functionalized graphene composites. The detachment of pyrene moiety as an 'unfolded' conformation could be achieved by sonochemistry with micellerization of sodium dodecyl sulfate (SDS) surfactant. This process was proven to be an effective way to prevent the long-term collapse of pyrene onto the GON. By time-resolved spectroscopic methods, ultrafast charge transfer behaviour (< 1 ps) was observed especially in 'folded' conformation. Interestingly, the fast decay component was diminished and finally disappeared in 'unfolded' conformation at the higher concentrations of SDS, which tightly organizes on the surface of GON. In addition, photocurrent analysis under white light illumination leads us to distinguish electron transfer behaviour in 'folded' and 'unfolded' conformations. In this experiment, effective charge separation occurs only in 'folded' conformation, and photocurrent does as well.


A
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Platinum layer
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Highly Sensitive and Fast Detection of Arsenic by Ultra-small Single Au Nanowire Electrode

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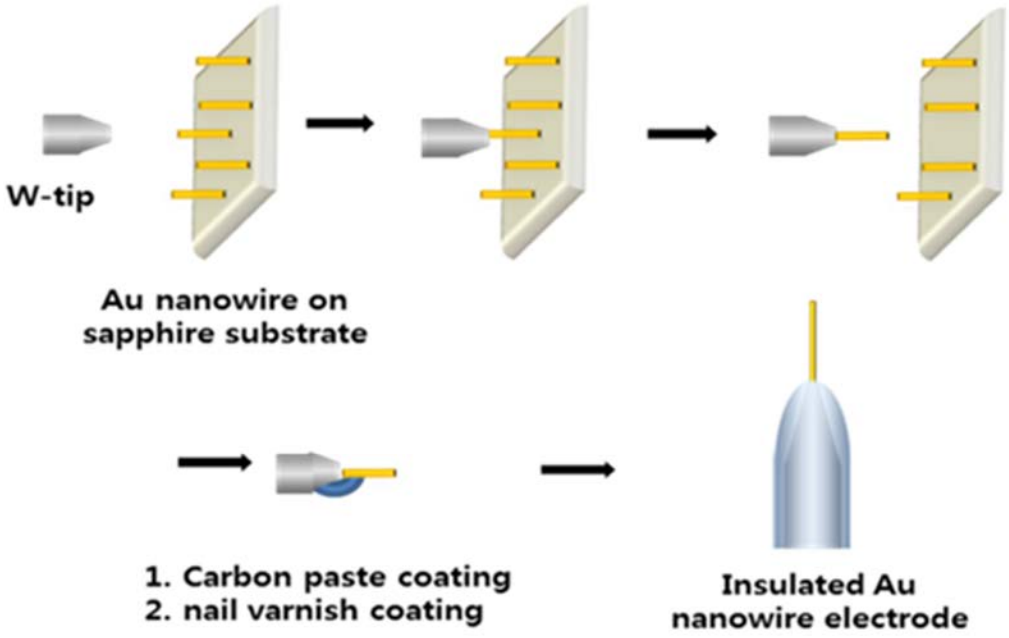
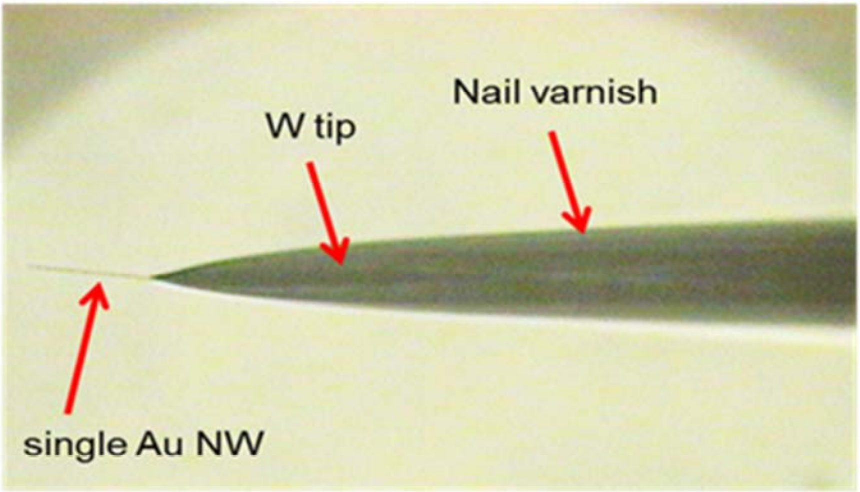
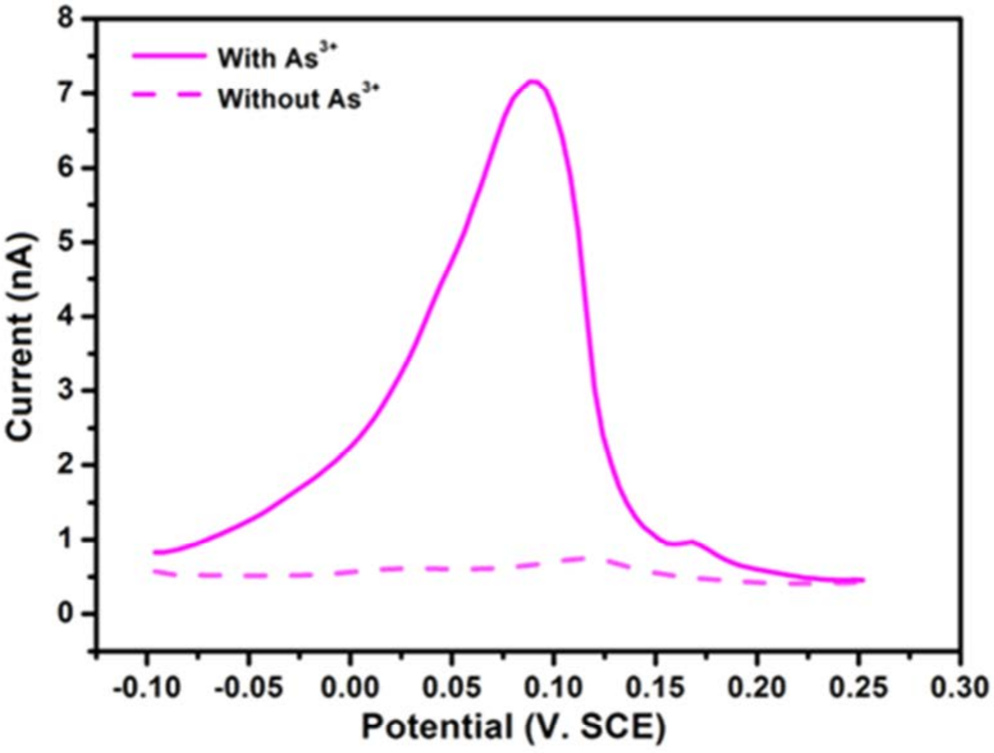
Arsenic is one of the abundant elements existing earth's crust but it is one of the toxic metals. Because of their good water solubility, contamination of drinking water by arsenic is found in many developing countries. The exposure of arsenic can cause many serious health problems. Thus, in-field detection of arsenic in drinking water is important for human health. World Health Organization (WHO) sets the permitted arsenic level in drinking water 10 ppb.In heavy metal detection, there are several analysis methods. Especially, electrochemical methods have attracted considerable attention in many studies. Recently, nano-sized electrodes are fast developed and used in electrochemical analysis due to some advantages like high signal-to-noise ratio (S/N) and low limit of detection (LOD). Also, due to their small size, bio-application such as intracellular detection of arsenic is possible since nano-electrodes can minimize cell damage during insertion of electrode.Recently, we have simply developed 1-dimensional nano-electrode using single-crystalline Au nanowires. The Au NWs are synthesized by chemical vapor deposition (CVD) method and then fabricated into an Au nanowire electrode (Au NWE) (Fig.1,2). To detect arsenic ions anodic stripping voltammetry (ASV) method is used. In this method, arsenic ions are firstly reduced and accumulated on the surface of electrode. Then reduced arsenic is oxidized. Sharp anodic current of arsenic is measured during this step. Using ASV method, ultra-sensitive detection of arsenic is possible (Fig.3). By this analytical application of Au NWE, we expect that it has potential to fabricate highly sensitive ultra-small devices for arsenic detection. Also, a single Au NWE makes it possible to detect heavy metal ions in very tiny volume.



<Fig 1> Fabrication steps of Au NW electrode



<Fig 2> Optical image of Au NW electrode



<Fig 3> Square wave voltammograms of Au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Hindered C-N bond rotation in triazinyl dithiocarbamate: The electron cascading down effect

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Variable-Temperature (VT) 1H-NMR spectra of benzyl(CH_2) region for compound 1 - 3. show two different peaks in room temperature, but as the temperature rises, two peaks collapse and finally turn to the one sharp peak in middle of the room temperature signals meaning the fast dithiocarbamate C-N bond rotation. The C-N rotational barrier of three compounds decreases down from compound 1 to compound 3. In order to define molecular origin of the retarded rotational dynamics, we performed Density Functional Theory (DFT) calculation at B3LYP/6-311G(d) basis level and Natural Bond Orbital (NBO) analysis. Our simulation data told us that the dibenzyl amino group substituted triazine ring can donate their electrons toward π* orbital of aromatic ring, and make lone pair on the sulfur atom in dithiocarmate strongly conjugate toward π* orbital of N-C=S, thiocarbamate group. The cascading down of electron population to thiocarbamate group from dibenzyl amino group causes more decreasing the rotational barrier of compound 3 than compound 1.

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Analysis of Terahertz absorption spectrum of Methomyl

황연희 곽경원*

중앙대학교 화학과

Terahertz (THz) spectroscopy can be used to distinguish between two crystalline isomers. Analyzing the lattice vibrational motions in experimental THz spectra is challenging, but can be achieved with the help of the computational methods. In this study, the THz spectrum of methomyl was obtained by a TPS spectra 3000 spectrometer (TeraView Ltd.). Pure HDPE pellets was used as the reference signal and the center of the methomyl pellets was used as the sample signals. Used methomyl was figured out (Z)-methomyl through the powder X-ray diffraction (PXRD) patterns. The vibrational motions of the observed absorption peaks were analyzed using solid-state density functional theory (DFT) calculations. The observed strong absorption peaks at 33.51, 54.50, and 63.18 cm-1 were well reproduced in calculations. Detailed normal mode analyses have been carried out and revels that those THz peaks from the intermolecular vibrations. The main difference in calculated terahertz spectra of (E)-, (Z)-methomyl is at below 40 cm-1 region. Only peak from (Z)-methomyl which is external translation vibrational mode was detected in that region and it would correspond to experimental value at 33.51 cm-1. The results demonstrate THz spectroscopy can be useful tools to determine crystalline isomers and the solid-state DFT at low-frequency regions gives the reliable vibrational motions.

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[발표취소] Temperature-dependent IR Spectroscopy and Computation of Thermodynamic study of Ion Solvation in Electrolyte

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중앙대학교 화학과 [1]군산대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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Humidity-resistance catalyst for toluene removal: NiO/TiO_2/SiO_2 prepared by atomic layer deposition

박은지 이주하 정명근 한상욱 김승연 김보라 박기정 김일희 김영독*

성균관대학교 화학과

NiO/SiO_2 and NiO/TiO_2/SiO_2 catalysts were prepared using ALD (atomic layer deposition) process and used for toluene oxidation under dry and highly humid (RH%= 70%) conditions at 250 °C and 350 °C, respectively. Under dry conditions, NiO/SiO_2 showed higher toluene removal efficiency as well as selectivity towards CO_2 compared to those on NiO/TiO_2/SiO_2. However, under highly humid conditions, toluene removal efficiency of NiO/SiO_2 significantly decreases due to the competitive adsorption of toluene with water and the decrease in the catalytic activity was much more pronounced at lower temperature. On the other hand, on NiO/TiO_2/SiO_2, most of its catalytic activity was maintained in the presence of water by the stronger interaction between TiO_2 and toluene, indicating that it can demonstrate a constant catalytic activity independent of humidity in the feed stream.

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Ultrafast Vibrational Spectroscopy on Fermi-resonance in Acetonitrile: Effects of ions

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고려대학교 화학과

The nitrile stretch (v_2) and the combination (v_{3+4}) modes of acetonitrile (CH_3CN) were found to be strongly coupled by Fermi-resonance. The frequencies of vibrational modes of acetonitrile in $CH_3CN…Li^+$ complex were significantly varied due to a strong ion?molecule interaction. The intensity of the combination mode of CH_3CN in the FTIR spectrum was substantially enhanced in $CH_3CN…Li^+$ complex because the combination band shifted closer to the nitrile stretch band. Here, Fermi-resonances in free CH_3CN and $CH_3CN…Li^+$ complex were studied by ultrafast infrared pump?probe (IR PP) and two-dimensional infrared (2DIR) spectroscopy. Spectral features of Fermi-resonance observed in IR PP and 2DIR signals were presented and the effect of Li^+ ion on Fermi-resonance were discussed.

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Adsorption of 2-MIB on Bare and PDMS-coated Activated Carbons

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성균관대학교 화학과

Polydimethylsiloxane (PDMS) was deposited on the activated carbon at two different temperatures of 150 ^{o}C and 300 ^{o}C using chemical vapor deposition (CVD). The adsorption behaviors of 2-methylisoborneol (2-MIB) with a concentration of 100 ppb on the bare and hydrophobic PDMS-coated activated carbons were evaluated using the gas chromatography (GC) with solid phase microextraction (SPME) sampling method. It was determined that total amounts of the adsorbed 2-MIB on the bare and PDMS-coated activated carbons in water for 60 min were almost same, although the adsorption rates of the 2-MIB on the PDMS-coated activated carbons in the initial stage of the adsorption process are reduced by the decrease of surface area after the PDMS coating.The bare and PDMS-coated activated carbon pretreated in water for 24 hour exhibited much different adsorption behaviors of the 2-MIB: the adsorption capacity and rate of the PDMS-coated sample for the 2-MIB were not changed compared with those of the as-prepared PDMS-coated activated carbon. In contrast, the bare activated carbon lost its original adsorption capacity and rate for the 2-MIB after the exposure to water for 24 hour. It is suggested that the hydrophobic coating on the activated carbon with PDMS can protect the adsorbent from water penetration, enhancing selective adsorption of the organic pollutants of low concentration in water.

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Low temperature carbon monoxide oxidation of NiO/mesoporous Al_2O_3 pre-annealed at various temperatures

한상욱 박은지 정명근 이주하 김보라 김승연 박기정 김일희 김영독*

성균관대학교 화학과

We fabricated 50-cycled NiO/mesoporous Al_2O_3 using atomic layer deposition (ALD) which can form homogeneous film on complex surfaces such as porous materials. Chemical and physical properties of the 50-cycled NiO/Al_2O_3 were analyzed by inductively coupled plasma-optical emission spectrometry (ICP-OES), X-ray photoelectron spectroscopy (XPS), energy dispersive spectroscopy (EDS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The 50-cycled NiO/Al_2O_3 was pre-annealed at various temperatures under air condition for 2 hours before the CO oxidation at 30 ^oC. All of the samples showed catalytic activity for CO oxidation at room temperature and they also showed about 90% CO consumption in the first 10 minutes of CO oxidation experiment. The catalytic activity of the deactivated 50-cycled NiO/Al_2O_3 catalyst during CO oxidation was regenerated after annealing at 450 ^oC for 2 hours under air condition. It implies that ALD-prepared NiO/Al_2O_3 could be one of the promising catalysts for low temperature CO oxidation.

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Fabrication of superhydrophobic cotton and its application for oil removal

송지수 정명근 박은지 한상욱 김보라 박기정 이주하 김승연 김일희 김영독*

성균관대학교 화학과

Removal of spilt oil from water has been essential task for environment science and technology. In this study, we used two types of cotton which are absorbent cotton and kapok for this matter. With simple dip-coating method, SiO_2 covered with PDMS (polydimethylsiloxane) can be attached to the surface of cotton and this makes the substrate superhydrophobic due to the formation of dual roughness and hydrophobic termination. Using adhesive solution consisting of PDMS and curing agent, the surface became more stable. Water contact angles for each surface were higher than 160º, corresponding to the superhydrophobicity. Cotton with superhydrophobic surface can be applied for oil spill because it does not wet in the water and it can absorb more oil than cotton without hydrophobicity. For example, in rotary oil case, the weight gain of coated kapok and coated absorbent kapok were 88 and 48 respectively.

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Fabrication of gas permeable superhydrophobic thin films on various substrates

김보라 박은지 이주하 한상욱 김승연 박기정 정명근 김일희 김영독*

성균관대학교 화학과

Membranes with superhydrophobicity and high gas permeability were prepared and characterized. Materials such as metal mesh, paper, fabric, and polytetrafluoroethylene allowing gas permeation were dip-coated in hexane-based solution of SiO_2 nanoparticles coated with polydimethylsiloxane (PDMS). The dip-coating provided superhydrophobicity to the surfaces of our membranes with water contact angles exceeding 160°. On the other hand, high permeability of CO_2 and dimethyl methylphosphonate vapor through the membrane could be obtained, indicating that our preparation method can be useful for the fabrication of shielding layers of gas sensors, which allow selective permeation of gas vapor from gas/aqueous-liquids mixture. Also, we observed that superhydrophobicity of fabricated films was maintained under acidic and basic conditions or UV irradiation.

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Reactivity and stability of TiO_2-shell/Ni-core catalysts for CO_2 reforming of CH_4

박기정 정명근 한상욱 김보라 박은지 이주하 김승연 김일회 김영독*

성균관대학교 화학과

TiO_2/Ni inverse catalysts were prepared using an atomic layer deposition (ALD) process. Scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) were used to analyze the physical, chemical characters of bare Ni, 100 and 500-cycled TiO_2 coated-Ni particles before and after the CO_2 reforming of methane (CRM) reactions. The 500-cycled TiO_2/Ni showed lower catalytic conversions and selectivity for the CRM reaction compared to that of bare Ni and 100-cycled TiO_2/Ni in the initial stage of the reaction experiment. However, the 500-cycled TiO_2/Ni showed the highest conversions and selectivity after 164 h of CRM reaction. All of the catalysts formed a coke caused by CH_4 cracking and the reverse-Boudouard reaction. However, the deposited shape of carbon on TiO_2/Ni was different from that of the bare Ni. The carbon atoms on 100 and 500-cycled were concentrated at the carbon filament structures. The graphitic carbons were formed on the bare Ni surface, blocking the catalytic active sites. However, the TiO_2/Ni catalysts could be more catalytically active due to the carbon filaments.

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Density Functional Theory and Ab Initio Calculation of OH Stretching Frequency in Water Monomer and Dimers

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충북대학교 화학과

The OH stretching frequency of water is very sensitive to surrounding environments and therefore useful information about the molecular structure and dynamics have been obtained from various vibrational spectroscopies probing the OH bonds. In those studies, theoretical works play an important role in interpreting experimental data, specifically by using mixed quantum-classical theories. In quantum mechanical part, density functional theory(DFT) is particularly useful for the accuracy and costs of calculations. However, being an empirical theory, it should precede to find what the most appropriate density functional for the OH stretching vibration frequency is. In this study, we performed DFT calculations with various functionals including recently developed ones incorporating dispersion interactions and long-range corrections. Those calculations are compared with the experimental frequencies and the results of CCSD(T) method. Since the OH frequency is the mostly influenced by the oxygen atom of the hydrogen bond acceptor, we studied a model system of water dimer by changing the distance of hydrogen bond between the two molecules. Since the anharmonicity of OH bond potential is known to be large, we fit the potential curve to a Morse potential to calculate the frequencies. We found that wB97 and wB97X predict the OH frequency in a quantitatively good agreement with the results of CCSD(T) and they will properly predict the change of OH frequency with the hydrogen bond distance. Interestingly, two hybrid functionals, B3LYP and X3LYP, which have been widely used in various areas, are less accurate in the prediction of the OH frequency than the former while the dependence of frequency on the hydrogen bond distance are predicted in a qualitatively correct way by the latter.

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Theoretical approach for the structures, energetics and spectroscopic properties of $(H_2O_5)_n$ (n=1~4) clusters

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한남대학교 화학과

본 연구는 $(H_2O_5)_n$ (n=1~4)에 대해서 다양한 기저집합과 범 밀도 함수이론(DFT)을 사용하여 최적화된 구조와 결합에너지, 조화진동수를 계산하였다. H_2O_5 의 여러 가능한 분자 구조를 최적화하고, 그 가운데 가장 열역학적으로 안정된 분자구조를 예측하였다. 이 때 이전의 DFT 방법에 대한 약점인 약한 결합을 갖는 클러스터들의 분자 구조를 보다 정확히 예측하기 위하여 CAM-B3LYP 및 MP2 방법 등을 사용하여 보다 정확한 구조적 특성 과 결합에너지를 확인하였다. 나아가 $(H_2O_5)_n$ 의 결합에너지를 다양한 기저상태의 구조와 결합하여 결합에너지를 보았으며, 보다 정확한 값을 도출하기 위해 영점 진동 에너지(ZPVE)와 바탕 집합 중첩 에러(BSSE)를 보정하였다.

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H_2O_4-$(H_2O)_n$ (n=1~5) 클러스터의 분자 구조 및 결합 에너지에 관한 이론 연구

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H_2O_4 는 HO_2 라디칼의 이중합체(dimer)의 구조로써 대기 중에서 전이 중간체로 오랫동안 알려져있었다. 그 후 최근 2011 년에 Levanov 등은 H_2O_4 의 Raman 분광학적 분석을 통하여 각 각 449, 589, 624, 827 과 865cm^{-1} 에서 H_2O_4 사슬 구조에 대한 특징적인 피크들을 얻어 H_2O_4 가 HO_2 라디칼의 이중합체가 아닌 사슬 구조를 밝혔다. 본 연구는 H_2O_4 사슬구조에 물 분자를 붙인 H_2O_4-$(H_2O)_n$ (n=1~5) 클러스터에 대해서 B3LYP, CAM-B3LYP, MP2 이론적 수준으로 기하학적 구조와 수용액 내에서의 안정성을 연구하였으며, local minimum 과 진동 주파수를 확인하였다. 정확한 binding energy 를 보정하기 위해서 영점 진동 에너지(ZPVE, zeropoint vibration energy) 와 바탕 집합 보정 에너지 (BSSE, basisset superposition error) correction 하였다.

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The dynamics of hydrogen atom release from vinyl radical on the gas-phase oxidation

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The dynamics of the gas-phase reaction between ground state oxygen atom (O(^{3}P)) and vinyl radical (C_2H_3) was investigated by applying a combination of vacuum-ultraviolet laser-induced fluorescence (VUV-LIF) spectroscopy in a crossed beam configuration and computational calculations. The radical reactants were respectively prepared by photolysis of NO_2 and supersonic flash pyrolysis of the precursor vinyl iodide (C_2H_3I). Doppler profile analysis of the nascent H-atom products in the Lyman-α region revealed that the average translational energy of the products and the average fraction of the total available energy released as translational energy were 7.03 ± 0.30 kcal mol^{-1}?and 7.2 %, respectively. The empirical data combined with CBS-QB3 level *ab initio* calculations and statistical calculations from RRKM theory demonstrated that an addition-elimination mechanism contributes a major reaction pathway resulting in oxygen-hydrogen exchange reaction O(^{3}P) + C_2H_3?→ H(^{2}S) + CH_2CO (ketene). On the basis of systematic comparison with several exchange reactions of small hydrocarbon radicals, the observed kinetic energy release can be explained in terms of the weak impulse at the moment of decomposition in the loose transition state with a product-like geometry and a small reverse barrier along the exit channel.

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Gas-Phase radical-radical reaction dynamics of $O(^3P) + C_2H_5 \rightarrow H(^2S) + C_2H_4O$

김장운 김진욱 최종호*

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The dynamics of the gas-phase radical-radical reaction between ground state oxygen atom ($O(^3P)$) and ethyl radical (C_2H_5) was investigated by applying a combination of vacuum-ultraviolet laser-induced fluorescence spectroscopy in a crossed beam configuration and *ab initio* calculations. The two types of radical reactants $O(^3P)$ and C_2H_5 were produced using photolysis of NO_2 and supersonic flash pyrolysis of the synthesized precursor azoethane, respectively. Doppler profile analysis of the nascent H-atom products in the Lyman-α region revealed that the average translational energy of the products and the average fraction of the total available energy released as translational energy were 5.01 ± 0.72 kcal mol$^{?1}$ and 6.1%, respectively. The empirical data combined with CBS-QB3 level *ab initio* theory and statistical calculations present that the title exchange reaction $O(^3P) + C_2H_5$ (ethyl) → $H(^2S) + CH_3CHO$ (acetaldehyde) is a major channel and proceeds via an addition-elimination mechanism through the formation of a short-lived, dynamical addition complex on the doublet potential energy surface. On the basis of systematic comparison with several exchange reactions of hydrocarbon radicals, the observed small kinetic energy release can be explained in terms of the loose transition state with a product-like geometry and a small reverse activation barrier along the reaction coordinate.

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Effect of MgO promotion on carbon dioxide reforming of methane reaction over Ni catalysts

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성균관대학교 화학과

MgO-promoted Ni catalyst was prepared using atomic layer deposition (ALD) method, and the catalyst was researched in terms of catalytic activity and stability for carbon dioxide reforming of methane (CRM) reaction using gas chromatograph (GC). X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and inductively coupled plasma-optical emission spectrometry (ICP-OES) were used to investigate the physical and chemical properties of MgO-promoted Ni catalyst before and after the CRM reaction. We focused on the effect of promoting MgO based on Ni catalyst compared with activity and stability of bare Ni. It has been suggested that MgO has a good affinity to CO_2 molecule which is one of the reactants in the CRM reaction due to its basicity, resulting in an increase of the adsorption probability of CO_2 on the surface of Ni. We showed enhanced the catalytic activity and stability of MgO-promoted Ni catalyst compared with that of bare Ni in CRM reaction.

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Ultrafast Excited-state energy relaxation dynamics of Porphyrin-[26]Hexaphyrin-Porphyrin Tape

이상수 김동호*

연세대학교 화학과

Organic π-conjugated systems have received considerable attention because of their numerous applications as organic conducting materials, non-linear optical (NLO) materials, near-infrared dyes, and highly efficient molecular photonic and electronic wires. Therefore, it is vital to understand the excited state dynamics for various applications. To understand excited state dynamics of π-conjugated molecular systems, we have investigated excited state dynamics in Zn(II)porphyrin-[26]hexaphyrin-Zn(II)porphyrin tape through femtosecond transient absorption spectroscopy. We think that this study will be a guideline for further investigations on the expanded π-conjugated systems in other molecular arrays for future applications as photonic devices.

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Photoinduced twisted intramolecular charge transfer in meso-diarylamino subporphyrins

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As an attractive feature that is not similar with porphyrins, meso-substituted subporphyrins show remarkably variable absorption and fluorescence spectra depending on meso-substituents. For instance, by twisting of the meso-substituents from its optimized orientation, there are strong perturbation of the electronic properties of subporphyrins by the interactions between subporphyrin core and the substituents.I recently discovered photophysical properties of meso-diarylamino subporphyrins 1, 2, and 3 (Figure 1), and especially, twisted intramolecular charge transfer (TICT) process for 2 and 3, respectively. In TICT, intramolecular charge separation occurs with twisting donor-acceptor arrangement to minimize the electronic interaction.

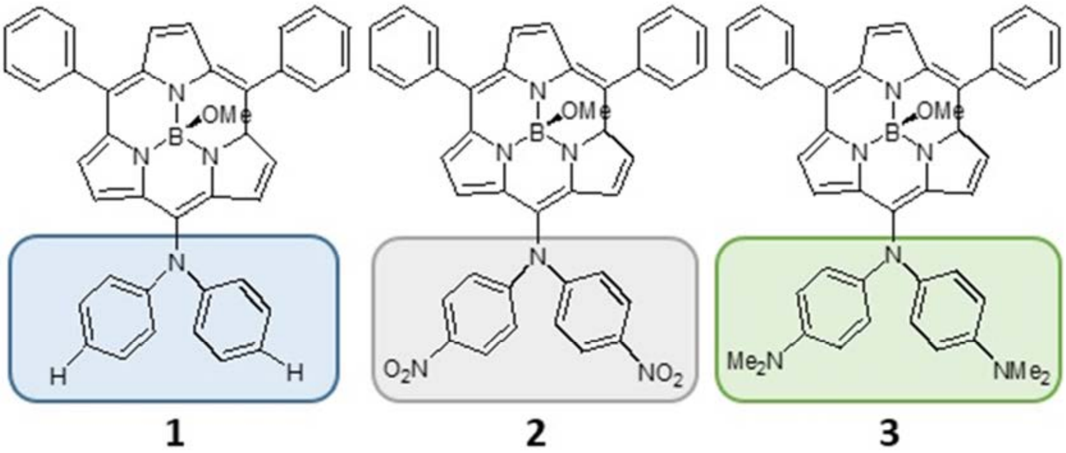

Figure 1. Molecular structures of meso-diarylamino subporphyrins.

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Linker Effects in π-conjugated Macrocyclic Oligothiophenes with Broadband Fluorescence Up-conversion Spectroscopy

김우재 김동호*

연세대학교 화학과

To date, π-conjugated polymers or oligomers have been widely utilized in various fields such as solar cells, OLEDs, OFETs and OPVs due to their high electrical conductivity. Especially, for improvement of the performance of these devices, many researchers have devised strategies to modify the structures of π-conjugated systems through various strategies.Among several approaches, the linkers between chromophore units play an important role in modifying the molecular structure because they can modulate the rigidity, π-conjugation length and charge transport characters. However, previous in-depth studies with regard to linker effects in the excited state have been only focused on linear systems. Such systems possess limitation known as chain-end effect, which inhibits electron delocalization along the entire of backbone. Cyclic systems exhibit no chain-end effect indicative of end-free electron delocalization and are more rigid as well as highly-ordered structure as compared to linear conjugated systems. Even supposing cyclic systems are relatively rigid and well-ordered, we can easily think that the linkers would alter not only the molecular structures and the degree of conjugation, but also exciton delocalization process in the excited state. Of many kinds of linkers, we wanted to investigate the effects of basic linkers which are ethynylene and vinylene in cyclic conjugated systems. In this respect, we have prepared π-conjugated macrocyclic oligothiophenes, consisted of twelve 2,5-thienylene units with ethynylene and vinylene linkers. In this work, time-resolved broadband fluorescence up-conversion measurement which can monitor transient fluorescence spectra was employed to track pure lowest singlet exciton dynamics.

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Unique Ultrafast Energy Transfer in a series of Phenylene-Bridged Subporphyrin-Porphyrin Hybrids

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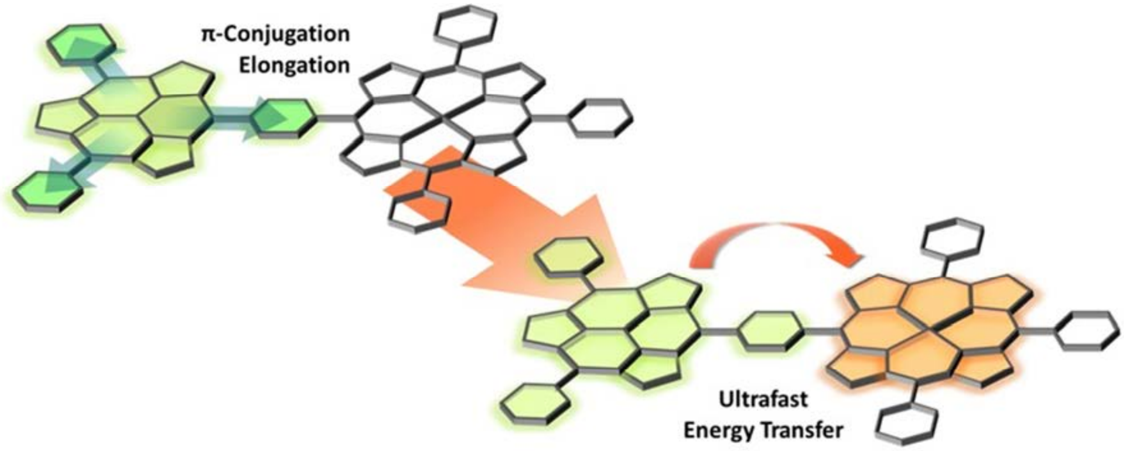
Recently, as ring-contracted porphyrin analogues, subporphyrins (SubPs) have emerged as a new class of promising functional dyes, displaying intriguing properties such as bowl-shaped nonplanar aromaticity. While the electronic properties of SubPs have similar features to those of porphyrins, SubPs display characteristically strong electronic interaction between subporphyrin core and meso-substituents, which leads to variable absorption and fluorescence features of SubPs.[1] These tunable electronic and optical properties of SubPs can serve advantageously to mediate efficient EET processes in artificial light harvesting molecular systems. In this regard, our group has reported the preparation and characterization of phenylene-bridged subporphyrin (SubP)-Zn(II) porphyrin (ZnP) hybrids,[2] which are thought of ideal molecules to reveal the characteristics of SubPs on the EET processes.In this work, we have explored intramolecular EET process of the phenylene-bridged SubP-ZnP hybrids. In the hybrids, the unique ring-contracted structure of SubPs promotes the electronic conjugation interaction between the SubP core and the phenylene-bridge, which efficiently mediates the electronic exchange interaction with SubP and ZnP. This feature provides a way for efficient energy transfer by through-bond effect, resulting in the remarkably accelerated intramolecular EET process.In summary, we have investigated the unique ultrafast EET process in the phenylene-bridged SubP-ZnP hybrids. We believe that this report has successfully identified the functional properties of SubP in the hybrid systems.


π-Conjugation
Elongation
Ultrafast
Energy Transfer

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Spectroscopic Evidence for Baird’s Rule: Reversal of H?ckel Aromaticity in the Lowest Triplet-states of Hexaphyrins

성영모 김동호*

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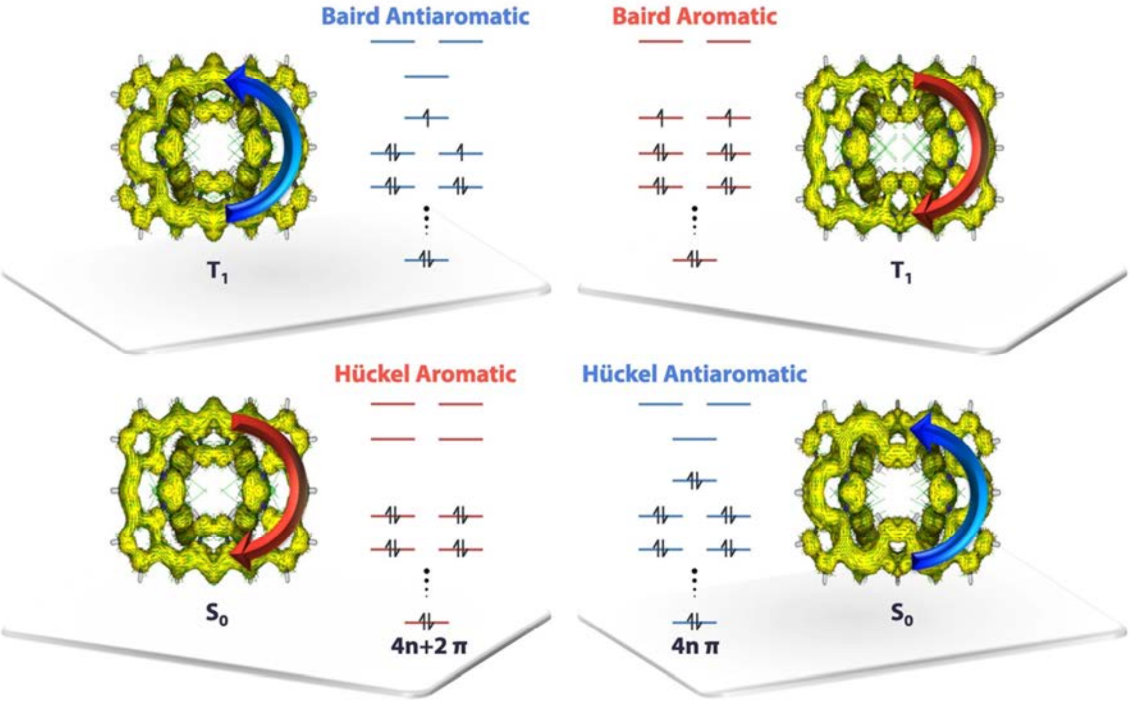
Reversal of (anti)aromaticity in a molecule’s triplet excited state compared to its closed-shell singlet ground state is known as Baird’s rule and has attracted the interest of synthetic, physical organic chemists, and theorists because of the potential to modulate the fundamental properties of highly conjugated molecules. Here we show that two closely-related bis-rhodium hexaphyrins containing [26]- (R26H) and [28]- (R28H) π-electron peripheries, respectively, exhibit properties consistent with Baird’s rule. In the ground state, R26H exhibits a sharp Soret-like band and distinct Q-like bands characteristic of an aromatic porphyrinoid, whereas R28H exhibits a broad absorption spectrum without Q-like bands, which is typical of an antiaromatic porphyrinoid. In contrast, the T-T absorption of R26H is broad, weak, and featureless, while that of R28H displays an intense and sharp Soret-like band. These spectral signatures, in combination with quantum chemical calculations, are in line with qualitative expectations based on Baird’s rule.


Baird Antiaromatic
Baird Aromatic
T_1
T_1
Hückel Aromatic
Hückel Antiaromatic
S_0
S_0
4n+2 π
4n π

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Investigation of size-dependence of the structural inhomogeneity in linear oligothiophenes by single-molecule spectroscopy

김태우 김동호*

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π-conjugated oligomers such as the oligothiophenes as well as their parent polymers continue to attract a great deal of attention as viable materials for a host of applications including light-emitting diodes, photodiodes, and field-effect transistors. Since examination of well-defined oligomers will provide intuitive knowledge about the electronic and photophysical properties of the π-conjugated polymer backbone, we have prepared a series of linear oligothiophenes (L-nTs) and they have been investigated with the single-molecule fluorescence detection techniques to reveal the chain-length dependency of their properties. Correlation studies between emission energies and the peak ratio of the emission spectra for single molecules of L-nTs provide the information of the inhomogeneities and fluctuations between the structural metastable states, which cause the variation of the lowest-energy excited state.

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Aptamer-Modified SERS Hot Spot for Sensor Application

김남훈

한국화학연구원 나노바이오융합연구단

A strategy for amplified SERS-based sensing using aptamer is described. The system is designed so that the aptamer’s conformational change following its interaction with one or two molecule leverages the position of a gold nanoparticle carrying 100 or more reporter molecules whose SERS intensities are altered as a result. This is illustrated using a bifunctional adenosine-sensitive aptamer which was used to create a SERS hot spot between a bulk Au surface or 80 nm Au nanoparticle (AuNP) and an 20 nm AuNP attached to the aptamer via a biotin-avidin linkage. The 20 nm AuNP was decorated with the Raman reporter (4-aminobenzenethiol). Introducing the target into the buffer in which this system is immersed increased the reporter’s SERS signal by a factor of ~3.5. In-situ atomic force microscopy (AFM) confirmed the fact that the mean height of the AuNP-bearing aptamer decreased by ~5.6 nm consistent with the observed SERS intensity change. The introduction of uridine, guanine, and cytidine produce no significant effect either on the SERS spectrum or the topographic AFM image.Reversible tuning of SERS hot spots was demonstrated using a bifunctional, adenosine-sensitive single-strand DNA aptamer with stem loop structure. Washing the sensor with buffer caused the SERS intensity and all details of its spectrum to revert to its pre-recognition-event levels, restoring the system’s activity towards adenosine.

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Dissecting protein configurational entropy into vibrational and conformational contributions

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숙명여자대학교 화학과

Protein configurational entropy is one of the major contributors to the thermodynamics of protein folding and protein-ligand binding. Quantifying how this important thermodynamic parameter is determined from underlying rugged free energy landscape is a challenging problem. Here, we present a computational method that classifies protein configurational entropy into “conformational” and “vibrational” parts. This is done by filtering out the short-term vibrational dynamics within individual free energy wells from the longer-term conformational transitions between them. The result of an application of this method to the folding thermodynamics of the protein villin headpiece subdomain will be presented.

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Studies on the fluorescence properties for the dermatophytes

박형련* 박유진 이준승 박기민[1]

전남대학교 화학과 [1]경상대학교 화학교육과

Dermatophytes are fungi that can cause infections of the skin, hair, and nails due to their ability to utilize keratin. Dermatophytes are spread by direct contact from other people (anthropophilic organisms), animals (zoophilic organisms), and soil (geophilic organisms), as well as indirectly from fomites. Dermatophyte infections can be readily diagnosed based on the history, physical examination, and potassium hydroxide (KOH) microscopy. Diagnosis occasionally requires Wood's lamp examination caused by fluorescent. However, their fluorescence properties are not clearly investigated. To understand the fluorescence behaviors of the dermatophyte, we studied on the spectroscopic properties of the four kinds of dermatophytes such as Microsporum Canis, Microsporum ferrugineum, Trichophyton Rubrum, and Trichophyton Schoenleinii which are well known as the common sources of human fungal infections. The dermatophytes emitted weak fluorescence intensities with the excitation of the around 320 nm light. However the fungus did not show the fluorescence with the excitation the light above 350 nm.

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Spectroscopic behavior of galangin in aqueous solution

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Galangin (3,5,7-trihydroxyflavone; GAL) is one of flavonoid compounds that exists in many plants. It is well known that they considered as an important bioactive compound incorporating specific interactions with nucleic acids, enzymes and protein. However, their antioxidant behaviors are still not clear. It is, therefore, examined about their antioxidants behavior in aqueous solutions using UV-vis absorption spectrophotometer and steady state fluorescence spectroscopy. The aqueous galangin reveal generally two maximum peaks at about 261 nm and about 350 nm in the absorption spectra and the shapes of them highly depend on the presence of hydroxide ions in aqueous solution. The intensity and position of the absorption maximum peaks are shifted to the long wavelength according as the increment of pH in the solution. Moreover, the shapes of the absorption spectra change with the storage time in the deaerated ammonium chloride buffer solution. Besides, their steady-state fluorescence emission spectra did also changed in aqueous solution both depending on the pH values and on the storage time of the solution. The UV-vis absorption spectra of the substances were changed as the content of metal ions increased. Their steady state fluorescence spectra changed also according as the concentration of metal ions. The fluorescence intensities of galangin are decreased when the amounts of metal ions increased in the solution. The metal ions acted as a dynamic quencher rather than static quencher forming acid-base complex.

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Study of Catalytic Effects of CO Oxidation Reaction for Spherical α-Fe_2O_3 Clusters by Photoacoustic Measerments

노중석 최중길[*] 이성한[1,*]

연세대학교 화학과 [1]연세대학교 화학 및 의화학과

The photoacoustic spectroscopy technique was applied to the kinetic measurements of the CO oxidation reaction on spherical α-Fe_2O_3 catalysts. The comparison of catalytic effects of spherical α-Fe_2O_3 clusters was discussed with those for α-Fe_2O_3 fine powder catalysts. The Catalysts were purchased or prepared by the solvothermal reduction method. Kinetic studies on the catalytic reactions were performed in a closed-circulation reactor system using a helmholtz photoacoustic cell at total pressure of 40Torr consisted of three gases such as CO, O_2, N_2. The variation of photoacoustic signals with the concentration of CO_2 produced during the catalytic reaction were recorded as a function of time. The CO_2 formation rates were then directly obtained from the change of the CO_2 photoacoustic signal. In the temperature range of 225~350℃, The apparent activation energy was determined from the initial reaction rate. The partial reaction orders of the catalytic reaction with respect to CO and O_2 were also investigated at various partial pressures of CO and O_2 at 350℃.

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The Ground and Low-lying Excited States of PtCN and PdCN: Theoretical Investigation including Spin-Orbit Coupling

문지원 김중한[*]

가톨릭대학교 화학과

Quantum chemical calculations of PtCN and PdCN were performed using density functional theory (DFT) and high-level *ab initio* methods such as the coupled cluster singles and doubles with perturbative triples (CCSD(T)) and multireference configuration interaction calculations including the Davidson correction (MRCI+Q). The molecular properties of the ground state and low-lying excited states of PtCN and PdCN are calculated. Spin-orbit coupling (SOC) is also considered in the DFT and MRCI+Q calculations. The electronic ground states of PtCN and PdCN are the $^2\Delta_{5/2}$ and $^2\Sigma^+_{1/2}$ states, respectively. The SOC as well as scalar relativistic effects contribute to the determination of the ground state of PtCN to be the $^2\Delta_{5/2}$ state.

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Theoretical investigation of the rearrangement reaction mechanism of *p*-hydroxyphenacyl diethylphosphate (HPDP) in water

문지원 김중한*

가톨릭대학교 화학과

The reaction mechanism of *p*-hydroxyphenacyl diethylphosphate (HPDP) in water was studied by density functional theory (DFT). The solvent environment was considered using both explicit and implicit solvent model. Total twelve water molecules were added to HPDP molecule as an explicit solvent model. The polarizable continuum model using the integral equation formalism variant (IEFPCM) was also used as an implicit solvent model. The intermediates (IMs) and transition states (TSs) on singlet and triplet states were optimized. The reaction mechanism from the triplet state of HPDP to *p*-hydroxyphenylacetic acid (HPAA) is elucidated.

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Two-dimensional electronic spectroscopy of Phthalocyanine derivative

송기희 김민석[1] 이한주* 한호규[1] 조민행[1]

한국기초과학지원연구원 서울센터 [1]고려대학교 화학과

Two-dimensional (2D) electronic spectroscopy provides a comprehensive insight for electron dynamics such as excitonic interaction, electronic coherence transfer and, excitation energy transfer by revealing correlation between multiple states in 2D frequency axes. A 2D optical spectrum can be obtained by detecting a third-order optical response signal created by three optical pulse-matter interactions. Various experimental techniques have been proposed and studied to realize the 2D optical spectroscopy. Among them, we adopt a quasi-collinear method based on two beam geometry. In this poster, we present a detailed explanation on the 2D spectroscopic system using an acousto-optic pulse shaper (Dazzler, FASTLITE), enabling programmable controls of intricate optical pulse sequences (time delay, phase & amplitude). We successfully obtained the time-resolved 2D electronic spectrum of phthalocyanine using the optical pulse shaper. Due to fast pulse shaping capability of our measurement scheme, a high-speed data acquisition can be achieved just in a few seconds for single 2D spectrum. Consequently, well-resolved cross-peaks indicating vibronic coupling are observed.

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Fluorescence Dynamics of Surface-Immobilized PBI in Solution Phase Probed by Single-Molecule Fluorescence Spectroscopy

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연세대학교 화학과

We have investigated the photophysical properties of surface-immobilized organic perylene bisimide (PBI) molecules in water and organic solvents by single-molecule fluorescence spectroscopy with confocal microscope at the single-molecule level. Unlike previous solution-based single-molecule study using immobilization protein, we utilized click chemistry to covalently link the PBI molecules on the glass surfaces by applying different linkers between the chromophore and the glass surface. By recording simultaneously the fluorescence intensity traces, lifetimes, and spectra of single PBI molecules, we found that PBI molecules show the more complex fluorescence intensity levels, broader distributions in the histograms of the fluorescence lifetimes and the spectral position in organic solvents compared to those in water. This clearly indicates that the photophysical properties of PBI molecules in solution phase are affected by hydrophobic and hydrophilic solvents. In addition, with increasing the length of the anchoring linker, the distributions in the histograms of fluorescence lifetimes and spectral position in organic solvents become broad and heterogeneous due to the increased flexibility by the long anchoring linker. In contrast, the histograms in water show the similar width in all the distributions regardless of the anchoring linker's length. This feature is attributable to the structuring water molecules around each PBI molecule by hydrogen bonding network. These results demonstrate that we directly observed the hydrophobic hydration as well as the fluorescence properties of each hydrophobic solute at the single-molecule level in solution phase for the first time.

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Selective Thiolation of Ground and Excited State Cyanine Dyes Studied by Time-dependent Density Functional Theory

임은학 허지영[1] 김성근[*] 권지웅[2] 박재완

서울대학교 화학부 [1]상명대학교 의생명공학과 [2]서울대학교 생물물리 및 화학생물학과

Photoswitching of cyanine dyes between a bright and dark state is an essential requirement for many fluorescence imaging methods such as STORM (stochastic optical reconstruction microscopy). Primary thiol is often essential for photoswitching of cyanine dyes as its anion makes a covalent bond to their C_2 carbon, which leads to the formation of a dark state. However, the mechanism for the formation of a specific C-S bond and the excited state dynamics of thiol adduct are not fully understood. In this study, we carried out density functional theory and time-dependent density functional theory calculations to investigate the thiolation mechanism and the excited state dynamics of the thiol complex. We determined the equilibrium geometries of C_2-thiolated cyanine dyes on both the S_0 and S_1 state and propose that thiolation requires internal rotation in the excited state.

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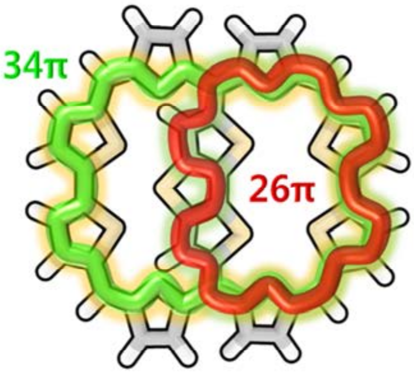
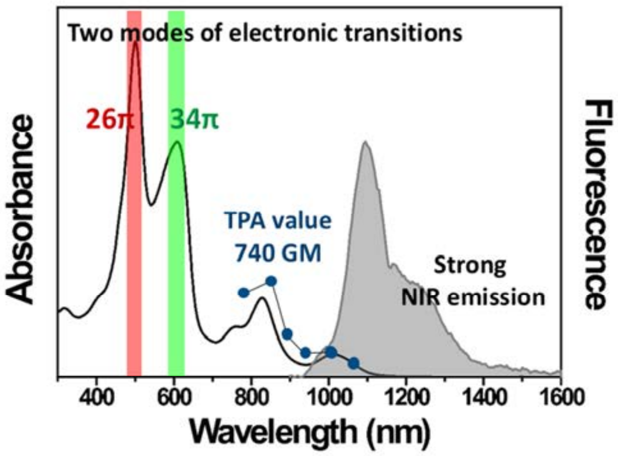
Realization of Three-Dimensional Aromaticity in Bridged Core-Modified Octaphyrin

차원영 김동호*

연세대학교 화학과

Over the years, a plenty of researchers on the characterization of H?ckel and M?bius (anti)aromaticity have been actively conducted by using various molecular systems. Recently, efficient multiple π-electron delocalizations within three-dimensional conjugated molecular framework represent an emerging research frontier for novel properties of both H?ckel- and M?bius-type porphyrinoid systems. Multiple pi-electron delocalizations can occur through multiple conjugation pathways in one molecule, and the development of new topologies that allow effective three-dimensional delocalization confronts a fascinating synthetic challenge. In this respect, expanded porphyrins have attracted considerable attention from organic and physical chemists due to their potential applications in light of their rich chemistry especially such as structural versatility and easy accessibility of [4n] and [4n+2] congeners for controlling the number of π-electrons through two-electron oxidation and reduction processes. Various modifications have been carried out on expanded porphyrins including core-modification and meso-meso connection with aromatic moieties. Throughout the studies on core-modifies and meso-bridged expanded porphyrins, we have observed the correlations between photophysical properties and three-dimensional aromaticity in measurements of the magnetic indices (chemical shift), temperature-dependent steady-state absorption and emission spectra, time-resolved excited-state dynamics, and computational calculations including NICS(nucleus-independent chemical shift), HOMA (harmonic oscillator model of aromaticity) and ACID (anisotropy of the induced current density).


34π
26π


Two modes of electronic transitions
26π
34π
TPA value
740 GM
Strong
NIR emission
Absorbance
Fluorescence
400
600
800
1000
1200
1400
1600
Wavelength (nm)

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Long-lived inhomogeneity of a dye dissolved in liquids at room temperature

김준우 주태하*

포항공과대학교(POSTECH) 화학과

Three pulse photon-echo peak shifts (3PEPS) is a unique method that gives inhomogeneity of a molecules in condensed phase. The 3 pulse photon echo (3PPE) signal that satisfies the phase matching condition, k3PPE=-k1+k2+k3, peaks when the second coherence time (t') is the same as the first coherence time (τ) because of the rephrasing process that takes place under the presence of large inhomogeneity. The position of maximum intensity for the 3PPE signal in a τ scan with fixed population time T gives the inhomogeneity of the system.We employed a diffractive beam splitter and a high resolution linear stage to enhance the spatial overlap and time-resolution for the 3PEPS measurements. For an infrared dye dissolved in methanol at room temperature, we established the existence of long-lived inhomogeneity much beyond the dielectric relaxation time of methanol.(1) We have attempted to reveal the origin of the long-lived inhomogeneity by employing various spectroscopic techniques and by varying solutes and temperature.(1)S. Park and T. Joo J. Chem. Phys. 131, 164508 (2009)

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Formation and Structure of Self-Assembled Monolayers of Otaneselenocyanates on Au(111) Prepared by Ambient-Pressure Vapor Deposition

한슬기 강훈구 성시천 한명수[1] 박희건 한진욱 노재근[*]

한양대학교 화학과 [1]한양대학교 나노융합과학과

Organic thiols are easily oxidized during the formation of self-assembled monolayers (SAMs) on gold in solution. To resolve this problem, we used the octaneselenocyanate (OtSeCN) molecules instead of thiol-based molecules. The formation of OtSeCN SAMs on Au(111) prepared by ambient-pressure vapor deposition was investigated by the scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). STM data show that the surface structures of OtSeCN SAMs contained the highly well ordered structure and were strongly affected by the deposition temperature and time. The number of vacancy islands and bright domains of OtSeCN SAMs decreased as increasing the deposition temperature or time. From XPS results, the high intensity of N1s peak in 399.1 eV was observed for OtSeCN SAMs formed at low temperature and short deposition time. These results show that the bright domains of OtSeCN SAMs were caused by the residue of CN species.

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Orientation change of 4-amino-4’-cyanobiphenyl under various pH conditions on silver surfaces: SERS and DFT study

엄소영 김홍래 권찬호*

강원대학교 화학과

Surface-enhanced Raman scattering (SERS) well-established as powerful spectroscopic tool for characterizing the adsorbate on metal surface was adopted for study on the adsorption behavior of 4-amino-4’-cyanobiphenyl (ACBP) according to the pH condition on silver surfaces. The observed Raman and SERS spectra were analyzed comparing with the Raman intensities and vibrational frequencies for the feasible structures of ACBP calculated at the density functional theory (DFT) level. In SERS spectra, the red-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 appearance of the C-H stretching bands in acidic condition should assume rather vertical orientation on silver surfaces.

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Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of thietane

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강원대학교 화학과

Thietane as a four-membered ring is a prototypical molecule for studying the equilibrium configurations of the neutral and the cation. The one-photon mass-analyzed threshold ionization (MATI) spectroscopy with vacuum ultraviolet (VUV) radiation generated by four-wave difference frequency mixing in Kr, was utilized to determine the ionization energy and cationic structure of thietane. The observed VUV-MATI spectrum demonstrated the twin peaks separated by 17 cm^{-1} with the FWHM of ~8 cm^{-1} for the lowest frequency band. It is assumed that the first peak should be originated from hot band transition for the ring-puckering vibrational mode. Then, the ionization energy of the ionic ground state of thietane was determined to be 69,762 ± 6 cm^{-1} (8.6493 ± 0.0007 eV) from the second peak of the lowest frequency band in the MATI spectrum. Most of the peaks observed in the present spectrum could be assigned by utilizing the Franck-Condon factors and the frequencies calculated through adjustments of the geometrical parameters of cationic thietane at the B3LYP/cc-pVTZ level.

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SERS and DFT study of the adsorption behavior 4-amino-4’-nitrobiphenyl on silver surfaces under various pH conditions

이진철 엄소영 김홍래 권찬호*

강원대학교 화학과

Surface-enhanced Raman spectra of 4-amino-4’-nitrobiphenyl adsorbed on silver surfaces under the various pH conditions were obtained to characterize the adsorption behavior. Also, ordinary Raman spectrum of neat sample was taken for comparison with the measured SERS spectra. Spectral assignments could be effectively achieved with an aid of density functional theory (DFT) calculations. In SERS spectra, absence or presence of the C-H stretching bands was conclusively about the orientations of the molecules adsorbed on silver surfaces.

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Quantum yields for H productions at 205 nm of carboxylic acids

박성만 윤상혁 권찬호 김홍래*

강원대학교 화학과

The quantum yields for H production channelsof acetic acid and trifluoroacetic acid at 205 nm have been measured from the Doppler broadened spectrum of H atom product. The spectrum of H atom was obtained measuring the laser-induced fluorescence (LIF) of the 2p state (Balmer-alpha line) from 3s or 3d, which was induced by two-photon absorption from the 1s state. The quantum yields are determined for the following dissociation channels CH_2COOD + H, CH_3COO + D, and CF_3COO + H, which are $\Phi_{CH2COOD + H}$(0.17±0.03), $\Phi_{CH3COO + D}$(0.07±0.03), and $\Phi_{CF3COO + H}$ (0.12±0.02), respectively.

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One-photon mass-analyzed threshold ionization spectroscopy of Oxetane

강도원 김홍래 권찬호*

강원대학교 화학과

The high-resolution one-photon mass-analyzed threshold ionization spectrum of oxetane has been measured using the VUV radiation in the 77570?81020 cm^{-1} region generated by four-wave difference frequency mixing ($\omega_{VUV}=2\omega_{UV}-\omega_{Vis}$) in Kr gas. The ionization energy of oxetane was determined to be 77976 ± 5 cm-1 (9.6678 ± 0.0006 eV) from the 0-0 band position in the MATI spectrum, which was measured by varying the PFI field to the zero-field limit. This value is in good agreement with the previous PES result of 9.65 eV.[1] Most of the peaks observed in the VUV-MATI spectrum could be assigned by utilizing the vibrational frequencies and the Franck-Condon factors calculated at the B3LYP/cc-pVTZ level. The Franck-Condon fitting method was adopted for the better to simulate the experimental spectrum. The cationic molecular geometry was considered as the fitting parameter in such calculation. Based on good agreement between the experimental and the calculated results, the cationic structure of oxetane in the electronic ground state was determined.Reference1.W. S. Koski et al, J. Phys. Chem. 1992, 96, 7226.

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One-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of tetrahydrofuran

박성만 김홍래 권찬호*

강원대학교 화학과

Vibrational spectrum in the 0-3100 cm^{-1} range of tetrahydrofuran (THF) cation in the electronic ground state was obtained utilizing vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. The VUV radiation for one-photon transition to the cationic states of tetrahydrofuran was generated by four-wave difference frequency mixing in Kr gas cell. From the position of the 0-0 band in the MATI spectrum measured with various pulsed fields, accurate ionization energy to ionic ground state of tetrahydrofuran was determined to be 9.4259 ± 0.0009 eV. This value is in good agreement with the previous PES result of 9.427 eV.

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Excited-state dynamics of alizarin and its derivatives studied by transient absorption spectroscopy

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광주과학기술원(GIST) 물리화학부

Alizarin, which is one of the dihydoxyanthraquinone, is known to stably form the intramolecular hydrogen bonding in the ground state. Upon photo excitation, the proton can be transferred from the hydroxyl group to the carbonyl oxygen with a change of molecular geometry, and the dual emission from the locally excited state and the excited proton transferred-state can be observed. With an increase of solvent polarity, the barrier between two excited states might decrease then the emission from the proton transferred-state dominates due to the fast transition between these states. In this work, to reveal the details of the proton transfer process upon photo excitation, the excited-state dynamics of alizarin in polar and nonpolar solvents are investigated by femtosecond transient absorption spectroscopy. Excited-state dynamics of alizarin derivatives including alizarin red S, alizarin yellow GG, alizarin violet R, and alizarin blue black B will also be studied.

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Energy Transfer and Bond Dissociation in Toluene by halogen molecules

이종백* H. K. Shin[1]

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Collision induced energy transfer and bond dissociation of C-H_{methyl} and C-H_{ring} in excited toluene in the collision with F_2, Cl_2, Br_2, and I_2 have been studied by use of classical trajectory procedures at 300 K. Energy lost by the vibrationally excited toluene to the ground-state halogens is not large, but the amount increases with increasing vibrational excitation from 5000 and 30,000 $cm^{?1}$. The principal energy transfer pathway is vibration to translation (V-T) in these systems, while the vibration to vibration (V-V) step is negligible. When the incident molecule is also vibrationally excited, toluene gains energy from halogens. The overall extent of energy loss is greatest in toluene + F_2 and that in in toluene + I_2 is lowest. The different efficiency of the energy transfer pathways in these collisions is mainly due to the mass effect. Collision-induced dissociation of C-H_{methyl} and C-H_{ring} bonds occurs when highly excited toluene (55,000-70,400 cm?1) interacts with the ground-state halogens. Dissociation probabilities are low ($10^{?5}$~$10^{?2}$) but increase exponentially with rising vibrational excitation. Intramolecular energy flow between the excited C-H bonds occurring on a subpicosecond timescale is responsible for the bond dissociation.

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Abstraction of Nitrogen Chemisorbed on a Tungsten Surface by Atomic Nitrogen

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전남대학교 화학교육과 [1]Department of Chemistry University of Nevada

We have calculated the probability of the N_2 formation and energy deposit of the reaction exothermicity in the newly formed N_2, particularly in its vibrational motion, in the gas-surface reaction $N(g) + N(ad)/W \rightarrow N_2(g) + W$ on the basis of the collision-induced Eley-Rideal mechanism. The translational and vibrational motions share most of the energy when the adatom-surface vibration is initially in the ground state. When the initial excitation increases, the vibrational energy of N2 rises accordingly, while the energies shared by other motions vary only slightly. The product vibrational excitation is significant in N_2 and the population distribution is strongly inverted. Flow of energy between the reaction zone and the solid has been incorporated in trajectory calculations. The amount of energy propagated into the solid is only a few percent of the available energy in the N_2 formation.

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Photoexcitation Dynamics of O_2-bound Heme Proteins Investigated by Time-resolved Vibrational Spectroscopy

박성철 박재홍[1] 임만호[*]

부산대학교 화학과 [1](주)코오롱 중앙기술원 분석평가센터

Time-resolved vibrational spectroscopy was used to investigate the photoexcitation dynamics of O_2-bound heme proteins in D_2O by probing the O-O stretch band in the time range from femtosecond to microsecond after excitation with a 575-nm pulse at 293K. Since the weak O-O stretch band is overlapped with the strong absorption bands in the 1200 ~ 1000 cm^{-1} region by water solvent, protein, and buffer molecule, difference time-resolved spectra (heme$^{16}O_2$ - heme$^{18}O_2$) were obtained to delineate O_2-related bands from the absorption changes due to conformational and thermal relaxation. In the early picosecond time scale, the fundamental bands of oxymyoglobin (MbO_2) and oxyhemoglobin (HbO_2) shift to lower frequency, showing a broadened absorption band, which decays on a 2.7 ps. After subtracting this contribution from the broadband absorption, the remaining bleaching bands decay with the same kinetics and were described by two (three) exponential functions plus an equation describing bimolecular reaction for MbO_2 (HbO_2). The recovered time constants for the exponential function were 6.7 ps (21%) and 36 ns (14%) for MbO_2 and were 2.1 ps (21%), 410 ps (13%), and 8 ns (6%) for HbO_2. The bimolecular rate constant of MbO_2 was 16×10^6 $M^{-1}s^{-1}$ (12%) and HbO_2 was 90×10^6 $M^{-1}s^{-1}$ (1%). The 2.7 ps decay of the broadened absorption band was attributed to thermal relaxation of six-coordinate heme subsequent to fast electronic relaxation without photodeligation. The cooling process for the six-coordinate heme group can be observed due to anharmonic coupling of low frequency modes with the observed O_2 stretching mode. We take the 6.7 ps (2.1 ps) decay of the MbO_2 (HbO_2) to be either partially or completely due to geminate recombination (GR) of O_2 after photodeligation. The 36 ns decay of the MbO_2 and 410 ps, 8 ns of the HbO_2 were attributed to GR of O_2 after photodeligation. When photoexcited in the Q-band, about 25~46% of MbO_2 undergoes photodeligation (quantum yield, QY = 0.25~0.46), about 25~46% of the deligated O_2 geminately rebinds in time constants of 6.7 ps and 36 ns, and the remaining O_2 escapes into solvent and bimolecularly rebinds with the rate constant of 16×10^6 $M^{-1}s^{-1}$. Fast and efficient GR of O_2 indicates that the heme pocket is efficient in trapping the deligated O_2. Conformation-independent dynamics of photoexcited heme-O_2 suggest that the O_2 binding characteristics is independent of conformational substates of heme-O_2.

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Surface-Enhanced Raman Study of Amino acids on gold and silver nanoparticles

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Surface Enhanced Raman spectroscopy (SERS) is an effective tool to study vibrational aspects of molecules adsorbed on noble metal surfaces. The origin of this enhancement is contributed by the local surface plasmons and the charge-transfer process between the metal and adsorbates. In this work, gold and silver nanoparticles have been synthesized by different reducing agents including sodium borohydride and citrate. Small amino acids including tryptophan, tryptamine and glycine are adsorbed on metal nanoparticles. These adsorbents have amine and carboxylate groups which are possible sites of attachment to the metal nanosurfaces. Concentration and pH dependent SERS spectra are measure to understand the changes in adsorption geometry. DFT calculations at level of B3LYP/6-311G(d,p) are also performed to compare simulated Raman spectra with experimental results.

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Rydberg series of $^1\Sigma_u^+$ and $^1\Delta_u$ states of the Li_2 molecule studied by the promotion model

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We studied the Rydberg series for the 12 $^1\Sigma_u^+$, 7 $^1\Delta_u$, and 1 $^1\Gamma_u$ states. This set consists of the seventeen states derivable from the Li(2s) + Li(*nl*) (*n*=2, 3, 4, 5) configuration, one $^1\Sigma_u^+$ state and one $^1\Delta_u$ state derivable from Li(2s) + Li(6p) and Li(2s) + Li(6d), respectively, plus one ionic state. We used the multireference configuration interaction method, combined with the Stuttgart/K?ln group's effective core potential/core polarization potential method, to calculate their potential energy curves (PECs). Four Rydberg series, $\sigma_u ns$ (n=3, 4, 5, 6), $\sigma_u np$ (n=2, 3, 4, 5), $\delta_u nd$ (n = 3, 4, 5, 6), and $\delta_u nf$ (n = 4, 5), are identified near the potential energy minima (referred to as the 'Rydberg region'). The promotion model is used to examine the behaviour of PECs and quantum defect curves (QDCs) by constructing diabatic PECs and QDCs. Besides QDCs, effective *n* and promotion curves are also used to directly examine the promotion. This reveals that the promotion model can be successfully applied to the singlet ungerade states of Li_2, indicating that the Rydberg region has the same characteristics as the united atom (UA) limit.Thus, the Rydberg region in Li_2 is much closer to the UA limit than the separated atoms (SA) limit.

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Rydberg series of the HeH molecule and correlation diagrams

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We study theoretically the 37 Rydberg states of HeH derivable from the $He(1s^2) + H(nl)$ configuration, with $n \leq 5$, and three more states with $n = 6$. The multireference configuration interaction method is used to calculate their electronic energy curves (EECs) for the internuclear distance *R* over the range of 0.0005 $28a_0$, the lower and upper ends of which are regarded as the separated-atoms and united-atom limits. Fifteen Rydberg series, *nsσ, npσ, ndσ, nfσ, ngσ, ndδ, nfδ, ngδ, ngγ, npπ, ndπ, nfπ, ngπ, nf?*, and *ng?*, are identified. Using Bingel's perturbation theory on the behavior of EECs for small *R*, we explain that the EECs of almost all Rydberg series show the same behavior because of the dominance of the core contribution. Thus, the small-*R* behaviors of the EECs of the many-electron molecular systems are quite different from those of one-electron molecular systems. However, core contributions are almost cancelled out in quantum defect curves so that their behaviors are like those of one-electron molecular systems. In addition, EECs show one-electron-molecule-like behaviors as *R* increases and the core effects disappear. The order of level energies in the equilibrium region is exactly the same as that in the one-electron molecular system at small *R*, except for the *nsσ* and *npπ* series. Core penetration of the *nsσ* orbital, facilitated by the core 1*s* orbital acting as a precursor, lowers the energies from the last position in the one-electron-molecule case.

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Structural Transition of Benzenemethanethiol Self-Assembled Monolayers on Au(111) at an Elevated Temperature

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The aromatic thiol self-assembled monolayers (SAMs) have drawn many attention because of its useful electrical properties come from its π?conjugated systems, which can be utilized for a number of technological applications such as electronic devices. The formation of benzenemethanethiol (BMT) SAMs on Au(111) were examined by means of scanning tunneling microscopy (STM) by changing the immersion temperature. The BMT SAMs formed at room temperature for 24 h exhibit hexagonally closed packed structure. As increasing the immersion temperature to 50 ℃, the surface structure of BMT SAMs shows the row structure and large-sized vacancy island. However as the increasing the immersion temperature to 75 ℃, the number of defects and disorder phase were increased. Whereas BMT SAMs formed at room temperature for 24 h exhibit the (√3 x √3) R30° structure, BMT SAMs annealed at 90 ℃ show long-ranged and striped phase structures with = (5/2 : 2√10) overlayer structure. From these results, we can find that BMT SAMs were strongly influenced by the immersion temperature.

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Excited State Intramolecular Proton Transfer Reaction Dynamics by Quantum Mechanical/Molecular Mechanical- Molecular Dynamics Simulations

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Proton transfer is one of the most important types of elementary chemical reaction in chemistry and biology. The reaction dynamics of excited state intramolecular enol-keto proton transfer tautomerism in 10-Hydroxybenzoquinoline (HBQ) has been investigated by QM/MM-MD simulation with four different solvents. The Excited State Intramolecular Proton Transfer (ESIPT) of HBQ proceeds in 20±8 fs in water and methanol solvents which is consistent with recent coherent time-resolved fluorescence measurements. In contrast, proton transfer occurs in other two solvents, CH2Cl2 and CHCl3 are 54±6 and 80±6 fs respectively. The QM/MM-MD simulation results indicates that the rate of proton transfer is inversely proportional to the polarity of the solvents. In addition, intramolecular hydrogen bonding capacity between the hydroxyl oxygen (proton donor) to the benzoquinolinic nitrogen (proton acceptor) plays important role for the ESIPT reaction.

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Photodissociation Dynamics of Aryl Halides Probed by Femtosecond IR Spectroscopy

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부산대학교 화학과

Femtosectond IR spectroscopy was used to probe the photodissociation dynamics of phenylchloride and phenylbromide in CCl_4 solution upon excitation at 266 nm. In the gas phase, photodissociation of aryl halide by a UV photon was known to produce phenyl radical, the C-C stretching bands of which are located at 1441 cm^{-1} and 1431 cm^{-1}. Upon excitation by a 266 nm photon, the phenyl radical was also formed in CCl_4 solution and the radical species disappears with a time constant of 1 ns for phenylchloride and 30 ps for phenylbromide. In addition to the phenyl radical bands, there are various transient absorptions in the region of 1390-1410 cm^{-1} for phenylchloride which decays with a time constant of 30 ps and 1388-1407 cm^{-1} for phenylbromide which decays with a time constant of 10 ps. Assignment of the transient absorptions and detailed photoexcitation dynamics of aryl halides in solution will be presented.

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Adsorptions and Reaction Mechanisms of NO2 on Ice Surface

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Theoretical calculations have been carried out regarding the adsorption and reaction mechanism of NO2 on ice surface with the help of MP2/6-31++G(d)//HF/6-31G(d) and DFT/6-31++G(d)//HF/6-31G(d) basis set using our QM/EFP scheme. At first NO2 physically adsorbed on ice surface and then H2NO3 formed by chemical adsorption. In the low concentration limit, single NO2 reaction mechanism on small and large ice surface models yields higher activation barrier. While in the high concentration limit, the reaction mechanism of NO2 dimer (cis and trans N2O4) yields relatively lower reaction barrier on 6 water model cluster. HONO and HNO3 can be obtained as product in NO2 dimer reaction mechanism on ice surface.

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Design of Explosive Systems in Molecular Size

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국방과학연구소 4본부 2부 [1]국방과학연구소 국방고등기술원

We have been interested in designing explosive systems in molecular size to understand the size limitation of explosion. As one of model systems, we utilize a carbon nanotube (CNT) as a container and nitromethanes as explosive molecules. By using both ab initio and molecular dynamics calculations, we try to comprehend the driving force in loading nitromethanes inside a CNT, and the optimized structure of nitromethanes loaded in a CNT. We calculate how many nitromathanes are able to be loaded, and how the structure of a CNT is deformed due to the change of loading pressure.

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Analogous metal-organic frameworks (MOFs) for the adsorption of organoarsenic compounds from aqueous solution: plausible mechanism and effect of central metal ions of analogous MOFs on adsorption

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경북대학교 화학과

p-Arsanilic acid (ASA) and roxarsone (ROX) are the two typical organoarsenic compounds have been studied to adsorbed onto metal-organic frameworks (MOFs) from aqueous solution for the first time. A MOF, iron-benzenetricarboxylate called MIL-100-Fe exhibited a much higher adsorption capacity for ASA and ROX than activated carbon, zeolite (HY), goethite, and other MOFs did. The adsorption of ASA and ROX over MIL-100-Fe was also much more rapid than that over activated carbon. Moreover, the used MIL-100-Fe could be recycled by simply washing with acidic ethanol. Therefore, it was determined that a MOF such as MIL-100-Fe can be used to remove organoarsenic compounds from spent water because of its high adsorption capacity, rapid adsorption, and ready regeneration. Interestingly, the porosity of the MOFs was not an important factor in the adsorption of organoarsenic compounds. Moreover, only one of analogous MIL-100s (MIL-100-Fe, rather than MIL-100-Al or MIL-100-Cr) was able to effectively remove the organoarsenic compounds. This selective and high adsorption over MIL-100-Fe, different from other analogous MIL-100s, could be explained (through calculations) by the facile desorption of water from MIL-100-Fe as well as large (absolute value) replacement energy (difference between the adsorption energies of the organoarsenic compounds and water) exhibited by MIL-100-Fe. A plausible adsorption/desorption mechanism is proposed based on the surface charge of the MOFs, FTIR results, calculations, and the reactivation results.

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Adsorptive removal of organosulfur compounds from fuel with ionic liquids supported to porous MIL-101, a typical metal organic framework

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There is a extensive command to reduce the content of sulfur-containing compounds in fuels like diesel and gasoline to a low level to prevent air pollution and deactivation of catalysts. Ionic liquid (IL)-supported metal-organic framework (MOF) was firstly demonstrated for the beneficial utilization of acidic IL in adsorptive desulfurization. For that, 1-butyl-3-methylimidazolium chloride (a typical IL) was introduced to one of the widely studied MOFs, MIL-101 (chromium-benzenedicarboxylate) via simple impregnation at ambient condition. A remarkable improvement in the adsorption capacity (~71%) was observed in IL-supported porous MIL-101 compared to the virgin MIL-101 for the adsorption of benzothiophene (BT) from liquid fuel. The improved adsorptive performance could be explained by the acid-base interactions between the acidic ionic liquid and basic BT. Moreover, from this study, it can be suggested that porous MOFs, supported with ionic liquids, may introduce a new class of highly porous adsorbents having the advantage of the imidazolium cationic sites for the efficient adsorption of various organics.

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Prediction of Heat of Formation of Nitro derivativesof Azoles using G4MP2-SFM scheme

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The nitrogen containing heterocycles, Azoles, are of high interest as the basis for a new generation of high energy density materials for use as propellants and explosives. The heats of formation of Pyrrole, Imidazole, Pyrazole, Triazole, Tetrazole and Pentazole with their nitro derivatives have been studied. A fast and highly accurate prediction procedure has been established to predict the heat of formation, using the parameterization scheme, G4MP2-SFM, combining SFM (Systematic Fragmentation Method) and high accuracy G4MP2 theories for these compounds. We suggest the parameterization scheme of groups (fragment) of SFM whose heats of formation are predicted by G4MP2. In the applications to 48 NO2 derivatives of azoles, our G4MP2-SFM (opt) yielded an overall MAD (mean absolute deviation) of 2.2 kcal/mol and RMSD (root mean square deviation) of 2.9 kcal/mol, as compared to full G4MP2 values, which determines its high prediction accuracy and statistical stability replacing the further quantum mechanical calculations with a set of simple calculation. This reliable method confirms that accuracy is not necessarily enhanced by greater complexity as well as gives the simplest and easiest pathway for the calculation of gas phase heat of formation of energetic compounds.

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Operating Mechanism of Carbon Nanotubes Coated Colloidal Sensors

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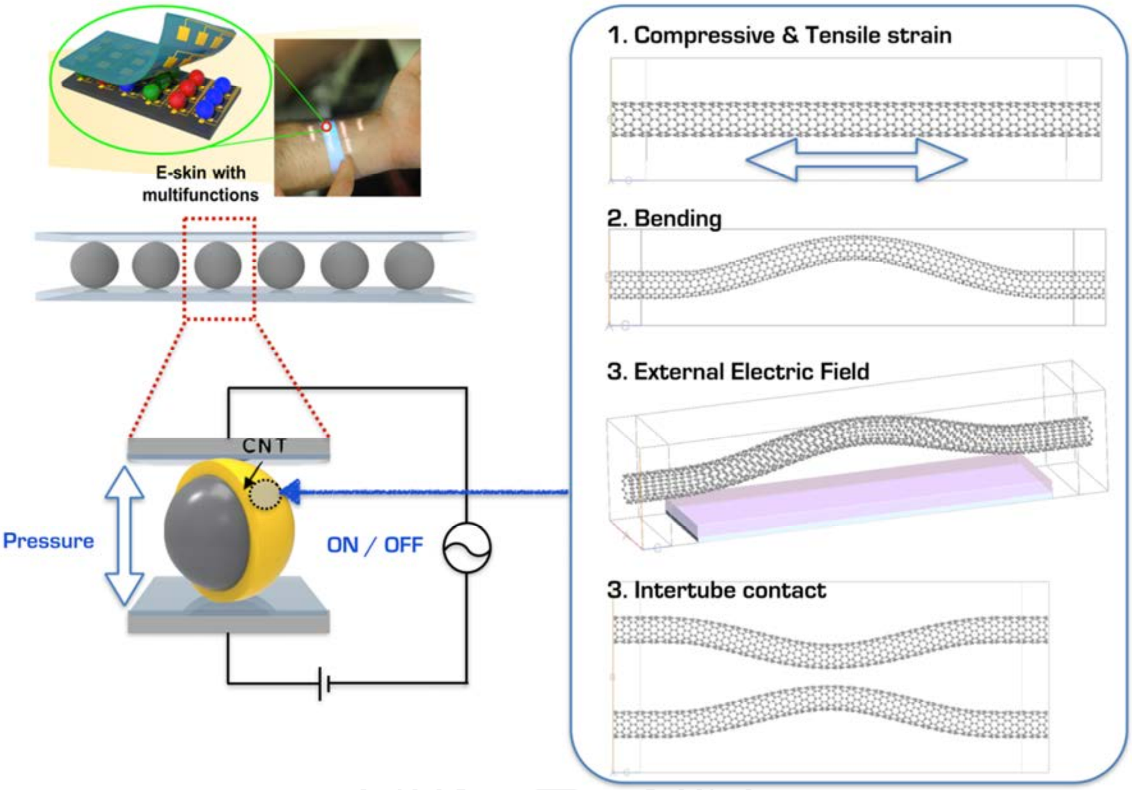
We have systematically investigated the electrical conductance change of Carbon Nanotubes (CNTs) coated polyurethane colloidal sensor under external pressure. The external pressure induces structural deformation of the colloidal sensors, especially coated CNTs. So, we have designed several models characterizing structural deformation of CNTs under compressive/tensile strains and investigated responding their electrical conductance. In addition, we have considered the effects of electrodes induced external electric field and CNT-CNT intertube contact stimulated by external pressure. In these works, we have clearly elucidated the operating mechanism of CNTs coated colloidal sensors is based on the electrical conductance changes of CNTs induced by structural deformations under external pressure, which strongly affects band structures and electron transport characteristics.


E-skin with
multifunctions
CNT
Pressure
ON / OFF
1. Compressive & Tensile strain
2. Bending
3. External Electric Field
3. Intertube contact

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Amino groups functionalized metal-organic frameworks for adsorptive removal of indole from model fuel via hydrogen bond formation

imteaz ahmed **Biswa Nath Bhadra 정성화***

경북대학교 화학과

Nitrogen-containing compounds (NCCs) are composed of basic materials such as quinoline (QUI) and neutral materials such as indole (IND). Because of the negative effect of NCCs on the environment and catalyst stability, NCCs should be removed from fuels. The NCCs can be removed by various methods including adsorption. Compared with basic NCCs, neutral NCCs are more difficult to remove through adsorption due to their less affinity towards adsorbents. In this report, adsorption of IND (as one of the representative neutral NCCs) was studied over the metal-organic frameworks (MOFs), UiO-66 and UiO-66-NH_2, which contain terephthalate and amino-terephthalate linkers, respectively. In spite of the reduced porosity of UiO-66-NH_2, the adsorption capacity of IND was improved upto 46% when compared with pristine UiO-66. Therefore, the additional amino group in the MOF imparts extra adsorption capability on the MOF. For a detailed investigation, adsorption of other NCCs such as QUI, pyrrole, and methylpyrrole was studied. The improved adsorption of IND over amino-functionalized MOFs could be attributed to the improved interaction of IND with the MOF via H-bonding because of the -NH_2 group. In addition to this remarkable improvement in IND adsorption, UiO-66-NH_2 could be regenerated several times for the adsorption of IND by simple solvent washing.

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Liquid phase adsorption of methylchlorophenoxypropionic acid (MCPP) with a metal-organic framework

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경북대학교 화학과

The adsorptive removal of methylchlorophenoxypropionic acid (MCPP) using metal-organic frameworks (MOF), namely Zr-benzenedicarboxylate (UiO-66), has been investigated for the first time to determine the applicability of MOFs in the removal of hazardous herbicides/pesticides from contaminated water. Compared with activated carbon, UiO-66 has a very high adsorption rate (kinetic constant ~ 30 times that of activated carbon). This rapid adsorption is remarkable because the pore size of UiO-66 is smaller than that of activated carbon. Moreover, the adsorption capacity of UiO-66 is higher than that of activated carbon especially at low MCPP concentrations (~7.5 times at 1 ppm of MCPP). These rapid and high uptakes by UiO-66 suggest that there is a special mechanism for interactions between MCPP and UiO-66. Additionally, the adsorbent can be reused for adsorptive removal by washing the spent adsorbent with a simple solvent. MOFs such as UiO-66 are therefore potential adsorbents for use in the adsorptive removal of MCPP from contaminated water. A plausible adsorption mechanism is suggested based on the effects of pH on the zeta potential of the adsorbent and on adsorption. Both electrostatic and π-π interactions might be important for the adsorption of MCPP by UiO-66.

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Computational Study on the Strong Binding Affinity of Cyclic Naphthalene Diimide to Tetraplex DNA

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숙명여자대학교 화학과

Ligands that strongly bind to tetraplex DNA are of recent biological interest since they potentially serve as specific anticancer agents. Cyclic naphthalene diimide (CND) is among such ligands, which exhibits greater affinity to tetraplex DNA than to a double stranded oligonuclotide. Here we report the molecular origin on this binding selectivity of cyclic naphthalene diimide toward tetraplex DNA over a double stranded oligonuclotide by using the quantum mechanical calculation and the integral-equation theory of liquids. We provide the interaction energies and the most stable binding site between CND and tetraplex DNA. The effect of metal 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 binding preference and the effect of solvent water upon complexation between tetraplex DNA and CND.

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Structure, Thermodynamics, and Water Dynamics of intrinsically disordered Tau Protein Fragment (Tau43) by Computational Study

임슬기 함시현[*]

숙명여자대학교 화학과

The abnormal aggregation of hyperphosphorylated tau protein into paired helical filaments (PHFs) is one of the hallmarks of Alzheimer's disease. We herein characterized structural and thermodynamic features of human tau protein fragment comprising 43 residues (termed Tau43), the minimal sequence of aggregating in tau pathology, by performing the fully atomistic, explicit-water molecular dynamics simulations followed by solvation thermodynamic analyses based on the integral-equation theory of liquids. Tau43 monomer displays conformational disorder in aqueous environments with fairly localized α-helical and β-sheet structures. Based on the solvation thermodynamic analysis, the lysine residues in Tau43 contribute favorably to the total solvation free energy with large negative values. Therefrom we investigate water dynamics behavior by constructing H-bond correlation functions of solvent water around the lysine residues of Tau43 to investigate the solvation thermodynamics-dynamics relationship of intrinsically disordered Tau43 in aqueous environments.

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Quantum Mechanics and Solvation Thermodynamic Calculations on the General Anesthetics

이진경 함시현*

숙명여자대학교 화학과

Anesthetics provide controlling of water flow in brain’s neuron transmittance and their binding sites are known as amphipathic in nature. While anesthetic-protein interaction has been demonstrated to be critically influenced by water, the detailed picture on the role of water in anesthetic mechanism remains elusive. Here, we studied general anesthetics (halothane, isoflurane, sevoflurane, enflurane, and fluorocyclobutane) by using quantum mechanical calculations and integral-equation theory of liquids. We have determined the electronic structure and optimized the geometries of these molecules in a gas phase. We then computed the solvation free energy on these systems based on the 3D-RISM integral-equation theory. Our work here thus provides a prerequisite to investigate anesthetic-protein interaction and the role of water involved therein.

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Computational Study on the Fluorescent Inhibitor for the Detection of Aβ Oligomers

임슬기 함시현*

숙명여자대학교 화학과

Soluble oligomers of amyloid-beta (Aβ) are considered to be the primary agent of neurotoxicity related with Alzheimer's disease (AD). In this regard, the development of the Aβ oligomer-specific sensor has been a great challenge since the chemical and topological characteristics of the Aβ oligomer have not been fully achieved. Here we report the structural and thermodynamic features of the Aβ oligomer-specific sensor called BDO-1, a BODIPY-based organic compound, as well as its complex with Aβ oligomer by using the combination of quantum mechanics, molecular docking simulations, and statistical mechanics. We also provide the molecular origin on why and how BDO-1 is Aβ oligomer-specific based on the binding free energy computation. We suggest the critical role of hydrophobic F19/V36 residues of Aβ oligomer in detecting BDO-1, which may render crucial information on the development of AD drugs.

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The effect of the surface structure of ZnO on the adsorption and bulk diffusion of hydrogen

MOTINABDUL 김창민*

경북대학교 화학과

We have compared thermal reactions of surface and subsurface hydrogen atoms on the (0001) and (10?0) surfaces of ZnO. When the ZnO surface is exposed to atomic hydrogen at 370 K, both surface and (0001) and (10?0) surfaces of the ZnO single crystal have been studied. Subsequent diffusion of surface hydrogen into the bulk and the migration of bulk hydrogen have been also investigated. Hydrogen diffuses into the bulk at 370 K through the surface adsorption state. Upon heating, bulk H atoms evolve as H2 molecules. In case of ZnO(0001), bulk hydrogen is completely remove below 750 K. Evolution of bulk hydrogen on (10?0) face of ZnO takes place at higher temperatures. Our observations confirm that the migration of H atoms in the ZnO crystal lattice takes place mostly along the c-axis.

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The Concentration Effectson the Interaction of PEO with SDS in Magnetized Water

이성현 전상일*

강릉원주대학교 화학과

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. 이러한 자화수는 또한 계면활성제의 CMC(critical micelle concentration)를 낮추는 것으로도 확인되었다. 고분자를 계면활성제에 첨가하면 이들 사이의 강한 정전기적 및 소수성 상호작용으로 인하여 계면활성제만의 CMC 보다 저 농도에서 마이셀을 형성하는데, 이를 CMC 와 구분하기 위하여 CAC(critical aggregation concentration)라 부른다. 이전 실험에서 다양한 농도의 비이온성 고분자인 PEO(polyethylene oxide)를 음이온 계면활성제인 SDS(Sodium dodecyl sulfate)에 첨가했을 때, CAC 및 C2 형성에 영향이 있음을 확인하였다. 본 연구에서는 물 대신 자화수를 사용함으로써 다양한 농도의 자화수용액 PEO 를 SDS 에 첨가함으로써 자화수가 CAC 및 C2 형성에 어떠한 영향을 미치는지 알아보고자 한다.

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Circular Dichroism Spectroscopy of Jet-cooled Chiral Molecules

홍아람 김남준*

충북대학교 화학과

Circular dichroism spectroscopy of jet-cooled chiral molecules provides a powerful tool to determine absolute configurations of different conformers present in the gas phase. We have obtained the resonant two-photon ionization (R2PI) CD spectra of jet-cooled pseudoephedrine (pED) and ephedrine (ED) with circularly polarized laser pulses generated using a photoelastic modulator (PEM). The R2PI CD spectra of pED and ED exhibit well-resolved CD bands, both of which are well-reproduced by theoretical calculations using the time-dependent density functional theory. We also apply laser-induced fluorescence (LIF) spectroscopic technique to measure the CD spectrum of ED. By comparing the LIF CD spectrum with the R2PI CD, we discuss the possibility of the state-selective isomerization of ED at the electronic excited state.

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Electronic Circular Dichroism Spectroscopy of 2-Amino-1-Phenylethanol in a Supersonic Jet

정창섭 김남준*

충북대학교 화학과

We obtained the electronic circular dichroism (ECD) spectra of (*R*)-(-)-2-Amino-1-Phenylethanol (*R*-AP) and its enantiomer (*S*)-(+)-2-Amino-1-Phenylethanol (*S*-AP) in a supersonic jet using resonant two photon ionization (R2PI) spectroscopy. CD spectrum of hydrated clusters of *R*-AP have obtained. *R*-AP and *S*-AP were irradiated by left and right-handed circularly polarized (LCP and RCP) laser pulses generated using a photoelastic modulator (PEM) and the difference between the ion signals produced by LCP and RCP pulses was recorded as a function of the wavelength to obtain the CD spectra. We identified the origin bands of the S_0-S_1 transition for two different conformers of *R*-AP present in the jet. Theoretical calculations were carried out to predict the structures of the conformers as well as the CD signs of their origin bands.

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Size-Dependence of Excitation Energy-Related Surface Trapping Dynamics in PbS Quantum Dots

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연세대학교 화학과 [1]한국기계연구원 나노기계연구본부

Using ultrafast transient absorption spectroscopy, we investigated the surface carrier trapping dynamics in various sized PbS quantum dots (QDs) when either a hot or cold exciton is photogenerated by different pump-energy. We observed that hot carriers exhibit distinctly different surface trapping dynamics from the cold exciton, in which their corresponding TA spectral evolutions show clear differences in the long wavelength region (< a band gap energy, Eg). We observed a rapid growth in the degree of surface trapping with an increase in the pump-energy. On the other hand, the degree of surface trapping in terms of the number of created excitons (?Nx?) shows negligible variation upon photoexcitation at any given wavelengths. The photoinduced electron-hole separation followed by carrier trapping was characterized by ultrafast trapping rate. The surface trapping rate was solely dependent on the PbS QD size; the surface trapping rate becomes faster as the QD size increases. Furthermore, we explain the dependence of QD size on the surface trapping rate in terms of the size-dependent exciton binding energy (Eeb).

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Excited-State Low-frequency Vibrational Coherence in Perylene Bisimide Probed by Femtosecond Pump-Probe Spectroscopy

박규형 손민정 김동호*

연세대학교 화학과

Coherent wavepacket dynamics have long been of tremendous interest, and recent studies focus particularly on observing such dynamics in photosynthetic complexes and protein macromolecules. On the other hand, research on similar coherent oscillations in small organic molecules remain rudimentary to date. Among various π-conjugated molecules, perylene tetracarboxylic acid bisimide (PBI) dyes with high chemical robustness and inherent high fluorescence quantum yield can be ideal candidates for the investigation of ultrafast photodynamic processes.In this regard, coherent oscillations of an N,N’-bis(2,6-dimethylphenyl)perylene bisimide (DMP-PBI) were studied using femtosecond pump-probe spectroscopy with a ~35 fs temporal resolution. Signature of coherent oscillation was observed upon probing stimulated emission, which can be attributed to wavepacket dynamics on the excited-state potential energy surface. Ultrafast wavepacket dynamics of two separate low-frequency modes at 140 and 275 cm^{-1} were extracted. DFT calculation indicates that the origins of the two modes are PBI deformation coupled to the motion of phenyl substituents. Phase jumps of the two modes occur at wavelengths displaced ~10 nm from the maximum of fluorescence, showing similar behaviours reported for photoactive biofunctional molecules.

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Zn(II) Production via a Pulsed Laser Ablation in Water: A Formation Mechanism of Zn and ZnO Nanoparticles

이슬기 안아름 최명룡*

경상대학교 화학과

Zn and ZnO nanoparticles were produced by a pulsed Nd:YAG laser ablation method in the absence of any surfactants and/or catalysts in deionized (DI) water via pulsed laser ablation in liquid (PLAL). In this paper, we present direct evidence for the production of Zn(II) ions induced from the plasma plume during the process of PLAL for the first time. Investigation of the absorption and emission spectra of zinc tetra(p-sulfonatophenyl) porphyrin (ZnTSPP) formed via the laser ablation on a Zn metal plate in TSPP solution showed a significant fluorescence quenching of ZnTSPP. This fluorescence quenching of ZnTSPP was further investigated with an aid of theoretical calculations. Based on these experimental and theoretical results, a plausible mechanism for the production of Zn and ZnO nanoparticles is proposed.

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Conformation-Specific Spectroscopic Studies of jet-cooled Acetaminophen-Water Clusters by Gas Phase

민아름 문철주 안아름 이지훈 최명룡* 김성근[1]

경상대학교 화학과 [1]서울대학교 화학부

Acetaminophen (AAP) is a widely used over-the-counter antipyretic and analgesic, a major ingredient in various cold and flu drugs, Tylenol. On the basis of the results with monomer, we would like to step further on the study of AAP-water clusters. For the water clusters, REMPI spectrum is responsible for the broad absorption with baseline. Then, we obtained UV-UV hole-burning spectra to idoentify the number of conformers in the AAP-water cluster system. Moreover, we investigated the vibrational mode of ground state using IR-dip spectroscopy. As well, we reports the structural information of AAP-water clusters by comparing the each experimental results and those from the theory. Further discussion of this system will be present in tthis poster.

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Conformation Specific Spectroscopy of Jet-cooled 3-Acetaminophen: REMPI, UV-UV Hole-burning and IR-dip Spectroscopic

이지훈 민아름 안아름 문철주 최명룡*

경상대학교 화학과

The conformational structures of jet-cooled 3-acetaminophen (3-AAP) were investigated in the gas phase by resonance-enhanced multiphoton ionization (REMPI), UV-UV hole-burning (UVHB) and IR-dip spectroscopy. We obtained sharply congested REMPI spectrum of 3-AAP and identified that 3-AAP has two conformers via UVHB (0-0 bands of the cis and trans isomers found at 35316.3 and 35237.3 cm^{-1}, respectively) and IR dip spectroscopy. Moreover, we also calculated the optimized structures of 3-AAP by density functional theory (DFT) with a 6-311++ G(d,p) basis set. This results show that 3-AAP has different structural characteristics compared to those of 4-AAP.

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Assignment of Jet-cooled Indole-3-carbinol by Laser Desorption Technique and Franck-Condon Simulations

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경상대학교 화학과

The excitation spectra of indole-3-carbinol (I3C) in the gas phase have been measured by mass-selected resonant two-photon ionization (R2PI) and UV-UV hole-burning (UVHB) spectroscopy for the first time using two different sample preparation methods, thermal evaporation and laser desorption. IR-dip spectrum was recorded to determine the conformational geometry of I3C; however, resulting ambiguous due to very similar predicted IR frequencies for the two lowest energy conformers. Further investigation using Franck-Condon simulations of the two conformers of I3C has led to a conclusive assignment of the observed conformer in the experiments as the global minimum structure of I3C.

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2D Correlation Analysis of pH-dependent IR spectra for HAMLET

김예슬 정영미* **Bogusława Czarnik-Matusewicz[1]** 박연주

강원대학교 화학과 [1]Faculty of Chemistry, University of Wroctaw, Poland

α-lactalbumin (ALA) can be transferred into intermediate state by physical or chemical agents. The intermediate state of ALA has an ablity to form with oleic acid (OA) the complex named, HAMLET (human α-lactalbumin made lethal to tumor cells). HAMLET possesses cytotoxic activity with respectr to tumor. However, the actual molar ratio of OA over protein in the complex are still poorly understood. In this study, to investigate structural change of ALA/OA complex having different molar ratio, principal component analysis (PCA) and 2D correlation spectroscopy were applied to pH-induced IR spectra of HAMLET . Details of this results will be discussed in this presentation.

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Spectroscopic studies of Jet-cooled Isocytosine

문철주 민아름 안아름 이지훈 최명룡*

경상대학교 화학과

Isocytosine(IC), 2-aminouracil, is a non-natural nucleobase, a similar structure of guanine; therefore, its spectroscopic investigation is worthy of attention especially for the natural/unnatural base pairs with guanine and isoguanine. In this study, mass-selected nanosecond(ns) and picosecond(ps) resonant two-photon ionization (R2PI) and UV-UV hole-burning (UVHB) spectroscopy using two different sample preparation methods, thermal evaporation and laser desorption. IR-dip spectra were recorded to determine the conformational geometries of IC. Further investigation using ab initio and density functional calculations for IC has led to unambiguous assignments for the observed conformers in the gas phase studies.

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Detection of UV and Visible Lights with Organic Bulk Heterojunction Photodetectors

정재훈 김화정 김영규*

경북대학교 화학공학과

Organic electronics are expected to create new applications because organic materials have great potentials in terms of molecular diversity leading to various optoelectronic properties as proven by the successful commercialization of flexible organic light-emitting devices (OLEDs). However, less attention has been paid on organic photodetectors (OPDs) even though OPDs have wide applications for cameras or sensors for smart phones, notebooks, security-monitoring systems etc. due to the their advantages including large-area, ultrathin, lightweight and flexible/bendable features. Recently, we have focused on the development of various OPDs by employing organic bulk heterojunction layers which are made with small molecular and/or polymeric semiconducting materials. In this presentation, we will show the optoelectronic properties of OPDs that are able to detect from UV to visible light ranges and discuss the physics behind the resulting device performances.

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Excited state dynamics studied by femtosecond time-resolved Raman spectroscopy

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Time-resolved femtosecond transient absorption spectroscopy which adopts narrow pump pulses and broadband super-continuum probe pulses with variable time delays has been successful in revealing details of the excited state dynamics. However, broad overlapping absorption bands with varying lifetimes over the wavelength make the kinetics analysis in the electronic excited states difficult and unclear. In this research, a femtosecond stimulated Raman spectroscopy (FSRS) based on a Ti:sapphire amplifier system has been built. The stimulated Raman process, which monitors all the vibrational transitions of sample, requires two pulses; picosecond narrowband Raman pump and femtosecond broadband super-continuum Raman probe. By combining actinic pump pulses with Raman pump/probe pulses with a certain delay time, time-resolved stimulated Raman spectrum of sample in the electronic ground and excited states can be obtained. Due to high spectral (

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Membrane introduction GC/TOFMS for real time monitoring of volatile organic compounds

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원광대학교 생명나노화학부 [1]원광대학교 화학과 [2]원광대학교 바이오나노화학 [3]한국표준과학연구원(KRISS) 첨단장비기술센터 [4]한국표준과학연구원(KRISS) 첨단측정장비센터

The benefits of membrane introduction GC/TOFMS (time-of-flight mass spectrometer) for real time monitoring of VOCs are well known, with such techniques increasing sample throughput and reducing the overall cost of pollution level monitoring. Characterization of membrane interface was performed using a TOFMS. Temporal evolution of VOCs through the two 127 ㎛ thick polydimethylsiloxane (PDMS) membranes were measured by monitoring the ion signal after a step change in the sample concentration. The transmission efficiency of each sample component was investigated as a function of membrane temperature and flow rate of carrier gas. The detection limits for VOCs were found to be in the range of ppb by volume. Initial results indicate that the membrane interface will be capable of use in a wide range of applications, particularly for real-time environmental monitoring.

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Ultrafast energy transfer between dyes and metal nanoparticles

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광주과학기술원(GIST) 물리화학부

Fluorescence of dye molecules in solutions or disperse in a polymer layer show strong enhancements (up to 30 folds), when a silver island film exists next to dye molecules. Excited-state dynamics of dyes near metal nanoparticles and ultrafast energy transfer between them have been studied by an ultrafast transient absorption technique and a time-correlated single photon counting (TCSPC) in visible wavelengths. The stimulated emission from the charge-transferred S1 (S1-CT) state of DCM in methanol solution shows an additional rise component of ~30 ps in the kinetic analysis, and the S1-CT lifetime gets longer with the existence of the silver island film. From the time-resolved fluorescence of rhodamine 6G and DCM in a thin polymer film coated on the silver island film, another dynamics with the ~400 ps lifetime is obtained. These results clearly show that the energy transfer between dyes and silver nanoparticles occurs in ultrafast time scales. The ultrafast energy transfer dynamics between dyes to nanoparticles might provide a clue to understanding the mechanism of metal enhanced fluorescence, which has shown many applications in biomedical photonics and engineering.

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A portable GC instrument for real-time monitoring of gas mixtures in air sample

유동욱 이재원[1] 오준식[2] 정광우[*] 박창준[3] 안상정[4]

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In the present study, we developed a portable GC instrument for real-time and quantitative determinations of gas mixtures in air sample. The instrument provides rapidly detection and quantitative determination in a compact and light in weight configuration. Significant reduction in peak tailing are accomplished by inject make-up gas with PID (photoionization detector), while retention time and peak width remain stable. We demonstrated the high sensitivity and selectivity of this device. The results indicate that the portable GC-PID module is expected to be used for a wide range of applications, particularly for in situ environmental monitoring, chemical processes, and regulation of contaminant emission.

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Dynamics of highly-polydisperse colloidal liquids

황지예 성봉준*

서강대학교 화학과

A cell contains a variety of macromolecules and they are caged by their neighbors, leading to dynamic heterogeneity. It is well known that diffusion of macromolecules in cells is qualitatively similar to that of glass-forming liquids near glass transition temperature. Threrefore, previous extensive studies on glasses might shed light on the protein dynamics in cells. However, most studies on glasses focused mainly on binary systems, whereas macromolecules in cells are highly polydisperse in size. Therefore, we conduct Langevin dynamics simulations for highly-polydispese colloidal systems to study the dynamic heterogeneity of macromolecules in cells. In general, displacement probability distribution function, $G_s(r,t)$, is Gaussian in case macromolecules undergo Browninan motion, while $G_s(r,t)$ may deviate from a Gaussian form in crowded cell environments. The degree of deviation from Gaussian distribution can be quantified by a non-gaussian parameter, $\alpha(t)$, of which the value is zero for Gaussian distribution. It has been well-known that $\alpha(t)$ increased monotonously with an increase in the density of binary liquids. In highly-polydisperse colloidal system, however, $\alpha(t)$ of macromolecules shows a non-monotonic behavior with density: $\alpha(t)$ increases up to a critical dentsity and decreases again to zero. And we also estimate both time and length scales of correlated region by calculating the relative angle distribution, $P(\theta, \Delta)$.

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Understanding Structures and Thermodynamics on Islet Amyloid Polypeptide Related with Type II Diabetes

조선희 함시현*

숙명여자대학교 화학과

Aggregation of islet amyloid polypeptide (IAPP) has been implicated as the primary cause of type II diabetes. However, the details on the molecular factors that promote aggregation potential of IAPP remain unclear. In this study, we have used various IAPP conformational ensembles identified by replica exchange molecular dynamics (REMD) simulations and Markov state models and have computed their solvation thermodynamics properties to elucidate structural and thermodynamic characteristics that potentially seed aggregation. We find that the metastable conformations with higher β-sheet contents exhibit larger hydrophobic surface area as well as higher solvation free energy than the most populated conformations. The structural and thermodynamic characteristics on the metastable state of IAPP provided herein may render a crucial information on the molecular origin that seed the aggregation process related to Type II Diabetes.

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Mutation Effects on FAS1 Domain 4 Related to Protein Aggregation by Molecular Dynamics Simulations and Solvation Free Energy Analysis

조선희 함시현*

숙명여자대학교 화학과

Mutations in fasciclin 1 protein (FAS1) are known to be the cause of several different corneal dystrophies, a protein aggregation disease in eyes. Despite the identification of the aggregation-prone mutations in FAS1 domains, no structural information has been provided for the mutants of this protein. In this study, we have investigated the structural characterization for the two mutants, R555Q and R555W, of the FAS1 by using fully atomistic, explicit-water molecular dynamics simulations. The MD simulation and three-dimensional reference interaction site model (3D-RISM) calculation results indicate that due to the non-native hydrophobic interactions in β2-β4-β5-β6 regions induced by the point mutation, the orientation of C-terminus is rearranged to block the YH binding motif in α6 region from integrins binding in the mutant structures. The atomic-level mutant structures and the molecular motif to trigger protein aggregation provided by MD simulations herein can be useful to design potential therapeutics and to block FAS1 aggregation related to corneal dystrophy.

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Photoexcitation Dynamics of Cobalttricarbonylnitrosyl Probed by Femtosecond Vibrational Spectroscopy

권다예 이소현 임만호*

부산대학교 화학과

Femtosecond vibrational spectroscopy was used to probe the photoexcitation dynamics of $Co(CO)_3NO$ dissolved in hexane. Upon dissolution into hexane, the C-O stretching modes of $Co(CO)_3NO$ vibrate at 2102 and 2035 cm^{-1}, red-shifted from those in the gas phase at 2108 and 2047 cm^{-1}, and its N-O stretching mode vibrates at 1808 cm^{-1}, red-shifted from that in the gas phase at 1822 cm^{-1}. The N-O stretching mode $Co(CO)_3{}^{15}NO$ vibrates at 1772 cm^{-1}, resulting in the ^{15}NO isotope shift by 36 cm^{-1}. When excited by a 266-nm photon, $Co(CO)_3NO$ in hexane shows immediate bleach at the three stretching vibrational bands. About 10% of the bleach decays with a time constant of 10 ps and the remaining bleach persists beyond 1 ns. The immediate bleach and the ps decay with the 10% magnitude in three stretching modes of the parent molecule suggest that about 10% of the photoexcited molecules relaxe without photodissociation and 90% of them immediately photodissociate. There were also rich transient absorptions in the region of 1760 ~ 1660 cm^{-1}, which show ps-dynamics. Assignment of transient absorptions and detailed photodissociation dynamics of $Co(CO)_3NO$ in hexane will be presented.

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Thermal Behavior and Molecular Interaction of P(HB-co-HHx)/PEG Blend Explored by 2D Correlation IR Spectroscopy

<u>Yujing Chen</u> 박연주 정영미*

강원대학교 화학과

Biodegradable poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (P(HB-co-HHx)) has recently received considerable attention owing to its potential applications in the environmental protection fields. Basic thermal properties of P(HB-co-HHx) copolymers have been studied extensively, while blends of P(HB-co-HHx) copolymers still lagged behind[1, 2]. This is of great importance for tailoring the mechanical properties and degradation kinetics to suit for various applications. In the present study, the blend system of P(HB-co-HHx) and polyethylene glycol (PEG) was selected and molecular interaction of P(HB-co-HHx) in its blends with PEG upon heating process have been investigated by infrared reflection absorption spectroscopy. 2D correlation spectroscopy was performed to further analysis for the thermal behavior change upon heating process[3]. The thermal behavior and molecular interaction of P(HB-co-HHx)/PEG blends will be discussed. [1]H.C. Choi, S.R. Ryu, H. Ji, S.B. Kim, I. Noda, Y.M. Jung, The Journal of Physical Chemistry B 114 (2010) 10979-10985.[2]M.K. Kim, S.R. Ryu, I. Noda, Y.M. Jung, Vibrational Spectroscopy 60 (2012) 163-167.[3]Y.M. Jung, I. Noda, Encyclopedia of Analytical Chemistry, John Wiley & Sons, Ltd, 2006.

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The Spectroscopic Study of Mice Serum under Radiation Exposure

박연주 정유진[1] 정영미[*]

강원대학교 화학과 [1]강원대학교 생명과학과

Acute radiation syndrome (ARS) is the collection of biological hazardous effects that present within 24 hours of exposure to high amounts of ionizing radiation. Because ARS symptoms are diverse and nonspecific, ARS cannot be diagnosed easily. For the early detection of ARS, we examined mice serum within 24 hours exposed to gamma radiation by using infrared (IR) and Raman spectroscopies in this study. The spectral changes in IR and Raman spectra of mice serum before and after radiation exposure can elucidate the structural changes of protein under the radiation-exposure damage of cells or animals. In this presentation, the results of IR and Raman spectra will be discussed in more detail.

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Quantum chemical study on the charge-transfer state of four-atom molecules as model PCET systems

문자연 안희선 백경구*

강릉원주대학교 화학과

The molecular structure and spectroscopic frequencies of four-atom anionic molecules with a non-covalent interaction were computed by various ab initio and DFT methods. The properties of their neutral ground electronic state were calculated too. Then the low-lying excited electronic states of the neutral systems were studied by applying IP-EOM, TD-DFT, CASSCF, CASPT2, and MRCI methods. Special emphases were placed on their charge-transfer state, i.e., its charge-distribution characteristics, possible dissociation limits, and non-adiabatic regions along the dissociation pathways. This study aims at finding proper model systems to extend a recent research on the quantum dynamics of proton-coupled electron-transfer (PCET) processes,[1] on the time scale of just a few femto-seconds.[2]

[1] Huynh, M. H. V.; Meyer, T. *J. Chem. Rev.* 2007, 107, 5004.
[2] An, H.; Baeck, K. K. *J. Chem. Phys. Lett.* 2014, 5, 1307.

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Au aggregates-4MBA@SiO2 core-shell nanoparticles as SERS tag for immunoassay

진실아 정영미* 박연주 **Bing Zhao[1] Zhi Yu[2] Lei Chen[3]**

강원대학교 화학과 [1]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun 130012, P. R. China. [2]Key Laboratory for Bionic Engineering of Ministry of Education, Jilin University, Changchun 130025, P.R. China. [3]Key Laboratory of Preparation and Applications of Environmental Friendly Materials, Ministry of Education, Jilin Normal University, Siping 136000, P.R. China.

Surface enhanced Raman scattering (SERS) based immunoassay has been extensively studied due to its high sensitivity and pingerprint information of molecules. developed by using SERS tag In this study, SERS tag which is combining Raman reporter-labeled Au aggregates on a SERS-active immune substrate was prepared. Au aggregates- 4-Mercaptobenzoic acid (4-MBA)@SiO2 core-shell nanoparticles functionalized antibody were used for detecting human immunoglobulin G. Details on sandwich-type SERS immunoassay will be discussed.

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Quantum wave-packet propagation study on the factors affecting the branching ratio of a photo-dissociation mediated by a $^1\pi\sigma^*$ state

안희선 백경구[*]

강릉원주대학교 화학과

The photo-induced hydrogen elimination reaction of thiophenol (PhSH) excited to $1^1\pi\pi^*$ state was investigated by the time-dependent quantum wave-packet propagation within two-dimensional (2D) space consisting of the S-H bond and the -SH torsion. In order to study the effect of several factors of 2D potential energy surfaces (PESs) on the branching ratio between the two dissociation channels to X and A states of PhS radical, the parameters of the previous analytic functions[1] for the 2D PESs of S_0, $^1\pi\sigma^*$ and $^1\pi\pi^*$ states were re-optimized. The effects of the reduced initial barrier to the $\pi\pi^*/\pi\sigma^*$ conical intersection (CI), the reduced torsional barrier on the $^1\pi\pi^*$ state, the mitigated slope of the $\pi\sigma^*$ state between the first $\pi\pi^*/\pi\sigma^*$ and the second $S_0/\pi\sigma^*$ CIs, and the reduced energetic splitting between two dissociation limits are discussed here.[2]

[1] Venkatesan, T. S.; *et al. J. Chem. Phys.* 2012, 136, 174312.
[2] An, H.; *et al. ChemPhysChem* 2015, DOI: 10.1002/cphc.201500060.

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Computational Study of the Optical and Electrochemical Properties of Coronene Derivatives as Hole Transport Material for Perovskite Solar Cells

GAPOL MAEBIENNE ANJELICA Mannix Balanay[1] 이상희 김동희*

군산대학교 화학과 [1]Dept. of Chemistry, Nazarbayev University

Organic-inorganic hybrid perovskite solar cells have attracted much interest as thin-film photovoltaic devices due to their high performance. The high cost and low performance of hole transporting materials (HTMs) hinder the advancement of perovskite solar cells. Development of new HTMs with high hole mobility and proper oxidation potential with respect to the energy level of perovskite is becoming an active area of research. In this study, with the aim of designing potential HTM, we investigate the properties of coronene derivatives. Coronene derivatives are reported to have good transport properties but have not been explored as HTM for perovskite solar cells. The energy levels, absorption spectra and electrochemical properties of the coronene derivatives were investigated using density functional theory and time-dependent density functional theory.

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Theoretical Study for Spin-Crossover in the C-H Activation of Methane by CoO+, NiO+ Cation

김상준 Mai Khanh Binh 김용호*

경희대학교 응용화학과

메탄올은 액체연료로도 사용되어지며 전 세계에서 가장 많이 생산되어지는 화합물들중 하나이다. 효율적인 촉매로 메테인을 메탄올로 전환하는 직접적인 방법은 순수, 응용 화학 학계에서 많은 주목을 받아왔다. 최근 NiO+와 CoO+에 의한 메테인 Hydroxylation 의 Knetic profiles 를 Spin-crossover 가 일어나는 Two-state reactivity (TSR)로 설명하는 연구가 진행되어왔다. 본 연구는 CoO+와 NiO+이온에 의한 메테인의 C-H 활성화에서 Spin-crossover 의 존재의 여부를 이론적 방법으로 연구하였다. CoO+의 Triplet 과 Quintet, NiO+의 Doublet 과 Quartet 에서의 수소이동의 포텐셜 에너지 표면을 구하고, 반응속도와 KIE 는 다차원적 터널링을 고려한 변분법적 전이상태 이론을 통해서 계산되었다.

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Theoretical Investigation of the Electronic and Optical Properties of Arylamine-based Organic Dyes as Sensitizer for Dye-sensitized Solar Cells

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군산대학교 화학과 [1]Dept. of Chemistry, Nazerbayev University

One of the most significant aspects in the development of dye-sensitized solar cells (DSSCs) is the exploration and design of various triphenylamine analogues in which the central nitrogen moiety is capable of establishing an sp2-hybridization which has shown to play an important role in assisting its charge-transfer properties. Density functional theory (DFT) and its Time-dependent counterpart for the calculation of excited states were utilized to investigate the geometry, electronic structure and UV-Vis absorption spectra of these dyes. Results show that the enhanced planarity between the phenyl rings of the donor moiety in relation with the π-conjugated bridge leads to a bathochromic shift and increase of molar extinction coefficient of the absorption spectra. Furthermore, the calculated ground-state and excited-state potentials indicated that all of the dyes have an efficient electron injection and dye-regeneration. These results suggest the potential use of these dye as sensitizer for DSSCs.

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Dicyanobenzene-based TADF(thermally activated delayed fluorescence) 물질에 대한 이론적 연구 : Carbazole의 개수와 위치에 따른 계산 결과

이경언 김동욱*

경기대학교 화학과

형광 OLEDs(Organic Light Emitting Diodes)는 엑시톤이 단일항 여기상태에서 바닥상태로 떨어지며 빛을 내는 방식을 말하는데 이는 최대내부양자효율이 25%밖에 되지 않는다. 하지만 TADF(Thermally Activated Delayed Fluorescence)는 삼중항에서 단일항으로 계간교차가 일어나게 하여 최대 100%의 내부양자효율을 이끄는 방법이다. 따라서 단일항, 삼중항 에너지 차이가 작을수록 계간교차가 일어나기 쉽기 때문에 더 좋은 내부양자효율을 가지게 되고 결과적으로 OLEDs 의 효율이 높아지게 된다. Carbazole 은 높은 삼중항 에너지와 좋은 정공 수송능력을 가져 OLEDs 의 정공수송물질로 널리 쓰이고 있다. 이 물질이 삼중항, 단일항 에너지 차이에 어떠한 영향을 미치는지 알아보기 위해 본 연구에서는 dicyanobenzene 을 기반으로 다양한 수의 carbazole 을 치환하고, 또한 4 개의 carbazole 일 경우 cyano 기를 ortho, meta, para 위치에 치환하여 이들의 단일항, 삼중항 에너지를 계산하여 보았으며 이로부터 TADF 물질들의 전자구조가 어떻게 영향을 받는지, 또 dicyanobenzene 자체의 cyano 그룹의 위치에 대한 영향도 조사하였다.

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The Measurement of Oxidation Potentials of Additives in Propylene Carbonate Electrolytes System

김성수 이경구[1,*] 곽경원[*]

중앙대학교 화학과 [1]군산대학교 화학과

Lithium-ion Batteries (LIBs) technology has been used for recent years. The oxidation potentials for LIBs are theoretically calculated by using Thermodynamic cycles that was studied and can be consistent with the experimental LSV results. In propylene carbonate system, we consider 5 additives for evaluating oxidation potentials. The calculations of oxidation potentials have 4 parts which consist of Gaseous and solvent, neutrals and cations, respectively. Only solvation energy of cations is difficult to be determined and controversial. The solvation energy of neutral additive, however, can be evaluated by GC we directly measured and Henry’s Law constant and logP ow by Minnesota database. And CBS-QB3 calculation is well understood in measuring ionization potentials in recent study.

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Single-molecule Studies of DNA Hybridization/Dehybridization Kinetics

한기림 김성근*

서울대학교 화학부

Although DNA hybridization and dehybridization are of utmost importance in molecular biology, their kinetics is too often overlooked. With their ubiquitous involvement in numerous biological processes and also due to the recent emergence of DNA nanotechnology, it is crucial to understand how DNA duplex association/dissociation rates depend on external variables. Studies in the past were mostly carried out at the ensemble level and thus were very limited since it was impossible to track single reaction trajectory. In this study, we adopted the single-molecule total internal reflection-fluorescence resonance energy transfer method to follow the forward and reverse reactions in real time and measure their kinetics during hybridization/dehybridization of DNA.

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Effect of Molecular Backbone on the Formation of Self-Assembled Monolayers of Dibutyl Diselenides and Dicyclohexyl Diselnides on Au(111)

정혜림 강훈구 박희건 한진욱 노재근*

한양대학교 화학과

Selenol-based self-assembled monolayers (SAMs) have drawn much interest in nanoscience and technology due to their superior structural and long-range order properties. We have investigated the selenol-based species having different tail group such as alicyclic and aliphatic systems by using scanning tunneling microscopy (STM), water contact angle (CA), cyclic voltammetry (CV) and reductive desorption (RD). In this study, we used dicyclohexyl diselenide (DCDSe) and dibutyl diselenide (DBDSe) having similar length. Bulky alicyclic ring and aliphatic backbone structure led different packing structure and adsorption density because of their different intermolecular interaction. Under the optimized condition of DCDSe SAMs formed at 50 ˚C for 12 h, we can obtain the high-resolution STM image of DCDSe SAMs with $(2 \times 2\sqrt{10})R27^\circ$ superstructure. Also, we have found that the concentration and deposition time strongly influence on the surface structure of DCDSe SAMs by the STM observation. Based on the results of DCDSe SAMs, we will characterize the formation and surface structure of DBDSe SAMs.

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Swing motion in the liquid ordered phase of lipid bilayers

오영훈 성봉준*

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Cellular membranes play crucial roles in biological processes such as signal transduction. There is a phase transition from a liquid disordered (Ld) to a liquid ordered (Lo) phase in single component lipid membranes. The dynamics of lipids in Lo phase lipid membrane is heterogeneous, which means that there are regions of fast and slow lipids. However, the physical origin of the heterogeneous dynamics of lipid membranes is poorly understood. Recent simulations suggested that the dynamic heterogeneity was intrinsic nature of lipids membrane because one could observe the dynamic heterogeneity even in single component lipid membranes. (Soft Matter, 2014, 10, 3036) In this work, we also investigate the transport mechanism of single component lipid membranes. Coarse-grained model lipid bilayers are constructed using the MARTINI, polarizable MARTINI, and BMW, models. All three models show similar dynamical behavior in the Ld phase although the transition temperature is model dependent. We find that the primary mode of transport in the Ld phase is the hopping of the lipid molecules. Hopping is seen in both the translational and rotational dynamics, which are correlated, i.e., the lipid molecules display a swing-like motion in the Lo phase.

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Improving potential energy surfaces in DFT: Stretched heteronuclear bonds

김민철 **Kieron Burke**[1] 심은지[*]

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Standard approximate density functional theory (DFT) calculations is known to give drastic failure in bond dissociation of heteronuclear molecules, including features like non-zero binding energy in the dissociation limit and fractional charged fragments. In this presentation, we use a recently introduced density-corrected DFT (DC-DFT) method to show that, by using more correct densities, even as simple as Hartree-Fock densities, one can get extremely accurate DFT potential energy surfaces for dissociation of heteronulear bonds. We present the potential energy surfaces of various heteronuclear diatomics using both self-consistent semilocal DFT and DC-DFT, comparing them to CCSD(T) results as reference.

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Synthesis of Zn_3P_2-Zn_3As_2 Nanowires

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Zinc phosphide (Zn_3P_2) and zinc arsenide (Zn_3As_2) belong to a unique pseudocubic tetragonal system, but their solid solution has rarely been studied. Here In this study, we synthesized composition-tuned $Zn_3(P_{1-x}As_x)_2$ NWs with different crystal structures by controlling the growth conditions during chemical vapor deposition. A first type of synthesized NWs were single-crystalline and grew uniformly along the [110] direction (in a cubic unit cell) over the entire compositional range ($0 \leq x \leq 1$) explored. The use of an indium source enabled the growth of a second type of NWs, with remarkable cubic-hexagonal polytypic twinned superlattice and bicrystalline structures. The growth direction of the Zn_3P_2 and Zn_3As_2 NWs was also switched to [111] and [112], respectively. These structural changes are attributable to the Zn-depleted indium catalytic nanoparticles which favor the growth of hexagonal phases. The formation of a solid solution at all compositions allowed the continuous tuning of the band gap (1.0-1.5 eV).

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Gallium Sulfide Selenide Ternary Alloy Nanobelts with Tunable Band Gaps

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Two-dimensional (2D) nanostructures are promising materials for next generation flexible electronic devices. Gallium sulfide selenide ($GaS_{1-x}Se_x$) ternary alloy nanosheets were synthesized by chemical vapor transport method. They exhibit a belt-type morphology (avg. thickness = 50 nm) and consisted of a mixed hexagonal/rhombohedral phases. The portion of rhombohedral phase increases with increasing x, and becomes equal to that of hexagonal phase for GaSe. Measurement of UV-visible absorption and photoluminescence (PL) show the tuned band gap of 2.0-2.5 eV that changes linearly with x. First-principles density-functional theory calculations for mono-, di-, and tri-layer GaS and GaSe predict that the band gap (indi-rect) of the GaS and GaSe monolayers is 3.33 and 3.01 eV, respectively, and the direct band is lying 0.5 and 0.01 eV above the indirect band. As the number of layers increases, the band gap decreases significantly; 2.65 and 2.20 eV for GaS and GaSe tri-layers, respectively, which are close to the experimental values. It also predicts that the hexagonal and rhombohe-dral phases have a similar band gap and the homogeneous mixing of S/Se occurs for the alloys. Furthermore, we calculate that the biaxial strain reduces the band gap significantly, and converges the indirect and direct band gaps for GaS. Photocur-rent measurements were performed on individual nanobelts by fabricating photodetector devices, suggesting that the incor-poration of rhombohedral phase induces the crystalline defects, which results in the lower photoconversion efficiency.

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Fabrication of efficient TaON and Ta3N5 photoanodes for water splitting under visible light irradiation

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호서대학교 그린에너지공학과 [1]고려대학교 소재화학과

The solar-driven photoelectrochemical splitting of water offers an attractive means of generating hydrogen fuel, which is free from environmental issues related to the combustion of fossil fuels. TaON and Ta3N5 with band gaps of 2.5 and 2.1 eV can be effectively used as novel visible photocatalysts. Herein, we developed unique synthesis method for high-yield TaON and Ta3N5 nanoparticles by combining a sol-gel method and a gas phase substitution reaction. We analyzed the electronic structure by transmission electron microscopy, electron-energy loss spectroscopy, and X-ray diffraction, and synchrotron X-ray absorption and photoelectron spectroscopy. The photoanodes for water splitting were fabricated on conducting glass support, which forms effective contacts, afforded a significant increase in the photocurrent and water splitting. The photoelectrochemical cells with these photoanodes show excellent visible-light-driven photocatalytic performance and stability for water splitting.

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Transition Metal Doping of Oxide Nanocrystals for Enhanced Electrocatalytic Oxygen EvolutionO_2

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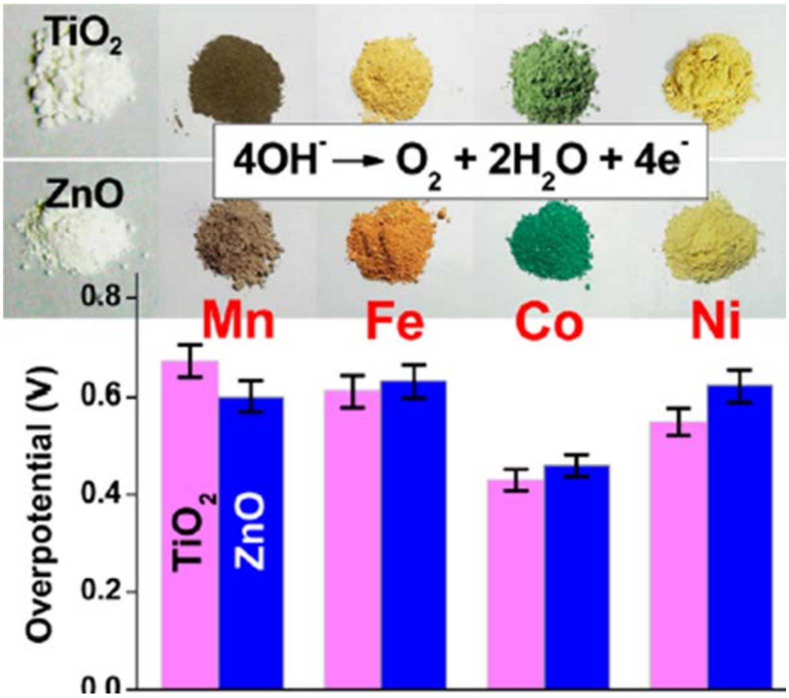
Catalysts for the oxygen reduction and evolution reactions are central to key renewable-energy technologies including fuel cells and water splitting. Despite tremendous effort, the development of oxygen electrode catalysts with high activity at low cost remains a great challenge. In this study, we report a generalized sol?gel method for the synthesis of various oxide nanocrystals (TiO_2, ZnO, Nb_2O_5, In_2O_3, SnO_2, and Ta_2O_5) with appropriate transition metal dopants for an efficient electrocatalytic oxygen evolution reaction (OER). Although TiO_2 and ZnO nanocrystals alone have little activity, all the Mn-, Fe-, Co-, and Ni-doped nanocrystals exhibit greatly enhanced OER activity. A remarkable finding is that Co dopant produces higher OER activity than the other doped metals. X-ray photoelectron and X-ray absorption spectroscopies revealed the highly oxidized metal ions that are responsible for the enhanced catalytic reactivity. The excellent OER activity of the Co-doped nanocrystals was explained by a synergistic effect in which the oxide matrix effectively guards the most active Co dopants at higher oxidation states by withdrawing the electrons from the metal dopants. The metal-doped NCs exhibit enhanced catalytic activity under visible light irradiation, suggesting their potential as efficient solar-driven OER photoelectrocatalysts.


TiO$_2$
ZnO
4OH$^-$ → O$_2$ + 2H$_2$O + 4e$^-$
Mn
Fe
Co
Ni
Overpotential (V)
0.8
0.6
0.4
0.2
0.0
TiO$_2$
ZnO

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Tin Germanium Sulfide Nanoparticles For Enhanced Performance Lithium Ion Batteries

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Germanium- or tin-based nanostructures have recently demonstrated outstanding lithium ion storage ability and are considered to be the most promising candidates to substitute current carbonaceous anodes in lithium ion batteries. Tin germanium sulfide ($Sn_xGe_{1-x}S$) ternary alloy nanocrystals (NCs) were synthesized by a gas-phase laser photolysis reaction with complete composition control ($0 \le x \le 1$). All of these composition-tuned nanocrystals showed excellent cycling performances in lithium ion batteries. Reversible capacities were in the range 800-1200 mAh/g after 70 cycles, which is close to the theoretical capacities of each composition. As the tin composition (x) was increased, the rate capability greatly enhanced, reaching a maximum at x = 0.8-0.9. This unique composition dependence of the electrochemical properties was explained by the lower charge transfer resistance due to the high conductivity of $Sn_xGe_{1-x}S$ NCs as well as Sn_xGe_{1-x} alloy NCs produced upon lithiation. Sn-rich $Sn_xGe_{1-x}S$ NCs are, therefore, promising candidates for applications in high-performance energy conversion systems.

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Synthesis of Atomatically Thin Copper Sulfide Sheets

권익선 박정희[1,*] 임형순 정찬수[1] 임영록[1] 박기동 곽인혜[1] 박충효[1] 오진영[1] 김예진[1] 서재민[1] 손창용[1] 김덕환[1]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

Atomically thin two-dimensional materials have attracted great attention in recent year owing to their intriguing properties originated from spatially confined electrons and holes within a finite thickness in 2D space. Many studies have been reported about various 2D material like transition metal dichalcogenide (TMDC). However, most of these materials have quantity and uniformity limitations since they have been synthesized via chemical vapor deposition or exfoliation. Copper sulfide is an important p-type semiconductor material with a band gap of 1.2~2 eV (bulk), depending on stoichiometric ratio, and has been the object of particular attention in photovoltaic applications. Here, we present the synthesis of atomically thin copper sulfide via solution based reaction in large quantity. These sheets have average thickness and size of 5 nm and 5 μm, respectively. Two dimensional copper sulfide can be applicable to photovoltaic cell, catalyst, thermoelectrics, gas sensor, even fabrication of 2D heterostructure.

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Ternary alloy nanocrystals of Sn and Ge Chalcogenides

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Tin (Sn) and germanium (Ge) chalcogenides have recently gained popularity as potential alternatives to the toxic lead chalcogenides, due in part to their relatively higher chemical and environmental stability, for use in photovoltaic devices. Herein, we report the synthesis of ternary composition chalcogenide, i.e., $Sn_xGe_{1-x}S$, $Sn_xGe_{1-x}Se$, GeS_xSe_{1-x}, and SnS_xSe_{1-x}, nanocrystals (NCs) by novel gas-phase laser photolysis. A full series of completely miscible alloy nanocrystals, the band gaps of which could be tuned to cover a wide range (0.9 - 1.6 eV), were obtained by facile composition tuning through adept control of the relative pressure of the precursors. Two cation alloy ($Sn_xGe_{1-x}S$ and $Sn_xGe_{1-x}Se$) NCs exhibited unique anisotropic bowing phenomena of the orthorhombic phase lattice constants, but the anion alloy (GeS_xSe_{1-x} and SnS_xSe_{1-x}) NCs did not. The cation alloy NCs showed optical bowing, which is well correlated with the bowing of the lattice parameters. The $Sn_xGe_{1-x}S$ and SnS_xSe_{1-x} NCs showed remarkably higher photoconversion efficiency in photovoltaic and photodetector devices when compared with that of end members.

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Controlled Chemical Vapor Deposition Growth of Single-Crystalline Galliun Selenide Monolayer

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Metal chalcogenide have attracted great attention owing to their two-dimensional (2-D) layer structure analogous to graphene. Gallium selenide (GaSe) is a typical layered metal monochalcogenide, which has a indirect/direct bandgap of 2.0 eV, and shows p-type semiconductor behavior. Hexagonal/rhombohedral phase GaSe has unique Se-Ga-Ga-Se layered repeating unit built by six-membered Ga_3Se_3 rings and adjacent layers are held together by van der Waals interactions. Synthesis of thin (including monolayer) layered GaSe is still challenging. Herein, we synthesized GaSe nanosheets via chemical vapor deposition method. The size, shape, and thickness of the GaSe nanosheets were controllable by growth duration, growth temperature, and gas flow rate. Large-area and single-crystalline GaSe monolayers were successfully synthesized with a thickness of 0.8 nm and a width of 30 μm. This GaSe monolayer is expect to next-generation flexible electronic and optoelectronic devices such as photodetectors and field-effect transistors.

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Optical Characteristics of $(GaP)_{1-x}(ZnS)_x$ 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 $(GaP)_{1-x}(ZnS)_x$ $(0 \le x \le 1)$ pseudobinary alloy NWs using the vapor transport method. Compositional tuning results in the phase evolution from the zinc blende (ZB) $(x < 0.4)$ to the wurtzite (WZ) phase $(x > 0.7)$. In the intermediate phase coexistence range, a core?shell structure is produced with a composition of $x = 0.4$ and 0.7 for the core and shell, respectively. The band gap (2.4?3.7 eV) increases nonlinearly with increasing x, showing a significant bowing phenomenon. The phase evolution leads to enhanced photoluminescence emission. Strikingly, the photoluminescence spectrum shows a blue-shift (70 meV for $x = 0.9$) with increasing excitation power, and a wavelength-dependent decay time. Based on the photoluminescence data, we propose a type-II pseudobinary heterojunction band structure for the single-crystalline WZ phase ZnS-rich NWs. The slight incorporation of GaP into the ZnS induces a higher photocurrent and excellent photocurrent stability, which opens up a new strategy for enhancing the performance of photodetectors.

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Morphology-Controlled Synthesis of Organometal Trihalide Perovskite Colloidal Nanocrystals

김덕환 박정희*

고려대학교 소재화학과

Organometal halide perovskites were first synthesized 1978, but have received much scientific attention after their recent introduction as a photovoltaic material with very low cost and intriguing properties. In recent years, methylammonium lead halide perovskites ($CH_3NH_3PbX_3$, X = Cl, Br, I) have attracted tremendous interest because of their outstanding photovoltaic performance, approaching a photoconversion efficiency of 19%. Previous studies have reported that these perovskites exhibit a large absorption coefficient over a broad spectral range, high charge carrier mobility, small exciton binding energy, and long exciton diffusion length. Herein, We synthesized $CH_3NH_3PbX_3$ nanocrystals with various morphologies (e.g., nanowires and nanosheets) by a novel solvothermal reaction using capping ligands. The photoluminescence spectrum of the film and solution (toluene), were monitored using a picosecond laser, in order to investigate the effects of morphology on the exciton lifetime. This exclusive strategy is an important milestone toward the broad commercialization of large-scale solution processes. High-purity, high-crystallinity thin films can be obtained by one-step drop-casting or spin-coating of a colloidal solution onto substrates, resulting in a new class of efficient optoelectronic devices.

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Metal Nanocrystal and Nitrogen-doped Graphitized Nanodiamond Hybrid for High-Efficient Electrocatalyst

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The large-scale practical application of fuel cells will be difficult to realize if the expensive platinum-based electrocatalysts cannot be replaced by other efficient, low-cost, and stable catalytic materials. Here we report the catalytic ability of metal (Pt, Pd, Ag, Au, Cu etc.) nanocrystal-N-doped graphitized onion-like nanodiamond (NC-NGND) hybrid nanostructures for oxygen reduction reaction. Metal NC-NGND hybrid nanostructures were prepared by laser-induced reduction reaction of metal precursor and nanodiamonds in solution. The NDs, transformed into the graphitized onion-like form during the reaction, were doped with the N atoms by the thermal annealing under NH_3 gas. The NC-NGND hybrid nanostructures exhibits low overpotential and selectivity for oxygen reduction reaction. The efficient performance is credited to the pyrollic-like N electronic structures of NGND that combined with the active metal NCs. This finding may lead to a new strategy to develop cost-effective electrocatalysts with superior efficiency for another electrocatalytic reactions such as hydrogen evolution reaction and CO_2 reduction reaction. In addition, rotating ring disk electrode hydrodynamic voltammetry was successfully used to determine the number of electrons underlying the high-efficiency reduction process.

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Metal Phosphide Nanowires for Hydrogen Evolution Reaction

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Production of molecular hydrogen by the electrochemical reduction of water is an important component of several developing clean-energy technologies. The hydrogen evolution reaction constitutes half of the water-splitting reaction. Currently, platinum is the best known hydrogen evolution catalyst with only small overpotentials and high reaction rates, but the scarcity and high cost may limit its widespread technological use. Recently, transition metal phosphides, including Nickel phosphide,Cobalt phosphide,and Iron phosphide, have been identified as promising hydrogen evolution reaction electrocatalysts. Herein, we synthesized vertically aligned metal phosphide nanowire arrays using chemical vapor deposition. We analyzed the morphology and structure by scanning electron microscopy, transmission electron microscopy, energy dispersive X-ray spectroscopy, and X-ray diffraction, and synchrotron X-ray absorption and photoelectron spectroscopy. Their electrocatalytic performance was tested for hydrogen evolution reaction, showing an excellent catalytic activity and stability.

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High-Yield Synthesis of Iron Nanoparticles and Their Application as Excellent Performance Electrocatalysts

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Employing a low-cost and highly efficient electrocatalyst to replace Pt-based catalysts for hydrogen evolution reaction has attracted increasing interest in renewable energy research. Herein we report the synthesis of Iron nitride that can efficiently electrocatalyze the hydrogen evolution reaction with activities close to that of Pt and function well under acidic medium. We synthesized iron(Fe) nanoparticles with high yield, using filament-assisted thermal decomposition of gas phase precursors. Iron nitride nanoparticles were synthesized by annealing of Fe nanoparticles at high temperature under a stream of NH_3. The morphology and structure of the products were analyzed by scanning electron microscopy, transmission electron microscopy, energy dispersive X-ray spectroscopy, and X-ray diffraction, and synchrotron X-ray absorption and photoelectron spectroscopy. Electrocatalytic activities of the samples were tested for hydrogen evolution reaction. Linear Sweep Voltammetry was done with scan rate of 1 mV/s from -0.2 to - 0.8 V. Iron nitride nanoparticles show excellent catalytic activity and stability in the acidic medium and serve as a promising new class of non-noble metal catalysts for practical hydrogen evolution reaction .

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Real-time observation of nanoparticles' behavior after endosome escape

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Upconverting nanoparticles (UCNPs) is an ideal optical probe for long-time particle tracking and imaging because UCNPs do not photobleach and photoblink. UCNPs absorb 980-nm near infrared photons which do not damage organelles and emit visible light by upconversion process. In most cases, it is well known that sub-100-nm sized nanoparticles interacting with cells follow endocytic pathway. We made UCNPs-Chlorine e6 (Ce6) complex which shows quenching of UCNP luminescence by energy transfer to Ce6. Subsequently, Ce6 generates reactive oxygen species (ROS) inducing endosome escape of UCNPs. We imaged such escape in real time by 980-nm excitation.

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Theoretical studies for the hydrogen binding to the Fullerenes doped transition metal

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탄소 60 개로 이루어진 Fullerene 이 발견된 이후, 다양한 분야에서 Fullerene 을 이용한 연구가 많이 진행되어 왔다. 특히, Fullerene 뿐만 아니라 Graphene, Carbon nanotube(CNT) 와 같은 탄소물질들을 이용하여 에너지 저장과 수소흡착에 대한 연구가 많이 이루어지고 있다.전이금속은 탄소물질의 수소흡착에 대한 능력을 증가시킨다는 점에서 착안하여, 본 연구에서는 전이금속(Ni, Pd, Pt)이 도핑된 fullerene 의 곡률에 따른 수소 분자와의 Binding energy 의 경향성을 알아내고자 하였으며, 곡률의 척도로는 전이금속이 도핑된 탄소의 Pyramidalization angle 을 선택하였다. Fullerene 은 Cn(n=탄소수, 20,26,30,36,60,70,84)에 따라 연구하였으며 Density functional theory 를 통하여 Binding energy 를 계산하였다. 그 결과, Pyramidalization angle 이 커질수록 Binding energy 가 작아지는 것을 확인하였으며 또한, 수소분자가 흡착하는 방향이 수직이 될 때, Palladium 이 도핑된 Fullerene 의 경우일 때, Binding energy 가 작아짐을 확인하였다.

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DC-ToF 비탄성 중성자 산란장치 개발 및 분자 동역학 연구에의 활용

소지용

한국원자력연구원 중성자과학부

비행시간 분광법 중성자 분광 장치는 중성자와 물질간의 준탄성 산란(quasielastic neutron scattering-QENS)과 비탄성 산란 (inelastic neutron scattering-INS)을 측정하여 물질의 동역학을 연구하도록 해 주는 실험 방법이다. 냉중성자를 이용한 비행시간 분광법 산란장치를 이용하여 준탄성 산란 및 비탄성 산란을 측정하면 수십 ueV 에서 수십 meV 까지의 에너지 영역에서 일어나는 동역학을 측정 할 수 있다. 비행시간 분광법 중성자 분광 장치는 다양한 상태 및 물성을 가진 물질의 동역학을 측정하는데 전 세계적으로 널리 이용되고 왔으며 분자의 diffusional/relaxational/rotational dynamics 와 magetism 을 연구하는데 중요한 기여를 해 왔다. DC-ToF 는 국내 유일의 연구용 원자로인 하나로의 냉중성자 가이드홀에 건설된 비행시간 분광법 산란 장치로서 2012 년 처음 입사 빔을 측정 한 이후 다양한 시험을 거쳐 장치의 건전성을 확인하으며 지속적인 성능 개선을 통해 충분히 경쟁력이 있는 성능을 보였다. 본 발표를 통해 DC-ToF 산란장치의 현황 및 시험 측정 결과 보여주며 다양한 물질의 동역학 연구에 이용될 수 있는 예를 제시한다.

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Efficient perovskite solar cells using blends of polymer/small molecule as hole transporting materials

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서울대학교 화학부

Perovskite(ABX_3) materials have recently attracted considerable interest due to its great optical and electronic properties. Thin film solar cells based on these materials promise to exceed the power conversion efficiency (PCE) of single-crystalline silicon. For developing efficient perovskite solar cells, many scientists have tested various hole transporting materials (HTMs) in order to find the most effective HTM. Among those HTMs, spiro-OMeTAD has a proper HOMO level for efficient charge transfer from perovskite to spiro-OMeTAD and has mostly been used as a HTM for perovskite solar cells. However, there are still possibilities of efficiency improvements by using different HTMs that have higher hole mobility than spiro-OMeTAD. In this study, we report efficient perovskite solar cells using blends of polymer/small molecule as HTMs.

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Theoretical Study for Multiple Proton Transfer in Calix[4]arene and Tetra Alcohol Cluster Systems

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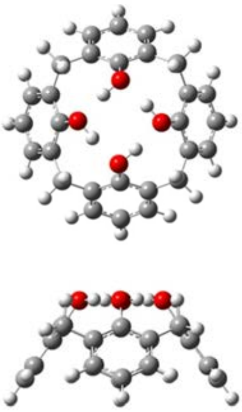
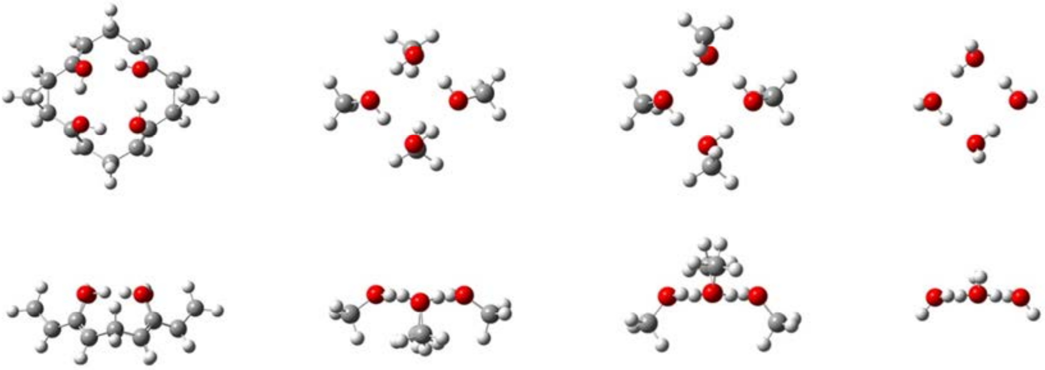
Multiple proton transfer plays an important role to many chemical and biological reactions. Calixarene, which has a possibility of being used in lots of industrial projects like developing cancer vaccines, chemical sensors, and high resolution electron beam lithography, experiences internal multiple proton transfer as well. In this study, we generated potential energy surfaces of quadrupole proton transfer in Calix[4]arene, tetra water cluster, and tetra methanol cluster, and calculated rate constants, tunneling effects, and KIE by variational transition-state theory including multidimensional tunneling. We found that four protons are transferred by jump mechanism. Interestingly, KIE in all the systems are small because the tunneling effect of deuterium is larger than that of hydrogen. This poster presents the reason for this very unusual observation.

Calix[4]arene



Tetra alcohol cluster



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Structural aspect of imogolite in gel matrix by deformation

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Nanocomposite materials has been developed to confer high performed mechanical property, and one of the efforts is preparation of hydrogel including iorganic particles. In this research, the gamma-ray irradiated imogolite-acrylic acid hydrogel was investigated with small angle X-ray scattering (SAXS) and small angle neutron scattering (SANS) in terms of particle concentration and deformation. SAXS and SANS were performed to probe the polymer contrast matched system and the ternary system, respectively. The SAXS analysis results present polymer dominant elongation, particle orientation and elongation of inter-particle distance as structural response against the external deformation. The neutron scattering analysis also supports the elongation of internal structure through the increase in correlation length of inhomogeneity of the system according to the magnitude of deformation.

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Photo-redox reaction between single-walled carbon nanotubes and surfactant

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When substances absorb light and reach high energy state, many reactions occurred such as photosynthesis, synthesis or changes of substrates, which are called photochemical reactions. Especially, photocatalysts such as Titanium oxide (TiO2) influence the reaction rate when they are exposed to light. Compare to other catalysts, photocatalysts have significant advantages such as room temperature reaction, controllability via light dose, and environmental benignity. Here we studied intimate redox relay between single-walled carbon nanotubes (SWNTs) and flavin mono-nucleotides (FMN) wrapping around them with possibility as photocatalysts. When aqueous FMN-SWNTs dispersion is exposed to 445-nm light in aerobic or anaerobic conditions, different oxygen-mediated photoredox reactions (Equation 1) can be observed with various tools such as photoluminescence and UV-VIS-NIR spectroscopy. nFMN + SWNT + nH2O ? nFMNH2 + SWNT2n+ + 1/2n O2(1)In anaerobic condition, when FMN is irradiated with 445 nm light, SWNTs lose electrons and are oxidized while FMN is photo-reduced to fully-reduced form, FMNH2. This is partially reversible after the introduction of molecular oxygen. In aerobic conditions, on the other hand, reduced FMN only exists when light is on and is easily oxidized with help of oxygen. Also, FMN is photodegraded and this causes that reduced FMN cannot completely oxidized as anaerobic condition. We speculate such photoredox relay in terms of energy diagram between SWNT and FMN in the presence or absence of oxygen.

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Coverage-Dependent Adsorption Selectivity of Leucine and Tyrosine Adsorbed on Cu(110) Surface

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The coverage dependent adsorption selectivity of leucine and tyrosine molecules adsorbed on the Cu(110) surface was investigated and compared to obtain the bonding configuration and stable adsorption structures at two distinct coverage (lower and higher) using density functional theory (DFT) calculations and their corresponding high-resolution photoemission spectroscopy (HRPES). We figured out that “O-H dissociation bonded structure” is the most stable structure of the Leucine on Cu(110), and “O-H dissociated and N-dative bonded structure” is the most stable structure of the Tyrosine on Cu(110) using DFT calculations. In addition, from HRPES results, we found that at lower coverage level (~0.20 ML), the Leucine on Cu(110) system shows “O-H dissociation bonded structure” whereas Tyrosine on Cu(110) system shows “O-H dissociated and N-dative bonded structure”. On the other hand, at higher coverage adsorption, we found the opposite result for the adsorption structures of two systems that the Leucine on Cu(110) system shows “O-H dissociated and N-dative bonded structure” whereas Tyrosine on Cu(110) system shows “O-H dissociation bonded structure”. This is consistent with the DFT calculation results that such adsorption geometry has the most stable adsorption energies at each coverage.

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Investigation of the interaction between novel unnatural chiral ligand and substrate on palladium for heterogeneous asymmetric hydrogenation

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The new chiral ligand 1 and substrate 2 (α, β-unsaturated acid) were synthesized and validated for their interaction in heterogeneous asymmetric hydrogenation with palladium catalysts in solution as well as in UHV conditions. First, NMR study identified the interaction both molecules with palladium nanoparticles in solution, and then STM with HRPES studies showed the adsorption geometry, spatial distributions and electronic structures on palladium metal surface in UHV conditions. Moreover, DFT calculations exhibited comparable to experimental results their reaction mechanism analogues. According to the results, these studies provide the broad scope of reaction and demonstrate detailed the mechanism of asymmetric hydrogenation.

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Liquid Exfoliation of Two-Dimensional 2H-Molybdenium Disulfide Using Covalent Surfactant

정미순 주상용*

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Two-dimensional transition metal dicharcogenides (TMC) such as molybdenum disulfide (MoS2) has outstanding optical, chemical, and electronic properties for various optoelectronic applications. MoS2 has two polymorphisms: metallic 1T and semiconducting 2H phases. Especially, 2H MoS2 upon either chemical and mechanical exfoliation methods exhibits strong direct-bandgap photoluminescence (PL) which is useful for photodetector and sensor applications. Up to date, chemical exfoliation useful for broadening applications includes Li intercalation, non-covalent and covalent chemical approaches. Especially, Li intercalation results in metallic 1T-phase MoS2 due to one electron addition to TMC lattice, which necessitates additional phase transformation process to 2H phase. Here, we present that chemical exfoliation method produces 2H-polytype of MoS2 having PL. Facile and scalable liquid exfoliation using covalent functionalization utilizes covalent replacement to chalcogen atoms of the TMC. Exfoliated few-layered MoS2 were characterized using solution- and solid state-based methodologies. The structure and chemical identity were confirmed by fluorescence. X-ray (XRD), Fourier-transform Infrared (FT-IR) spectroscopies, demonstrating covalent bonding between functional surfactant and chalcogen atoms. Exfoliation using functionalization is more convenient way to make few-layered MoS2.

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Effect of stochastic reactivity switch on the fluctuation dynamics of the product counts in the birth-death process

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Reaction networks in living cells are often regulated by stochastic reactivity switch. However, still missing is the general understanding of how the stochastic reactivity fluctuation of an intracellular reaction network affects the dynamics of the product number statistics. In this study, we propose the time correlation function of the product number as an experimental observable and establish the quantitative relationship between the experimental observable and the dynamics of the stochastic reactivity switch by considering a general reaction network model. The theoretical result enables one to extract microscopic information about the reactivity fluctuation, which is often beyond direct observation, from the time correlation function of the product number. Correctness of the obtained result is confirmed by an accurate stochastic simulation. On the basis of the obtained results, we discuss physiological consequences of the stochastic reactivity switch.

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Individualized Single-Walled Carbon Nanotube Assembly Using Functional Self-Assembled Monolayer for Facile Field-Effect Transistor

장명수 김소민 주상용*

연세대학교 화학과

Transistor based on single-walled carbon nanotube (SWNTs) has drawn a lot of attention owing to its high performance such as high current on/off ratio and excellent electrical conductivity. However, as-synthesized SWNTs typically contain both metallic and semiconducting tubes and, thus, additional elimination or separation steps to remove metallic tubes are necessary for SWNTs transistor manufacturing. Complex process including the aforementioned separation, selective assembly on a substrate is obstacle for various device applications. Here, we propose simple, highly-efficient one-step method for individualized SWNTs assembly using functional self-assembly monolayer (SAM) method. Acetylene-terminated flavin (FC6), SWNT-interacting moiety, is introduced into a silane-terminated hydrocarbon chain via simple click chemistry for SAM. By dipping the SAM-containing substrate in sonicating SWNTs dispersion, individualized SWNT trapping on SAM occur spontaneously. SWNTs trapped by SAM form uniform and randomly-oriented network arrangement, suitable for device array fabrication. SWNTs network are confirmed by AFM and UV-vis-NIR spectrometry.

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Application of cross polarization-single pulse to solid-state 13C NMR characterization of some natural organic matters

오세웅

목포대학교 화학과

C-13 ramped-CPMAS (Cross Polarization under Magic Angle Spinning) NMR represents the most powerful experimental approach to collect information on the structural and conformational characteristics of natural organic matter. Recently Simpson et al (Geoderma 226-227, 405-414, 2014) published an improved technique, so called ramped-CPSP (Cross Polarization Single Pulse) under magic angle spinning, which can bring considerable advantages but does not have associated drawbacks. In this work, this new technique is applied to some different natural organic matters such as plant and soil samples, and the results obtained from two techniques are examined using a 9.4 T NMR spectrometer.

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Conformations of an Isolated β-amino acid: Double-resonance Spectroscopy of Laser-desorbed L-β-homotryptophan

김정진

아주대학교 화학과

L-β-homotryptophan (HTrp) is a β-amino acid with one more methyl group than tryptophan (Trp) between the asymmetric carbon and the carboxylic group. HTrp was found to have UV absorption in the same region as Trp but showed quite different vibronic progressions, suggesting different Franck-Condon activity and/or different distribution of conformers than Trp. To find out the effect of a more flexible backbone on the structure of amino acids with the same indole chromophore, conformations of isolated HTrp was investigated by UV-UV hole-burning (HB) spectroscopy and quantum mechanical calculation. 14 conformers were found by UV-UV HB spectroscopy and quantum chemical computation at M05-2X/6-31G** level suggests there are 15 conformations below 6 kJ/mol, while Trp has 6 conformers at a similar experimental condition. Further structural assignments are underway to reveal the intramolecular hydrogen-bonding pattern of each conformer with the aid of a conformer-specific vibrational spectrum by IR-UV double resonance spectroscopy.

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Raman Study of the Effect of Residual Polymer on Chemical Vapor Grown Graphene

구은혜 주상용*

연세대학교 화학과

As transferring chemical vapor deposition (CVD) grown graphene on arbitrary substrate, various polymers are generally used which inevitably leave residual layers on graphene. In spite of its importance, the role of residual polymers is not well-known. In this study, we report the effect of residual poly (methyl methacrylate) (PMMA) on CVD grown hexagonal graphene grain via Raman spectroscopy. As a result of analyzing bare-, PMMA-covered supported and PMMA-covered suspended graphene, the positions of G and 2D bands are gradually downshifted in that order. It displays residual PMMA on graphene exports compressive strain maintaining its doping level. In addition, residual PMMA has a dominant effect on CVD grown graphene as compared to substrate.

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Unraveling Reaction Intermediates in Proton Transfer of Strong Photoacids in Alcohols

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기초과학연구원 첨단연성물질연구단 [1]울산과학기술대학교(UNIST) 화학과 [2]울산과학기술대학교(UNIST) 자연과학부 화학과

In general, chemical reactions are considered to be ones between molecules. However, in aqueous solutions, water molecules get together via extensive hydrogen (H)-bonded networks to form clusters, and the water cluster usually behaves as a molecule resulting in unique chemical reactivity of water especially in acid-base reactions. While three-dimensionally H-bonded networks form in water, linear H-bonded networks form in alcohols. In this study, we have revealed the three-step mechanism of acid-base reactions, using a strong photoacid of N-methyl-7-hydroxyquinolinium iodide and weak bases of alcohols. We have investigated the dynamics of excited-state proton migration through H-bonded alcohol networks in acid-base reactions with variation of alcohols having different basicity and polarity. From time-resolved measurements, we have found out that exited-state equilibrium between the cationic photoacid and its neutral conjugate base is established and that transient intermediate species form during proton dissociation from the photoacid to a base alcohol. At the first step, the proton of the photoacid transfers to an adjacent H-bonded alcohol molecule, and the protonated alcohol molecule forms a contact pair (tight encounter complex) with the conjugate base of the photoacid by H-bonding; the re-protonation of the conjugate base, as the back reaction of the first step, also takes place. In succession, another adjacent alcohol molecule stabilizes the protonated alcohol molecule by forming a dimer via H-bonding, and then, the protonated alcohol dimer and the neutral conjugate base of the photoacid form a loose encounter complex. Finally, proton migration through H-bonded alcohol networks takes place to scavenge the proton, resulting in the separation of the loose complex to complete the acid-base reaction.

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Continuous time random walk coupled to dynamically heterogeneous environment

송상근 김지현* 성재영*

중앙대학교 화학과

We investigated a nonrenewal continuous time random walk (CTRW) model describing stochastic transport in dynamically disordered media. The two major statistical parameters, mean square displacement (MSD) of a random walker and non-Gaussian parameter (NGP) of the displacement, could be identified once we know statistical properties about jump event counting statistics (JECS). To confirm the relationship between JECS and CTRW, we performed nonrenewal CTRW simulations, where each jump process accompanies multiple internal transitions coupled to dynamic environment. Theoretical and stochastic simulation results are in excellent agreement with each other. The statistical properties of displacement characterized by MSD and NGP are modulated by the inverse relaxation time scale λ of environmental process and the number of multiple internal transitions, l. MSD initially shows the super-diffusive behavior ($\sim t^l$) and approaches the normal diffusion ($\sim t$) as time flows beyond the mean jump time. In contrast to the renewal counterpart whose NGP indicates near-Gaussian distribution of displacement at long times such that MSD is seemingly Fickian, NGP of the current non-renewal CTRW shows a substantial non-Gaussian feature that persists over quite a long time for slow environmental relaxation, though it finally reaches zero in the long-time limit.

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Consistent description of fluctuation of turnover times in single-enzyme reaction kinetics

정인춘 김대현 송상근 김지현* 성재영*

중앙대학교 화학과

Enzyme is an extremely important molecular machine because of its role as catalyst. Enzymatic reaction kinetics has been studied decades ago, and the well-known way to describe the activity of enzyme is the Michaelis-Menten mechanism. However, the Michaelis-Menten equation could not explain the fluctuation of enzymatic turnover times observed with advanced experimental techniques, while it still could be used for mean turnover time. In order to overcome its shortcoming, the static disorder was introduced to the Michaelis-Menten equation for explaining the turnover time distributions at several substrate concentrations. However, it fails to explain the randomness of turnover times. It was recently reported that the non-Poisson renewal description of the Michaelis-Menten mechanism could provide an excellent quantitative interpretation of the turnover time randomness. on the basis of the non-Poisson renewal theory, we show that a super-Poisson distribution for lifetime of enzyme-substrate complex can provide a quantitative and consistent explanation of mean and randomness of turnover times, and even turnover time disributions at several substrate concentrations within the limit of the renewal theory.

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Optimized expression, purification and structural analysis of human transmembrane proteins

김지선 김용애*

한국외국어대학교 화학과

Human transmembrane proteins (hTMPs) are closely linked to diverse cellular functions such as transport, channel formation, signaling and cell to cell interaction, so they are assume to be crucial therapeutic targets. In order to study the structure and function of these hTMPs, it is important to prepare reasonable amounts of proteins. However their preparation is seriously difficult and time-consuming due to their relatively hydrophobic surface, absence of stability, flexibility. We tried to produce large amounts of human amyloid-β (hAβ) that is related to the dementia and human melanocortin-4 receptor (hMC4R) that is related to the severe early onset obesity. The hAβ transmembrane protein shows that the nonfibrillar hAβs form the Ca2+-permeable ion channel in the cell membrane and these channels would enable disrupt the normal cellular calcium homeostasis. It plays a central role in pathogenesis of dementia and Alzheimer disease. The hMC4R is critical regulator of energy homeostasis like the energy intake and expenditure. Heterozygous mutation D90N located in second transmembrane domain of hMC4R results in human obesity, hyperphagia and insulin resistance. In this research, we succeed to produce the transmembrane domain of the hAβ and second trans-membrane domain both of the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). To assess the structural characterizations of these proteins in the membrane-like environments, we were obtained enough quantities of proteins by using a recombinant DNA technologies and highly purified proteins were applied to a few analysis techniques like PAGE, CD, MASS, solution and solid-state NMR spectroscopy. In addition, we could get 1H-15N 1D, 2D SAMMY and SMAPI spectra using home-built solid-state NMR probe.

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Excited State Proton Transfer Dynamics of Coumarin 183 in solvents

정준영 이치호 이주형 박성남*

고려대학교 화학과

Coumarin 183 (C183) is a model compound of the active site of Δ^5-3-ketosteroid isomerase (KSI) which is important in isomerization of 3-oxo-Δ^5-srteroids to their Δ^4-conjugated isomers because C183 mimics the change in charge density like a substrate in catalytic site of KSI by photoexcitation. C183 is known as a photoacid that its pKa changes from ~7 to ~2 when C183 is electronically excited. In this work, we have studied the excited-state proton transfer of C183 in chloroform, ethanol, and water by using a picosecond time-correlated single photon counting (TCSPC) method. It was found that the proton transfer did not occur in chloroform while it occurred in ethanol and water. Time-resolved spectra obtained from the TCSPC method was analyzed with different kinetic models by using global fitting method that allowed us to extract the proton transfer rate constants of excited state C183 in different solvents. The reversible reaction model of the proton transfer between acidic and basic states of excited C183 was found to be more reliable than the irreversible model. The proton transfer rate constants were determined to be 0.28 and 3.30 ns-1 for ethanol and water, respectively. The proton transfer rate constants were found to be mainly dependent on the dielectric constant of solvents.

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Optimization of expression, purification and Structural investigation of syndecan-4

김태형 김용애*

한국외국어대학교 화학과

Syndecans as cell surface receptors participate in biologically important cell-cell and cell-matrix interactions. The syndecan protein family has four members. One of them, syndecan-4 is a transmembrane heparin sulfate proteoglycan (HSPG) belonging to the syndecan family and they has more widespread distribution than other syndecans on most cell types. They may affect extracellular matrix, anticoagulants, and growth-factors as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4 (Syd4) consists of 25 hydrophobic amino acids and has dimer or oligomer formation to perform crucial for transduction of signals. However, a lot of efforts to elucidate the structure and function of syndecan-4 have been hindered by insufficient yields and low solubility. Thus, we demonstrated an optimized method for recombinant expression and purification of syndecan-4 (Syd4). The three types of Syd4 that are wild type Syd4-TM (wSyd4), mutant Syd4-TM (mSyd4), and Syd4-eTC were investigated in our research. The mSyd4 has a partially modified sequence of Syd4-TM and Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of syndecan-4. All peptides were released from the fusion protein, and then purified by semi-preparative reversed-phase HPLC. Enough amounts of purified Syd4 analogous (wSyd4-TM, mSyd4-TM, Syd4-eTC) for the analysis of peptides was obtained from 1L of M9 minimal media under optimal conditions. Their biophysical properties of peptides were studied by circular dichroism (CD), mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy. Analysis of CD spectra presents that all types of Syd4 analogous adopt a stable α-helical structure in micelle environments. The solution NMR studies show wSyd4 and Syd4-eTC form an asymmetric dimer in micelles and mSyd4 present monomer. Optimized structure of Syd4 based on 2D SAMPI4 Solid state NMR investigates Molecular Dynamics Simulation.

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The synthesis of CdSe@ZnS quantum dots using the hydrolysis of soybean-oil

이희재 이성훈*

서울대학교 화학부

Quantum dots(QDs) have received great attention for the past 20 years because of their unique electrical and optical properties. Because of their excellent luminescent properties, QDs are of great interest in various applications, such as light-emitting diodes, lasers, biological fluorescent tags. Especially in the case of CdSe@ZnS (core@shell), the single-step synthesis approach has become generally known as the synthesis of highly luminescent quantum dots. Although CdSe is a extensively-known material in hot-injection synthesis of quantum dots, only a few studies are reported for the manufacturing quantum dots using eco-friendly solvent and surface ligands. So, in this work, We presented the highly luminescent blue, green, red CdSe@ZnS using hydrolysis of the soybean oil as eco-friendly solvent and surface ligands, instead of any artificially materials like ODE and Oleic acid. The soybean oil(mainly composed by triglycerides) consists largely of unsaturated fatty acids like linolenic acids, linoleic acids and oleic acids. The fatty acid ligands with long hydrocarbon chains play a vital role in encapsulating the CdSe core as surfactants. Those fatty acids are produced by hydrolysis of soybean oil at high temperature and high pressure with a little alkaline water, called saponification. So, the adjustment of the hydrolysis conditions could easily change the ratio of the fatty acids and be able to tune the size of quantum dots too. Finally, a wide range of emission wavelengths(453-623nm) with a narrow fwhm(

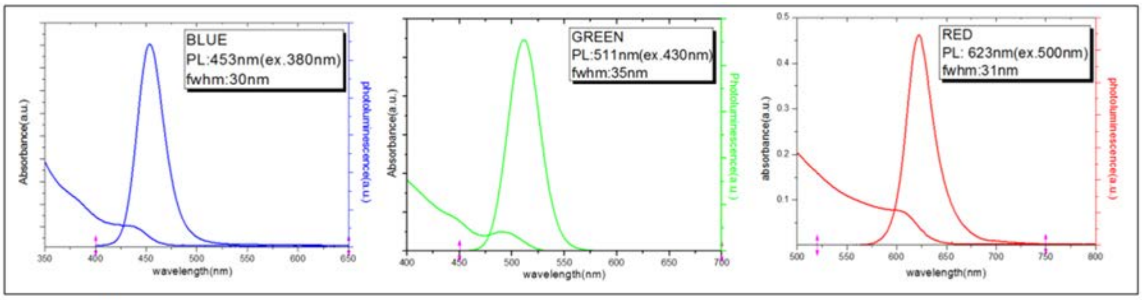

Figure. Absorption and photoluminescence of CdSe@ZnS(core@shell) quantum dots

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Charge Transfer Rates in Nanocrystal Arrays

최완 심은지*

연세대학교 화학과

We investigate charge transfer rates in nanocrystal arrays with respect to the properties of composing quantum dots and capping molecules. For the successful applications of semiconductor nanocrystal arrays, it is important to develop materials with the high carrier mobility. By examining nanocrystal arrays with the size-dependent coupling energies and activation energies, we found that the conflict between the electronic coupling and the charging energy produces the non-monotonic size-dependent trend of carrier mobility that was reported in experiments. We calculated time-evolution of the density matrix using the on-the-fly filtered propagator functional path integral method, which is then used to extract charge transfer rates as well as the carrier mobility. We constructed a simple formula based on path integral calculations and compared the formula with existing theories that were formulated for bulk systems and with experimental measurements. We also discuss various factors that define the crossover nanocrystal diameter where the carrier mobility reaches its maximum.

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Topology of [32]Heptaphyrin: H?ckel vs. M?bius

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We investigate H?ckel and M?bius topology preferences of [32]heptaphyrin in various solvents and temperatures using molecular dynamics simulations. Unlike the H?ckel's rule, molecules have unstable anti-aromatic character if it has [4n] π electron system. However, [4n] π molecule also can be stable by changing their topology as twisted M?bius [4n] aromatic conformation. To study the stability and the preference of the conformation, we introduce a simple definition of the degree of planarity. In an expanded and planar conformational porphyrin molecule, π-electron delocalization readily occurs among p-orbitals leading to stabilization of the molecule. Therefore, higher the degree of planarity, more stabilized, and preferred, the conformation. We performed molecular dynamics simulations for each structure of H?ckel and M?bius [32]heptaphyrin at various solvents and temperatures. In non-polar solvents, like toluene, the H?ckel conformation indeed has the higher planarity than that of the M?bius topology agreeing with the experimental observations that [32]heptaphyrin prefers H?ckel topology in non-polar solvents. As the temperature decreases, the M?bius topology molecule has the higher planarity than that of H?ckel conformation, which also agrees with the experimental findings. Such agreement suggests that simple molecular dynamics simulations using CHARMM force field is simple yet sufficient to model and study the stability and topology of π-conjugated expanded molecules.

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Synthesis of stable dispersion of ZnO quantum dots in aqueous solution

김재욱 유정열 김종규* 이동혁 이유로 정상화 장연재

단국대학교 화학과

Aqueous dispersion of >10nm size stable ZnO quantum dots exhibiting luminescence in the visible region have been used as capping agent to control the particle size as well as to achieve uniform dispersion of QDs in aqueous medium. X-ray diffractometer (XRD) analysis reveals formation phase pure ZnO particles having wurzite (hexagonal) structure. field emission scanning microscope (Fe-SEM) images show that the particles are spherical in shape, having average crystalline sizes 4, 5.5 and 8 nm for samples prepared at pH values of 10, 12 and 14, respectively. From the optical absorption studies, the band gap energy of QDs is found to be blue shifted as compared to bulk ZnO (3.36 eV) due to the quantum confinement effect and is consistent with the band gap calculated by using effective-mass approximation model. The photoluminescence (PL) observed in these QDs has been attributed to the presence of defect centers.

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Ordered dispersion of ZnO quantum dots in SiO2 matrix and its strong emission properties

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단국대학교 화학과

ZnO nanoparticles in the form of quantum dots (QDs) have been dispersed in SiO2 matrix to form ZnO QDs-SiO2 nanocomposites. Addition of tetraethyl orthosilicate (TEOS) to an ethanolic solution of ZnO nanoparticles produces random dispersion. On the other hand, addition of ZnO nanopar- ticles to an already hydrolyzed ethanolic TEOS solution results in a chain-like ordered dispersion. The photoluminescence spectra of the as-grown nanocomposites show strong emission in the ultraviolet region. When annealed at higher temperature, depending on the sample type, these show strong red or white emission. Interestingly, when the excitation is removed, the orderly dispersed ZnO QDs-SiO2 composite shows a very bright blue fluorescence visible by naked eyes for few seconds indicating their promise for display applications. The emission property has been explained in the light of structure-property relationship.

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Fabrication of perovskite solar cell based on self-organized regular arrays TiO_2 nanotubes

이경섭 이성훈*

서울대학교 화학부

Solar cells have been in the spotlight because of depletion of fossil fuel and environmental problems. A lot of solar cell types have been studied such as CdTe, Silicon, CIGS but especially perovskite solar cell has recieved a great deal of attention. Absorption coefficient of lead organohalide perovskite has 10 times higher than that of ruthenium-based dyes and the band gap of the material is 1.5eV so it can absorb near-infrared region. Moreover, fabrication process is easy and not expensive. Compared to the other solar cells, Perovskite solar cell has excellent efficiency with low fabrication cost. For improving efficiency, various approaches is in progress. one of the things to improve efficiency is surface area. TiO_2 is one of the semiconductor materials used as electrode in the solar cell and has various shapes such as nanotube, nanorod, nanoparticle, nanowire. The nanoparticle shape is generally used due to high surface area and easy fabrication. Therefore, more perovskite materials are adsorbed on the TiO_2 surface and it can absorb much solar energy. However, There are limitations about fabrication of thick nanoparticle layers for more surface area. Nanoparticle layers are fabricated by spin coating process and micrometer thickness is impossible with spin coater. In case of nanotubes, TiO_2 nanotubes have more surface area due to no limitation of thickness within micrometer scale and have the exact path of electrons compared to the TiO_2 nanoparticle. Here, we report fabrication of the perovskite solar cell based on TiO_2 nanotubes.

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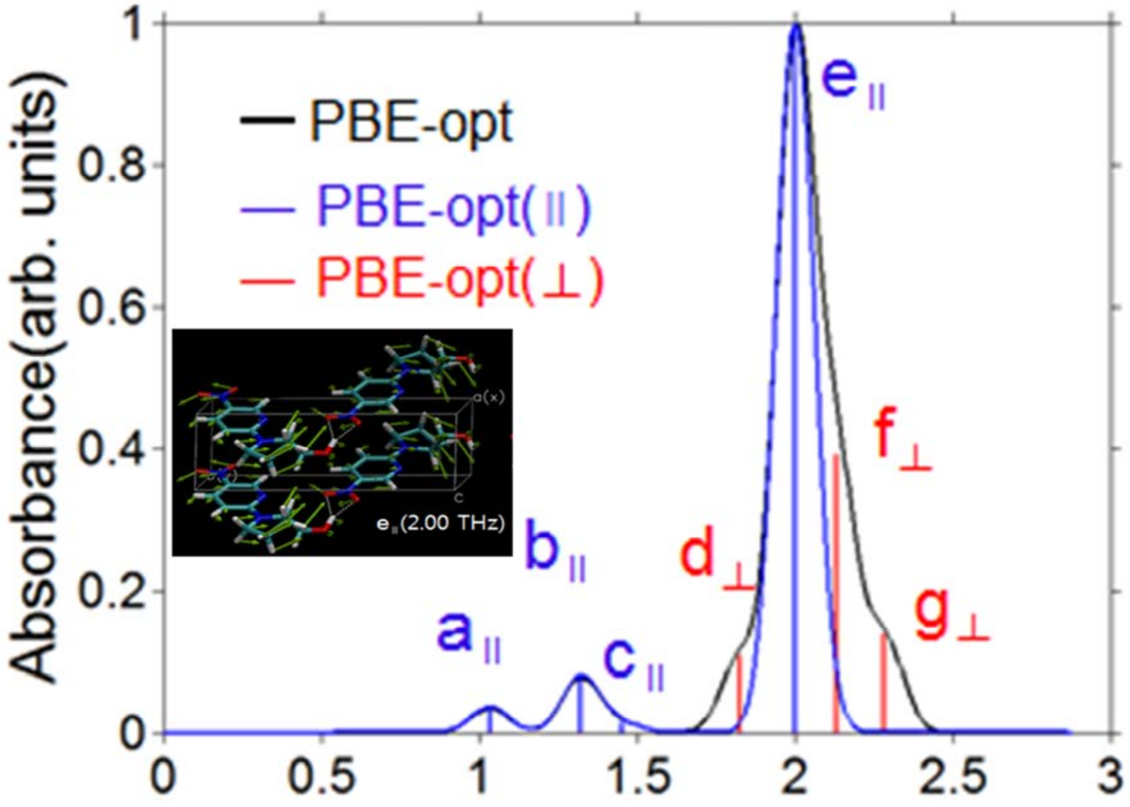
First-Principles Calculation of THz Absorption of PNP crystal

김종택 권오필[1,*]

공군사관학교 교수부 [1]아주대학교 분자과학기술학과

We investigate theoretically the phonon modes of organic electro-optic crystal, PNP. THz phonon modes significantly influence the characteristics of THz wave generation and detection. The electro-optic 2-(N-prolinol)-5-nitropyridine (PNP) molecular crystal containing a relatively small numbers of atoms in the unit cell is chosen for phonon mode calculation. THz phonon modes with its frequency and intensity are calculated by periodic density functional theory and the resulting spectrum exhibits a good agreement with the experimental spectrum measured by THz time-domain spectroscopy. Therefore, the phonon mode identification is very important for optimizing and designing new THz source and detection materials as well as THz spectroscopy


Absorbance(arb. units)
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5
3
PBE-opt
PBE-opt(∥)
PBE-opt(⊥)
$a_{\parallel}$
$b_{\parallel}$
$c_{\parallel}$
$d_{\perp}$
$e_{\parallel}$
$f_{\perp}$
$g_{\perp}$
a(x)
c
$e_{\parallel}$(2.00 THz)

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Programmed Transformation from 2D into Higher-Order Architectures: Role of Internal Phase of Self-Assembled Sheets

한민우 심은지*

연세대학교 화학과

We investigate the relationship between the internal phase of sheets and the formation of higher-order structures. In particular, we focus on the self-assembly of rod-coil molecules to two-dimensional structures and their spontaneous transformation into higher-order architectures through the Frustrated Aggregate Internal Rearrangement (FAIR) mechanism.[J. Phys. Chem. B 2013, 117, 7763] The FAIR mechanism plays a crucial role for systems with slow internal phase transition rates which often caused by non-covalent molecular interactions such as pi-pi interactions, directional dipole-dipole attractions including hydrogen bonding, and entropic coil-coil repulsion. Previously, we reported that the sheet anisotropy driven by the internal phase induces transformation into higher-order architectures including tubules, curved layers, and various shapes of micelles. Here, we demonstrate that the specific internal phase with a maximum frustration can be attained by controlling the balance between the coil-coil repulsion and rod rigidity. The internal transition rate measured through the time-evolution of the number of intermolecular bonds shows that the semi-flexible rods give rise to the slowest internal phase transition.

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Direction-controlled chemical doping for reversible G-Phonon mixing in ABC trilayer graphene

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이중층 그래핀(graphene)의 한쪽 표면에 전하를 주입하면 반전 대칭(inversion symmetry)이 깨지며 라만-비활성 진동모드가 활성화되면서 라만 G 봉우리가 G^-, G^+ 봉우리로 갈라진다고 알려져 있다. 삼중층 그래핀은 그래핀이 적층되는 방식에 따라 ABA(Bernal), ABC(rhombohedral) 그래핀으로 나뉘며, ABC 그래핀은 ABA 와는 달리 반전 대칭성을 가지고 있다. 본 연구에서는 화학적인 방법을 이용하여 ABC 그래핀의 반전 대칭을 제어하고 그에 따른 라만 스펙트럼의 변화를 탐구하였다. ABA 그래핀과는 달리 이중층 그래핀과 ABC 그래핀에서는 저진공 열처리 또는 요오드 흡착반응을 한 후에 G 봉우리가 갈라지는 것을 관찰하였고, 전하밀도가 증가 할수록 G^-, G^+ 봉우리의 위치 차이는 증가하는 것을 관찰하였다. 물과 메탄올에 의한 세척 반응으로부터 열처리는 복층 그래핀과 기판 계면에 그리고 요오드 흡착은 그래핀의 상단 표면에 잉여전하를 유발하여 반전 대칭을 깨트린다는 사실을 확인하였다. 또한 상단 및 하단에 잉여전하를 유발하면 복층 그래핀의 반전 대칭이 회복되었고, 전하를 거의 전달받지 않은 층 때문에 발생하는 G^o 봉우리를 관찰하였다. G^-, G^+ 봉우리의 진동수 차이가 반전 대칭을 유발한 전하밀도의 그래디언트에 대한 척도가 될 가능성을 제시하였다.

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Optoelectronic Properties of Bare and Ligand Passivated CdSe: An Electronic Structure Study

김효진 한민우 김민철 심은지*

연세대학교 화학과

In this presentation, we establish the relationship between white light emission of CdSe nanoparticles with composition and coverage of ligands. It is known that ligands like TOPO, phosphonic acid, and amine quench the broad trap state emission, whereas thiol amplifies the trap state emission. This indicates that tuning white light emission is possible by means of ligand exchange, which indeed has been observed in many experiments. We performed density functional theory calculations to observe total and partial density of states of bare CdSe, OPH_3 passivated CdSe, and SCH_3 passivated CdSe as well as mixed ligand models. We demonstrate that the band gap, *i.e.*, white light emission, is influenced by ligands not only because of their chemical properties but also because of composition and coverage of ligands.

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Mechanistic Role of Copper Step Sites of $Cu/ZnO/Al_2O_3$ Catalyst during Methanol Synthesis Reaction

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$Cu/ZnO/Al_2O_3$ is industrially used methanol synthesis catalyst at elevated pressures P (50 to 100 bar) and temperatures T (473 to 573 K) using $CO_2/CO/H_2$ syngas mixture. Although the recent investigations have been described that active sites of this catalytic system are Cu step sites and stacking faults, circumstantial mechanistic routes are still unknown and debated even its initial state. In this study, we investigated the CO_2 hydrogenation mechanism at the step sites of Cu using Cu(775) surface at 1 bar with varying temperature from 298 to 450 K by reflection absorption infrared spectroscopy (RAIRS). At the edge of step, CO_2 is initially adsorbed as carbonate species and transformed to formate species via the bicarbonate. At elevated temperature above 323K, bicarbonate species completely disappeared with appearance of formates on terrace sites. Interestingly, only formate species on the step edge was continuously decreased with step-wise heating up to 400K and it forms CH_2, CH_3 vibration. These phenomena is strongly attributed that the formate, especially on the step, is initial intermediate and is desorbed by hydrogenation reaction because thermal desorption temperature of formate (~470K) is much higher than desorption temperature. Furthermore, adsorbed CO_2 as carbonate species is easily transformed to CO molecules at the edge of step by reverse water gas shift (RWGS) reaction.

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NiS-coated TiO_2 nanoparticles for supercapacitor electrodes

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국민대학교 생명나노화학과

Nickel sulfide (NiS) has attracted growing attention as an electrode material for supercapacitors due to its good capacitive properties, high electrical conductivity and low cost. The fabrication of electrode nanostructures has also been widely studied to enhance the capacitive performance of the supercapacitors because the increased surface area can improve the charge transfer and energy storage processes occurring at the electrode surface. However, most nanofabrication techniques require complicated and delicate nanoprocesses, and hence are not suitable for practical use. In this work, we developed a simple method to fabricate nanostructured NiS electrodes by depositing NiS onto TiO_2 nanoparticles. First, the TiO_2 nanoparticles were spin-coated on a fluorine-doped tin oxide (FTO) substrate, and then NiS layers were deposited onto the TiO_2 nanoparticles by consecutive dip-coatings in the solutions containing nickel and sulfur precursors. This nanostructured NiS electrode showed significantly improved capacitive properties compared to the electrode of NiS films deposited without TiO_2 nanoparticles.

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Effects of Plasma Treatment on Structural and Dynamical Properties of Model Lipid Bilayer Cell Membranes: Atomistic Molecular Dynamic Simulation Studies of Oxidized DOPC Membrane Systems

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광운대학교 화학과

The oxidization of phospholipids has been a topic of interest in physiological and biological studies for a long time. It has been recently shown by experiments that the dielectric barrier discharge (DBD) plasma treatment can be applied as cancer therapy by specifically oxidizing the cancer cell lines. Especially, it is also observed by experiments that the 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) lipids can be oxidized into damaged molecules (OX1, OX2, OX3, and DSPC) through the plasma treatment. [1, 2]

In this study, in order to mimic the biological lipid bilayer cell membrane damaged by the DBD plasma treatment, we built up model membrane systems that consist of various damaged species. We have observed that the oxidized species of DOPC lipids significantly affect membrane properties such as area compressibility modulus, tail angle distribution, density profile, and order parameter. Especially, in the OX3 system, it was observed that OX3 lipids not only induce the water pore formation but also escape from the membrane, which leads to the considerable alteration of the membrane properties.

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Sonochemical synthesis of ZnO nanoparticles The effect of Molar ratio and sonication times

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Nanostructured ZnO was synthesized by the sonochemical method with zinc acetate dihydrate and sodium hydroxide at room temperature. Different moles of Zinc Acetate dihydrate(Zn(CH3COO)2·2H2O) and Sodium Hydroxide(NaOH) were separately dissolved in 100 ml de-ionized water each, and then mixed under magnetic stirring. The mixtures turned into white gels, which were sonicated for 120min and 360min afterward under magnetic stirring. The white precipitates were centrifuged and washed with the methanol several times to remove ionic impurities and finally dried at 50℃ and 24h. The strucural investigation was carried out by field emission scanning electron microscopy(FESEM). The crystallinity and crystal phases of the synthesized nanostructures were analyzed by the X-ray diffraction spectroscopy(XRD).

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dbALP: database of annotated ligands and pockets

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Ligand is the key to perform a protein function in protein-ligand interaction. Protein can function itself, however it can have more functions according to combined various ligands. Therefore, researching protein-ligand interaction is helpful to understand protein functions and mechanisms. The dbALP is a database to inform what kind of ligands combine to protein, and provide joinable ligand as well as known protein-ligand complex information to know other protein functions. The dbALP has used 84,600 protein structures in PDB (Protein Data Bank), and provides pocket information and ligand which can combine with proteins. Geometry method is used to calculate protein pocket site, and sequence alignment with conserved protein sequence is also used to predict ligand position. DPSP score is applied to evaluate suitability between pocket and ligand and to find appropriate ligands. All calculated information is showed in the dbALP result page that includes basic protein information, three dimensional structure of proteins and ligands, calculated information of proteins and ligands, information of protein-ligand interactions, and literature. Particularly, heat-map system is easy to understand protein-ligand interaction, so we introduced heat-map system to see protein-ligand complex information easily by any researchers. The dbALP is expected to use drug candidate development research because it can predict unknown protein ligands as well as known protein ligand through comparing conserved protein sequences.

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Refinement of protein homology models through molecular dynamics simulations and model selection

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The refinement of low-resolution protein models derived from homology modeling still remains a challenge in protein structure prediction field. We have previously developed knowledge-based potential and structural-derived distance potential, and these showed successful results on NMR protein structure refinement. In this study, we tried several refinement simulations with 35 homology models obtained from the refinement category of the CASP11 competition. The molecular dynamics (MD) simulation was performed based on three different target energy potentials; with two developed energy potentials, without these energy potentials, and with harmonic restraint potentials on well-defined secondary structure regions. Moreover, simulated annealing (SA) was also performed for refinement. Selecting the near-native structure from decoy set is a significant task in protein structure refinement. We selected the native-like structure in decoy set using several criteria: (1) “protein-like scores”, such as protein packing quality associate scores (nDOPE, dDFIRE and WHAT_CHECK packing scores), steric clash and Ramachandran plot appearance, (2) “protein-like score” weights scaling, (3) structural clustering, and (4) structural averaging.

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Folic coated Gadolinium Oxide Nanoparticles as a Cancer Cell Targeting MRI Contrast Agent

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경북대학교 화학과

The choice of the tumor cell folate receptor as the target. Folate recptor up-regulation or over-expression is associated with a broad variety of tumor types. In this poster, I synthesized folic acid coated gadolinium oxide nanoparticles which were synthesised in triethylene glycol as a cancer cell targeting MRI contrast agent. They were characterized with FT-IR, TGA, XRD, MPMS, ICP-MS, TEM and MRI instrument. We hope that they can mostly target the cancer cells but not normal cell. These nanoparticles have enhanced relaxivity. Hence, it can be used as a MR imaging contrast agent.

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Investigation of magnetic properties of $NaFePO_4$ on the basis of density functional theory

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Magnetic properties of $NaFePO_4$ which is rechargeable battery insertion compound were examined by energy-mapping analysis based on density functional theory calculations. Our results show that spin exchange interactions through superexchange paths are antiferromagnetic and hence one-dimensional antiferromagnetic chain is formed. These antiferromagnetic chains are coupled antiferromagnetically through super-superexchange paths.

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Adsorption of surfactants in hydrophilic mesoporous silica from aqueous solutions of different neutron scattering length density

신태규

한국원자력 연구원 중성자과학연구부

Adsorption of nonionic and cationic surfactants in the cylindrical nanopores of mesoporous SBA-15 with a pore diameter of ca. 8 nm was studied as a function of pH, electrolyte concentration and neutron scattering-length density(SLD) of the solvent. The dependence of the surfactant adsorption on the pH of the solution and electrolyte concentration has been extensively studied and is well known, while that of surfactants on the solvent SLD is not the case. We found that the adsorption amount of investigated surfactants measured by using TGA differs from that of direct adsorption measurement and also from SLD to SLD for identical surfactant. In this presentation, these findings will be reported and dicussed by supplementary results of Small-angle neutron scattering curves of the surfactant-adsorbed SBA-15.

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The Mechanism : Hydrolysis of Formamide

백용수 최철호*

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The reaction mechanism for the neutral hydrolysis of amides in water has been investigated using QM/MM (quantum mechanics/ molecular mechanics) molecular dynamics simulations. The corresponding reaction mechanism is controversial in the previous researches although there are some experimental evidences that hydrolysis mechanism occurs without any catalysis in neutral. In this work, we have investigated the possible mechanism of the hydrolysis of formamide in aqueous solution. A combined QM/TIP5P-MD simulation utilized with umbrella sampling has been performed to generate the free energy surface of this reactions. Overall, it is found that the most favored mechanism is water assisted step-wise mechanism with two reaction steps in both ab-initio calculation and QM/TI5P-MD simulation. In the first step of the step-wise mechanism, the carbonyl group of the formamide molecule is hydrated to form a diol intermediate. From this intermediate, a water-assisted proton transfer occurs from one of the hydroxyl groups to the amino group. In both reactions, we observed that water plays a role to assists the proton transfer. The diol intermediate is significantly stable in QM/TIP5P-MD simulation, which is inconsistent with the results of ab initio calculation. It has been also found that water assisted stepwise reaction is preferred rather than concerted one.

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Non-Aqueous Acid-Base Reactions Between a Strong (Photo)Acid and Weak Protic Bases

이영민* 박선영[1] 김희수 권오훈[2,*]

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Proton transfer plays its important role in diverse biological and chemical phenomena such as water ionization, fast proton diffusion, acid-base reactions, proton pumps, DNA mutagenesis, and enzyme catalysis. In organic synthesis, acid catalysis is described to be a key for alcohol dehydration to produce alkenes, ethers, or alkyl halide.[1] When alcohol captures a proton from an acid catalyst such as HCl or H_2SO_4, it forms an alkyl oxonium ion (ROH_2^+) which is believed to be the key reaction intermediate.[2] Thus, the time-resolved spectroscopic studies of acid-base reactions in alcohol may allow understanding reaction mechanisms and development of efficient synthetic methods. In this study, we address the fundamental mechanism in the proton transfer to alcohol using a photoacid, *N*-methyl-7-hydroxyquinolinium ion. The clustering of alcohol molecules is found to be critical for alcohol to act as a BrØnsted base should be considered. We also identified bimodal reactivity of the photoacid resulting in the proton transfer reactions with monomeric and dimeric alcohol, simultaneously.[3] Details of our study will be presented in the poster.References[1] Morrison, R. T.; Boyd R. N. Organic Chemistry, 6th ed; Prentice Hall: New Jersey, 1992.[2] Han, H.-L.; Camacho.; Witek H. A.; Lee, Y.-P J. Chem. Phys. 2011, 134, 144309.[3] Y. M. Lee, S.?Y. Park, H. Kim, and O.-H. Kwon, to be submitted.

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A density functional study on permittivities of ordered noble-metal alloys

류설

조선대학교 화학과

Permittivities and electronic band structures of ordered binary-component noble-metal alloys, i.e., intermetallic compounds such as $CuAg_3$, $CuAu_3$, CuAu, and Cu_3Au, were calculated using density functional theory methods with plane-wave basis sets. Convergence tests on permittivities and electronic band structures of ordered binary alloys were performed with respect to calculation parameters and functionals used. In addition to normal linear-response-regime permittivities, improved permittivity values corrected with local-fields effects were also calculated for discussion of calculation time, quality of results, and comparison with random-alloy cases.

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Ultrasmall Mixed Gadolinium Dysprosium Oxide Nanoparticles for MRI Contrasting Agent

tirusew tegafaw 이강호*

경북대학교 화학과

Several mechanisms have been proposed to synthesize water soluble lanthanide oxide based MRI contrasting agents. We report here a biocompatible d-glucuronic acid coated ultrasmall mixed gadolinium?dysprosium oxide nanoparticles with an average particle diameter of 1 nm were synthesized and applied for T1, T2 MRI in vivo and in vitro. cytotoxicity test was measured by using NCTC 1469 and DU145 cells showing that D-glucuronic acid coated ultrasmall mixed gadolinium?dysprosium oxide nanoparticles are non toxic up to 200 ?M.This level of cytotoxicity implies that the synthesized material is a promising candidate for biomedical applications. The water soluble and biocompatible D-Glucuronic acid coated GdDy mixed oxide nanoparticles have drawn tremendous attraction in the application of magnetic resonance imaging.

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Modeling Multi-Enzyme Reaction using Hybrid Langevin/Monte Carlo Simulations

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광운대학교 화학과

Multi-enzyme systems can boost up the reaction rate of a sequential chain reaction by arranging the corresponding enzymes in space. The multi-enzyme system in this study consists of a formate dehydrogenase (FDH) and a mannitol dehydrogenase (MDH), which are directly linked by poly ethylene glycol (PEG) oligomers. In this system FDH converts NAD^+ into NADH by producing CO_2 from formate ions and then NADH is used as a cofactor in MDH to produce a mannitol from a fructose. Experimental results showed that this system dramatically accelerates the production rate of mannitols, compared to the case where the enzymes are not linked. We first performed Langevin Dynamics (LD) to obtain structural parameters such as distance between enzymes and relative orientations of active sites. Next, using the parameters from LD, we calculated the reaction rate using Monte Carlo simulations of simplified multi-enzyme models. The simulation results were in good agreements with the experimental results.

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Direct Observation of Intermediate Steps in the Excited-State Proton Transfer of N-Methyl-7-Hydroxyquinoline Iodide in Ethylene Glycol

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The excited-state proton transfer (ESPT) of the photoacid N-methyl-hydroxyquinolium ioidide (NM7HQ-I), in ethylene glycol has been explored by steady state and time-resolved fluorescence spectroscopy. To find the size of ethylene glycol clusters as photoacid-alcohol reactions, we followed the population change of the photoacid during the reaction with varying the content of ethylene glycol in an aprotic solvent. Previously it was found that dimeric clusters of mono-ols (methanol, ethanol, n-propanol etc.) are required for proton dissociation from this photoacid.[1] In the present study from analysis of fluorescence kinetic profiles we have shown that, for the photodissociation of a proton from NM7HQ-I, dimeric cluster is essential for di-ol (ethylene glycol) as well. The solvation dynamics of NM7HQ-I in ethylene glycol is found to be much slower compared to other alcohols which may be attributed to the high viscosity of the concerned solvent.[2] Due to this slowed down dynamics we could trap one of the intermediate species during the proton-transfer process. We propose that the intermediate is either a tight ion-pair or a solvent separated ion-pair.References1. Alcohol as an Effective Brønsted Base in Solution Due to Hydrogen-Bond Clustering, T. G. Kim, M. J. Ajitha, S.-Y. Park, K. Kwac, Y.M. Lee, H. Kim, Y. Jung, and O-H. Kwon (Submitted)2. The Dynamics of Solvation in Polar Liquids, M. Maroncelli, J. Mol. Liq., 1993, 57, 1-35.

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Potential dual imaging nanoparticle: Gd2O3 nanoparticle

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Gadolinium (Gd) is a unique and powerful element in chemistry and biomedicine which can be applied simultaneously to magnetic resonance imaging (MRI), X-ray computed tomography (CT), and neutron capture therapy for cancers. This multifunctionality can be maximized using gadolinium oxide (Gd2O3) nanoparticles (GNPs) because of the large amount of Gd per GNP, making both diagnosis and therapy (i.e., theragnosis) for cancers possible using only GNPs. In this study, the T1 MRI and CT dual imaging capability of GNPs is explored by synthesizing various iodine compound (IC) coated GNPs (IC-GNPs). All the IC-GNP samples showed stronger X-ray absorption and larger longitudinal water proton relaxivities (r1 = 26?38 s-1mM-1 and r2/r1 = 1.4?1.9) than the respective commercial contrast agents. In vivo T1MRand CT images of mice were also acquired, supporting that the GNP is a potential dual imaging agent.

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Apoferritin Encapsulated gadolinium oxide nanoparticles for MRI Contrasting Agent

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경북대학교 화학과

Magnetic nanoparticles with appropriate surface coatings can be used for various biomedical purposes, such as drug delivery, hyperthermia, tissue repairing, cell and tissue targeting, and magnetic resonance imaging. In this study Apoferritin is used as a surface coating to make biocompatible and water soluble.The structural, morphological and magnetic properties of these synthesized products were characterized by using X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy (FTIR), TGA, and SQUID magnetometer.

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DFT Study of SNAr fluorination:N, N', N''-tetra-Boc Guanidine System

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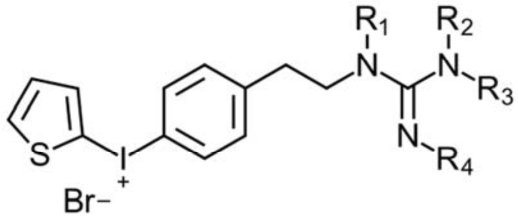
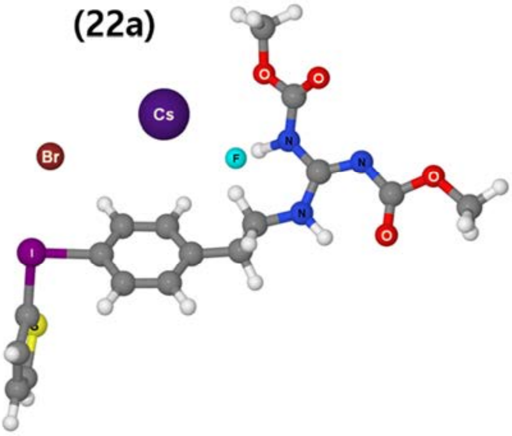
We calculated the model system for (22a), (22b) and (22c) with a level of theory M06-2X/6-311G**. The guanidine moiety of (22a) and (22b) is protected by two Boc groups, and that of (22c) is fully protected by Boc groups. From the computational result, We figure out that the position of fluorine and the thermodynamic properties affected the fluorination yield. The global minimum structure of pre-reaction complex (22a) is difficult to occur the reaction because the position of fluorine is far away from the reaction carbon center. however, In the case of (22b), the position of fluorine is good to ready to S_N2 reaction with thermodynamic stability. There is a similarity in guanidine moiety between (22a) and (22b), but the difference is that the oxygen in Boc affected the Cs cation or not. In the (22c), the fully protected guanidine moiety act as a ligand for Cs cation due to the interaction between Cs cation with lone pair electron of oxygen atoms in Bocs. Finally we calculated the reaction pathway and compared the activation barrier with experimental result.

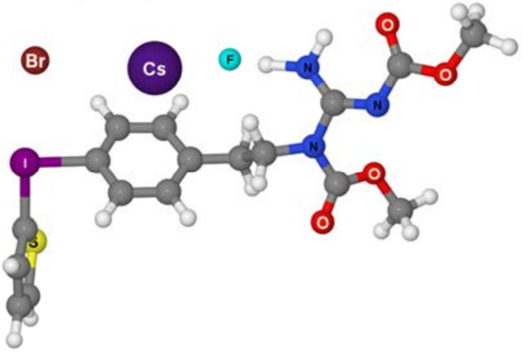


	R1	R2	R3	R4
(22a)	H	H	Boc	Boc
(22b)	Boc	H	H	Boc
(22c)	Boc	Boc	Boc	Boc

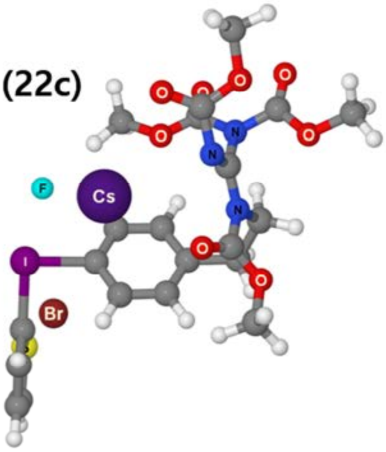
(22a)



(22b)



(22c)



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Computational Basis to evaluate Ni-S covalency in relation to H_2 evolving Ni catalysts

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Many catalysts mimicking the active site of [NiFe] hydrogenases have been synthesized to acheive H_2 production from water with low activation energy, but their properties are still far from optimal due to the lack of a molecular-level understanding of their reaction mechanisms. As an effort to search for electronic and geometric structural factors that govern its H_2-evolving chemistry, we test the relation between the covalency of Ni-S bonds and the efficiency of H_2 evolution. For a systematic search, structurally simple, synthetic H_2-evolving Ni catalysts with β-mercaptoethylamine, pyridine-2-thiolate, or bipyridine lignads have been selected. To establish computational methodologies for later-on spectroscopic analysis, we first compared B3LYP and BP86 DFT functionals to find which reproduces the Ni-S covalency better. This validation is based on various spectroscopic data, which will be used to aid the interpretation of spectroscopic and kinetic data and to construct corresponding reaction coordinates.

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Bovine serum albumin (BSA) and cleaved-BSA conjugated ultrasmallGd2O3nanoparticles: Synthesis, characterization, and application toMRI contrast agents

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경북대학교 chemistry [1]경북대학교 화학과

Bovine serum albumin (BSA) (Mn= 66.5 kD, size = 14 × 4 × 4 nm) is an attractive biological molecule forbiomedical applications because of its water-solubility and bio-compatibility. It can also bind manyultrasmall nanoparticles (NPs) as confirmed in this study. We synthesized polyethylene glycol diacid(PEGD) coated ultrasmall Gd2O3nanoparticles (PEGD-GNPs, the core davg= 2.0 nm), which were then con-jugated to BSA and cleaved-BSA (C-BSA) (i.e. BSA-PEGD-GNPs and C-BSA-PEGD-GNPs) through amidebonding. Large relaxivities were observed in both aqueous sample solutions (r1= 6.0 s?1mM?1andr2= 28.0 s?1mM?1for BSA-PEGD-GNPs and r1= 7.6 s?1mM?1and r2= 22.0 s?1mM?1for C-BSA-PEGD-GNPs). Three tesla T2magnetic resonance imaging (MRI) in a mouse after the injection of an aqueoussample solution of BSA-PEGD-GNPs into a mouse tail vein revealed significant negative contrast enhance-ments. Large relaxivities and in vivo MR images prove that BSA-PEGD-GNPs and C-BSA-PEGD-GNPs arepotential MRI contrast agents.

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Plasma oxidation of single and few-layer MoS_2

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직접띠간격(direct bandgap)을 갖는 단일층의 MoS_2 는 구조적 결함(defect)이 발생하면 전자구조가 절연체(insulator) 특성으로 변화하게 된다. MoS_2 의 발광 특성을 제어하기 위해 원자 크기 수준의 두께와 물성을 조절할 수 있는 화학적 표면개질법에 대한 연구가 필요하다. 최근 MoS_2 의 고온 산화반응을 통해 표면에 MoO_3 가 형성되었다는 연구결과가 보고되었으나 반응 메커니즘은 알려져 있지 않다. 본 연구에서는 산소 플라즈마에 의한 단일층 및 복층 MoS_2 의 산화반응을 원자힘 현미경(AFM), 광전자 분광법(XPS), 광발광 및 라만 분광법을 통해 관찰하였다. 플라즈마로 생성된 산소 라디칼과의 반응시간이 증가함에 따라 E^1_{2g} 와 A_{1g} 진동모드에서 기인하는 라만 신호세기, 그리고 A 와 B 엑시톤에서 유래하는 광발광의 세기가 감소하였다. XPS 측정에서 산화반응 이 후 Mo^{4+}는 Mo^{6+}로 변화하여 MoO_3 가 생성됨을 관찰하였다. AFM 을 통해 반응 전 MoS_2 의 단일층 단차가 0.7 nm 에서 반응 후 1.7 nm 로 증가하였다. 이 결과는 플라즈마 산화반응을 이용하여 초박형 MoS_2 표면에 구조적 결함 생성과 동시에 MoO_3/MoS_2 이종구조체가 생성됨을 보여주었다. 본 연구는 광발광 특성 제어를 위해 원자 크기 수준의 표면 화학 반응을 이용하여 MoS_2 의 전자구조를 조절할 수 있다는 가능성을 보여준다.

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Enantioselective Hydrogenation of (E)-alpha-Phenylcinnamic acid using Carbonaceous Support-based Pd catalysts: Influence of the Support Acidity

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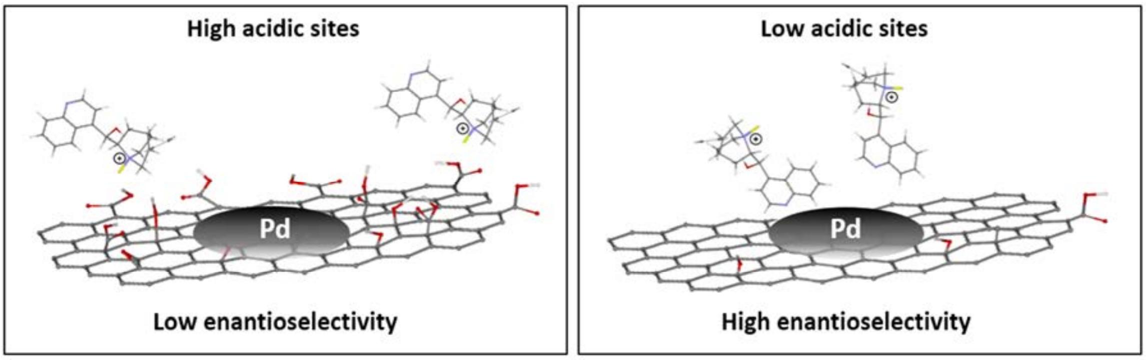
한국과학기술원(KAIST) 화학과 [1]숙명여자대학교 화학과

A systematic comparative study of carbonaceous materials as catalyst supports for the asymmetric heterogeneous hydrogenation of (E)-alpha-phenylcinnamic acid (PCA) was performed to investigate the influence of the supports on the reaction enantioselectivity. A series of Pd-based catalysts supported on activated carbon (AC), graphene oxide (GO), or carbon nanotubes (CNTs) was prepared using deposition methods, and their physicochemical properties were characterized. The results demonstrated that the textural structure of the supports had a trivial effect on the enantiomeric excess (ee). The TGA, FT-IR, and TPD-NH3 data revealed an abundance of acidic sites present on the Pd/GO catalyst, unlike the other catalysts, and these sites reduced the enantioselective hydrogenation of PCA. In addition, the effect of the support acidity on the enantioselectivity was ascribed to the preferential adsorption mode of cinchonidine (CD) on the GO surface via electrostatic interactions between the negatively charged oxygen functional groups present on the GO surface and the positively protonated amine groups present in the CD molecule.



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Long-range proton relay shows an inverse linear free energy relationship depending on the pK_a of the hydrogen-bonded wire

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경희대학교 응용화학과

The long-range proton transfer dependence on the pK_a of hydroxyl molecules in hydrogen (H)-bonded wires was investigated using quantum mechanical calculations. The triple proton transfer takes place in an asynchronous and concerted fashion between carboxylic and imidazole groups linked by two H-bonded chain molecules. Four hydroxyl molecules with different acidities, water, 2-fluoromethanol, 2,2,2-trifluoromethanol, and phenol, were used to construct sixteen H-bonded wires. The proton transfer rate increased with the acidity of the chain molecules. The rate was found to be more dependent on the particular chain molecule with relatively small structural changes in the wire, which can act as a solvent, rather than molecules with larger O-H bond cleavage in the TS. An inverse linear free energy relationship was recognized for the first time in the multiple proton transfer with a change in hydroxyl molecules. The activation and reaction free energies decreased and increased, respectively, with respect to the acidity of the chain molecules. This inverse LFER can be explained by the pK_a slide rule, in which the pK_a dependence of H-bond strength in a wire has an opposite trend for chain molecules that donate and accept a H-bond. Therefore, the pK_a of wire molecules can have different roles, which leads to the very unusual relationship between the activation and reaction free energies.

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Fitting atomic charges with dynamical information from molecular dynamics simulations

김창우 이영민*

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Atomic partial charge is one of the key parameters for molecular dynamics (MD) simulations and is parametrized to represent the overall electrostatic effect induced by both nuclei and electrons. There are a number of schemes to obtain it from quantum chemical calculations. Methods such as Mulliken or natural bond orbital (NBO) analyses obtain the atomic charge directly with the electron density from quantum calculations, while others like charges from electrostatic potentials using a grid based method (CHELPG) and restrained electrostatic potential (RESP) fit the atomic charge to reproduce the electrostatic potential in the vicinity of the molecule. In condensed phase simulations, electron density of a system fluctuates constantly, mainly due to electrostatic interactions with nearby solvent molecules and due to the conformation change of the system itself. This makes the atomic charges derived from existing schemes somewhat unrealistic, because most of the methods rely on a single (usually energy minimum) conformation of the molecule with the continuum solvent model at their best. In this work, we devised a new charge-fitting protocol which can implement dynamical information from the molecular dynamics simulation. Unlike traditional methods which use the electrostatic potential, it fits the solute-solvent interaction energy of the classical MD model to the results from quantum chemical calculations. Molecules of various types and sizes are tested. We adopted multiple initial guesses in some situations to test the convergence of our proposed scheme.

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The catalysts of Pd/CeO2 nanoparticles synthesized by pulsed laser ablation in liquid phase

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부산대학교 화학과

Recently, the importance of nano-technology is increased due to properties of nano-compounds such as high surface area and catalytic effect. So it is frequently investigated in various parts of science. Specially, metal nanoparticles are successfully used in a wide range of applications like catalysis, sensing, capacity and so on. NPs can be obtained by top-dowm and bottom-up method. Also, there are many methods to synthesize nanoparticles like pulsed laser ablation, photo-reduction and spray pyrolysis. The pulsed laser ablation in liquid phase (PLAL) is one of top-down method. This method is attractive to be easy to synthesize NPs and eco-friendly in comparison with other propulsive techniques. A method of PLAL is used to synthesize Pd/CeO2 nano-catalysts in deionized (DI) water with CeO2 powder and Pd plate. The target is irradiated by a Q-switched pulsed Nd:YAG laser at wavelength (1064 nm) and energy density (8.8 J/cm2). Products are analyzed by field emission transmission electron microscopy (FE-TEM) and UV-vis spectroscopy. Also, Pd/CeO2 composites are shown as efficient catalysts for reacting the reduction of NO2 to NH2 by using 4-nitrophenol and NaBH4.

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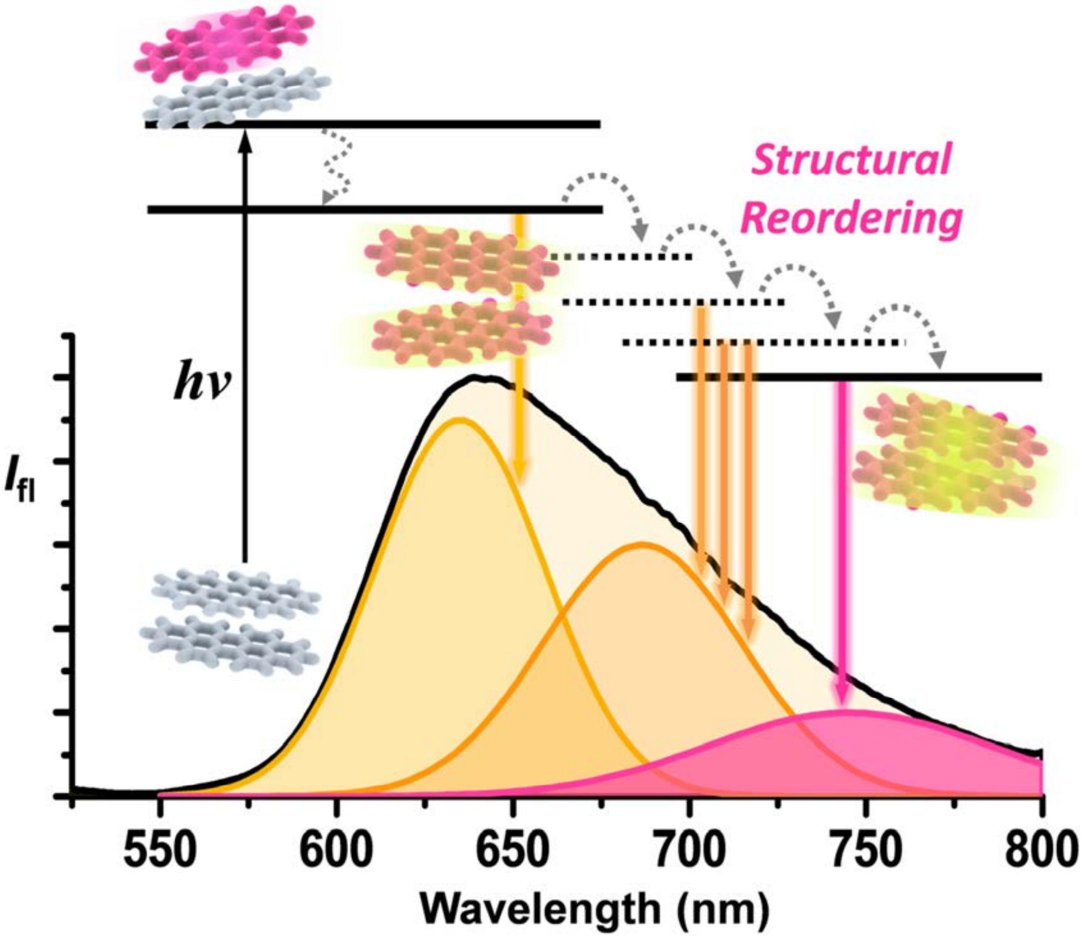
Spectroscopic Demonstration of Exciton Dynamics and Excimer Formation in a Sterically Controlled Perylene Bisimide Dimer Aggregate

손민정 김동호*

연세대학교 화학과

While it is commonly accepted that H-type PBI aggregates give rise to a broad, red-shifted excimer fluorescence with considerably longer fluorescence lifetimes than observed for the monomers, the underlying mechanisms of excimer formation and other relevant exciton dynamics in such π-stacked systems are still far from being understood. In this context, herein we demonstrate a thorough spectroscopic investigation on the exciton relaxation pathways, including excimer formation, in a perylene-3,4:9,10-bis(dicarboximide) (PBI) dimer aggregate by using time-resolved fluorescence and transient absorption spectroscopy combined with excitation-power and polarization dependence. It was found that the excited dimer formation process followed by structural rearrangement is approximately two times faster than observed within larger PBI aggregates. Excitation-power dependent transient absorption decay profiles revealed the fully delocalized nature of excitons in the dimer aggregate as opposed to larger stacks.


Structural
Reordering
hv
I_{fl}
550
600
650
700
750
800
Wavelength (nm)

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Computational Study on the Origin of Fluorescence Red Shift in Yellow Fluorescent Protein

박재우 이영민*

포항공과대학교(POSTECH) 화학과

Many mutants of wild-type green fluorescent protein (wtGFP) have been developed to change the fluorescence emission maximum. Some variants were generated by changing protein environment near the chromophore. One representative example is the yellow fluorescent protein (YFP). This slightly red-shifted mutant was generated by replacing the Threonine 203 residue into Tyrosine. With this one point mutation, the fluorescence emission maximum shifts by 0.08 eV. Yet, the reason for this red shift has not been investigated in a detailed manner, although in the previous experimental works, it was supposed to be coming from π-stacking and conformational change. In this work, the fluorescence emission spectra of wtGFP and YFP are calculated with the excited state molecular dynamics simulations using interpolation of diabatic Hamiltonian. Simulated fluorescence emission peak was shifted by 0.04 eV, which was mainly due to the conformation change of the chromophore. Additionally, excited state quantum chemical calculations of the geometries which possess π-stacking between the chromophore and Tyrosine 203 gave another 0.04 eV red shift of the fluorescence emission. By assuming these effects as additive, the total emission maximum shift would be 0.08 eV, reasonably agreeing with the experimental results. Thus, we attribute the red shift to the conformational change of the chromophore and π-stacking between the chromophore and Tyrosine 203.

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Monte Carlo Study on the Cassie-Baxter to Wenzel Transition of the Water Droplet Deposited on Domed Pillars

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We studied how the water droplet sitting on top of domed pillars penetrates down into the gap between the domed pillar walls as the spacing between the pillars or the pressure of droplet increases. This penetration pertains to the Cassie-Baxter to Wenzel transition of the droplet. By using the lattice gas Monte Carlo simulation, we simulated pillars with various shapes ranging from normal dome-shaped to needle-like pillars. Regardless of the shape, the penetration between the parabolic pillar walls was always smooth, which is in stark contrast to the abrupt filling found for the gap between rectangular or cylindrical pillars. This smooth behavior was also found for the Cassie-Baxter to Wenzel transition induced by increasing the pressure of the droplet. We related the pressure susceptibility of the density of the water confined between the pillar walls to the fluctuation in the density of the confined water.

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A Single-molecule Photoswitch: Self-photoswitchable Cyanine Dye Working in Thiol-free Solutions

박상원 권지웅 김성근[1,*]

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Optical transition between fluorescent and non-fluorescent states is the most essential and important feature in super-resolution imaging. Photoswitchable cyanine dyes are most widely used due to their brightness and fatigue-resistance, but require concentrated thiols that may do harm to living biological bodies and affect the activities of biomolecules therein. Here we introduce a novel, advanced single-molecule photoswitch capable of switching even in thiol-free solutions. A general click reaction between cysteamine and Cy5-NHS ester makes thiolated-Cy5 that shows a switching behavior and promising photophysical properties.

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Pd/C nanoparticles produced by pulsed laser ablation in liquid

김유진 김태규* 마로리

부산대학교 화학과

Nanoparticles have attracted much attention because of their new physical and chemical properties from bulk materials. Many techniques have been used for preparing NPs. Pulsed laser ablation in liquid (PLAL) that is one of these techniques is interesting because it is a green technique and available in various metals, solvents, stabilizing agent. Also core/shell NPs are attracting much interest, since they show different properties from either core or shell NPs. We generated Pd/C core/shell NPs via pulsed laser ablation of a Pd target in acetonitrile without adding stabilizing agent. The target is irradiated by a Q-switched pulsed Nd:YAG laser at wavelength (1064 nm) and energy densities (8.4 J/cm2). Pd/C NPs formed by PLAL was analyzed by high resolution transmission electron microscopy (HR-TEM), selected area electron diffraction (SAED), cyclic voltammetry (CV). CV results show Pd/C NPs are good electrocatalysts.

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Effect of Annealing Temperature on Photocurrent Density of Hematite Thin Film on Fluorine Doped Tin Oxide Substrate

조은수 강영수*

서강대학교 화학과

Among various candidate materials, hematite has emerged as a promising photo-electrode due to many advantages for photoelectrochemical water splitting. It has narrow band gap about 2.2 eV and it can absorb almost 40% of the sunlight. Also, it is inexpensive, abundant in nature, and very stable in electrolytes over pH 3. In this research, deposition and annealing (DA) method was used to synthesize hematite thin film. Hematite was deposited by spin-coating on the fluorine tin oxide (FTO) as a substrate, and the drying and annealing procedures were followed. Then, the hematite thin film was annealed at various temperature conditions. As the annealing temperature went up from 550 ℃ to 700 ℃, the photocurrent density was increased. The film annealed at 700 ℃ has the maximum photocurrent of 0.6 mA/cm2 at 1.23 V vs. RHE under 1 sun illumination. This work deals with which temperature is optimum for synthesizing the hematite film and the reason why the photocurrent density increased.

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Synthesis of Sintered Sm2Fe17N3 Magnet for Exchange-Coupled Nanocompostie Magnet

안재우 강영수*

서강대학교 화학과

Nowadays, Nd2Fe17B is the most popular permanent magnet. It has stronger magnetic energy product than any other hard magnet materials. But, this material has low curie temperature (585 K), so it is unstable in high temperature. On the other hand, Sm2Fe17N3 has high curie temperature (749 K) and this can replace Nd2Fe17B with higher stability at high temperature.Usually, Sm2Fe17N3 can be synthesized by Ball-milling method (Top-down). But as-synthesized magnet shows phase separation at high temperature (>1473 K). But, in case of sintered Sm2Fe17N3 magnet synthesized by wet chemistry (Bottom-up), purity of material is much more higher and also size can be controlled. So the magnetic energy product of sintered Sm2Fe17N3 magnet can be enhanced than that reported in the previous report. With this sintered Sm2Fe17N3 magnet, final goal is the self-assembled hard/soft nanocomposite magnet for magnetic for higher maximum energy product than 55 MGOe by exchange-coupling effect.

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Fabricate (002)-oriented Monoclinic WO3/Reduced Graphene Oxide Film for CO2 Reduction to Methanol

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The reactivity of a photocatalyst is influenced by its surface atomic structure. Therefore controlling crystal facet will be very important to enhance the reactivity of the photocatalyst. In my work, I synthesized rectangular shape of monoclinic tungsten trioxide (WO3) as potential photocathodic materials. Actually monoclinic tungsten trioxide WO3 has a bandgap of 2.7eV where its conduction band is little lower than CO2 reduction potential (CH3OH/CO2 at ?0.38V, NHE, pH=7). But among (002), (020) and (200) of WO3 three main facets, the (002) dominant rectangular sheet like WO3 crystal has an elevated conduction band where its CB band is suitable for CO2 reduction. Therefore I fabricated WO3 nanoplate thin film with dominant crystal facet of (002) by spin coating. And also I deposited reduced graphene oxide on the top of WO3 film to do engineering of reduction potential more properly. I expect that (002)-oriented monoclinic WO3/rGO film could be applied well as photocathode for methanol production which is our final purpose in artificial photosynthesis.

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Synthesis of Y2Si3:Pr3+ Phosphor Nanoparticles and its Application to Enhanced Photochromic Window Film

강하례 강영수[1,*]

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For photochromic materials, organic compounds have been attracted interests because of its better photochromic efficiency than inorganic compounds. However, inorganic photochromic materials have an advantage of durability. To enhance photochromic efficiency of inorganic photochromic film, upcoversion film which converts the visible light into the UV light could be attached on the top of photochromic film as most photochromic film absorbs the UV light around 290 nm. Pr3+ was been chosen for activator due to its proper emission peak (280-400 nm). Also, for the host material, monoclinic-Y2SiO5 was selected for its optical and mechanical stability. Y2SiO5:Pr3+ nanoparticles were fabricated via co-precipitation decomposition and sol-gel method.

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Changed Photoelectrochemical Activity of α-Fe2O3 Nanostructured Thin Film by Cu Doping

안나현 강영수*

서강대학교 화학과

a-Fe2O3 has attracted attentions due to its good properties such as visible light absorption and stability.1 Powder type of Cu-doped hematite was synthesized and deposited on the FTO substrate. Purposely adjust the amount of Cu dopant (1, 2, 3, 5 mol% of Fe precursor) to study the effect of Cu doping. The photocatalytic activity of Cu-doped hematite was investigated by measuring photocurrent. The properties of the film were characterized by many methods such as XRD, TEM, SEM, IPCE, PEC, and UV-vis absorption spectroscopy. Fe3+ ions in a-Fe2O3 nanocrystal structure are substituted by Cu2+ ions. This leads to lattice distortion and increase in hole trapping sites.2 XRD pattern shows that crystal structure remains as almost same when adjusting the amount of Cu2+ ions. Due to charge imbalance and crystal distortion, when Cu2+ ions occupied Fe3+ sites, hole trapping occurred leading to the decrease in PEC value. Furthermore, electrochemical impedance value was increased as Cu doping increased, which was consistent with PEC data. Also, incident photon to electron conversion efficiency has decreased by doping.

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CRASY: Photochemical reactions of cytosine tautomers

이종찬 남경현 SCHULTZ THOMAS[1,*]

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) Natural Sciences

Mass-Correlated Rotational Alignment Spectroscopy (mass-CRASY) combines information from mass spectrometry with that from high-resolution rotational spectroscopy. It thereby allows the single-step characterization of multiple molecular species in heterogeneous or impure samples. The rotational structure is analyzed through the impulsive excitation of a coherent rotational wavepacket and the time-delayed probing thereof by resonant multi-photon ionization (a weak measurement). Resulting ion masses are characterized by mass spectrometry (a strong measurement). Electron-CRASY utilizes the same principle as mass-CRASY but reveals information about the electronic structure of the molecules. This poster presents photochemical reaction dynamics of excited state cytosine and the planned use of CRASY to explore photochemical reactions of DNA bases. The keto form of cytosine is the biologically relevant tautomer and theoretical calculations proposed particular photochemical properties for this tautomer.

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Asymmetric-Potential-Well Model for CdSe Quantum Dots in Dielectric Media

정화준 신승구*

포항공과대학교(POSTECH) 화학과

We employed the finite-potential-well model with a dielectric boundary to calculate the optical properties of CdSe quantum dots (QDs) in chloroform. The bandgap and oscillator strength of CdSe QD obtained from theory were compared with experiments. The kinetic energies of electron and hole in finite potential wells were calculated by using the effective mass approximation. The Coulomb potential energy was treated as a perturbation. The Coulomb potential energy included the effects of dielectric boundary set by the size-dependent dielectric constant of QD, the static dielectric constant of solvent, and the continuously varying dielectric constants at the ligand-covered interface between QD and solvent. To calculate the bandgap of Cd- or Se-rich QDs, we modified the finite-potential-well model by asymmetrically expanding the confined region of either electron or hole. In the case of Cd-rich (or Se-rich) QD, the conduction (or valence) band region was expanded by one Cd (or Se) atom. The oscillator strength of CdSe QDs was obtained by taking account into the atomic transition moment of CdSe unit calculated from time-dependent density functional theory. The present asymmetric-potential-well model provides the bandgap and oscillator strength that are in good agreement with experiments.

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Enhanced photocatalytic activity and anti-photocorrosion of AgI nanostructures by coupling with Graphene-analogue Boron Nitride sheets

<u>최지하</u> 김태규* devulapalliamaranathareddy 이승희 마로리

부산대학교 화학과

Graphene-analogue boron nitride(BN) covered with AgI nanocomposites were successfully synthesized by a template-free in situ ultrasound-assisted method at room temperature. A set of characterizations technics like X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), Field Emission Scanning Electron Microscope (FE-SEM), transmission electron microscopy (TEM), UV-VIS Spectrophotometer, Fourier transformed infrared spectroscopy (FT-IR), and photoluminescence spectroscopy (PL) have been employed to know the structural and morphological nature. The results showed that the AgI nanostructures were grown on graphene analogue boron nitride sheets. The photocatalyst studies show that BN-AgI nanocomposites exhibit much higher photocatalytic activity and anti-photocorrosion than the pure AgI under visible-light irradiation. Among the BN/AgI nanocomposites (wt% of BN = 0.1, 0.2, 0.3, 0.4), BN/AgI (0.2wt%) has the highest photocatalytic activity by the degradation of Rhodamine B (RhB). And its catalytic efficiency goes up to 100% within 70 min. According these results, we are able to know how good the BN/AgI nanocomposites have photocatalytic efficiency under visible-light.

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Atomic and electronic Structure of multifunctional heterocyclic compound on Ge(100)

김도환

대구대학교 화학교육과

We have performed density-functional theory (DFT) calculations in order to investigate the atomic and electronic structure of purine on Ge(100). As a multifunctional heterocyclic molecule, purine molecules form double dative bonding with surface germanium atoms through the lone pair electrons of two nitrogen atoms at room temperature. Another surface germanium atom reacts with carbon or nitrogen atom of purine ring to stabilize the positive charge of the datively bonded nitrogen atom. The reaction with nitrogen atom induces further N-H bond dissociation, while the C-H dissociation is unfavorable. The electron donated from the surface Ge atom stabilizes the structure through resonance. Simulated STM images from the optimized configurations show characteristic features of the adsorption structures.

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Gas Phase Photodissociation Dynamics Studies of Oxalyl Bromide near 265 and 234 nm

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부산대학교 화학과

In gas phase photodissociation dynamics of oxalyl bromide (C2O2Br2) have been studied near 265 and 234 nm by employing [2+1] resonance-enhanced multiphoton ionization (REMPI) with time-of-flight mass spectrometer (TOF-MS). Both two wavelengths state selective detection of Br (2P3/2) and Br* (2P1/2) were detected after photolysis of C2O2Br2. At two pump energy, the nascent Br (2Pj , j=1/2, 3/2) atoms stem from the primary C-Br bond fission as well as secondary dissociation of their corresponding C2O2Br radicals which are energized from the ultrafast primary C-B bond rupture. In this study at first we get 2D images and from these images we can calculate total translational energy distributions, recoil anisotropic parameters, and relative quantum yields. From this result the excited state translational energy distribution can be fitted by single Guassian distribution, whereas at ground state three Guassian functions found and the average translational energies about high velocity compounds are of 11.9 and 12.49 kJ/mol near 265nm. At 265 nm the quantum yields for Br* is 0.42 and translational anisotropy parameter, β, values are 0.90 for Br and 1.38 for Br*. On the other hand, at 234 nm the quantum yields for Br* is 0.33 and translational anisotropy parameter, β, values are 0.79 for Br and 0.97 for Br*.

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Fabrication of (002)-Facet Dominant WO3 Films for Enhancing Photoelectrochemical Properties

Zheng jin you 강영수*

서강대학교 화학과

Tungsten trioxide, WO_3, is a very important $5d^0$ transition metal oxide with a relatively narrow band gap (~2.8 eV). It can utilize the solar light in the visible range. WO_3 has attracted a lot of interest due to its photosensitivity, good electron transport properties, and stability against photocorrosion. However, its conduction band minimum is below the hydrogen evolution redox potential, which indicates that WO_3 photoanode can only drive half of the water splitting reaction for O_2, rather than H_2 evolution. In addition, enhancing the photocurrent of WO_3 film for solar water splitting by many methods, such as doping, crystal engineering and so on, are intensively considering. By using the theory calculation, the surface energy order of the monoclinic WO_3 (γ-WO_3) is {002} > {020} > {200}. The most reactive surface is {002} plane in the γ-WO_3 crystal. Therefore, fabrication of {002} facet dominant WO_3 films is very important for enhancing the photoelectrochemical properties. The (002) dominant films can be fabricated by hydrothermal method[1], rubbing method[2], and spin-coating method. Especially, the (002) dominant thin film made by the spin-coating method shows the high transmittance and nice photocurrent performance.

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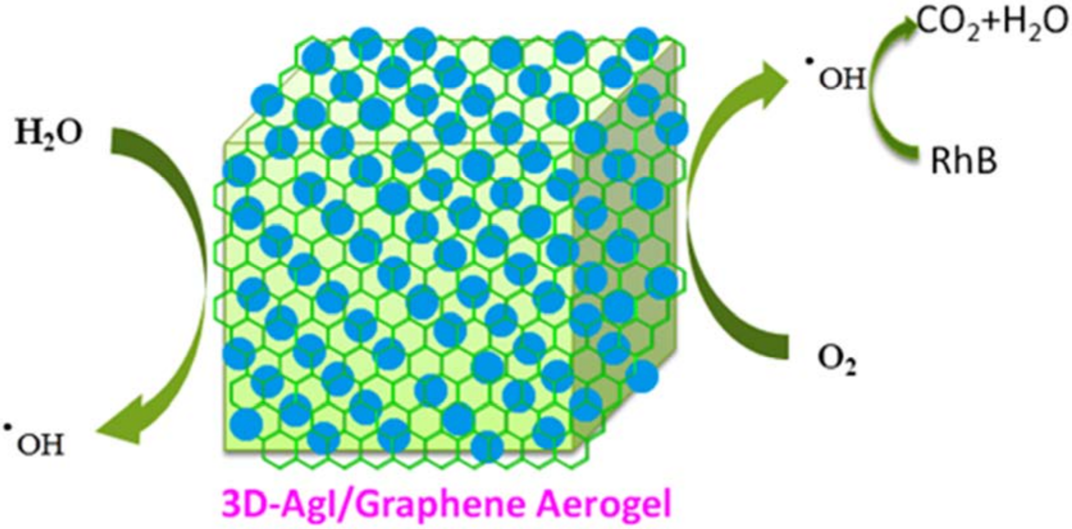
Self-Assembled Three-Dimensional Graphene-Based Aerogel with Embedded AgI Nanoparticles and Its Excellent photo catalytic Activities

devulapalliamaranathareddy 김태규* 최지하 이승희 마로리

부산대학교 화학과

AgI nanoparticles functionalized self assembled graphene aerogel is constructed using vitamin-C as the reducing agent. A set of characterizations including FESEM, TEM, XRD, XPS, Raman, FTIR, optical absorption and photoluminescence techniques confirm that the aerogel is formed with ultradispersed AgI nanocrystals and self-assembly of graphene nanosheets into porous hydrogel structures. The obtained aerogels exhibits high adsorption and photocatalytic degradation ability toward organic dye (Rhodamine-B) due to abundant visible light active nature of AgI and the higher specific surface area of graphene nanosheets with three-dimensional interconnected pores. The well wrapped graphene nanosheets on AgI nanostructures could promote the transfer of photo-generated electrons, which not only inhibited the recombination of electrons and holes effectively, but also suppressed the photocorrosion of AgI, resulting enhanced photocatalytic activity and stability. This study brings a novel approach to develop multiresponsive graphene aerogels by co-assembly of various semiconductor nano components for efficient water remediation.


H_2O
$^{\bullet}OH$
$^{\bullet}OH$
CO_2+H_2O
RhB
O_2
3D-AgI/Graphene Aerogel

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Synthesis, structure, photoluminescence and anticancer activity of mononuclear copper(II), zinc(II) and palladium(II) complexes of Isoxazolones

MAHIMALURUJAGADEESH 김태규*

부산대학교 화학과

A series of ionic, mononuclear copper(II), zinc(II) and palladium(II) complexes of isoxazolone ligands have been synthesized and characterized by FT-IR, FT-Raman, ESI-MS, 1H NMR and fluorescence spectral techniques. The ligands 3-phenyl-4-(4-fluorophenyl)-5-isoxazolone L1 and 3-phenyl-4-(4-toulyl)-5-isoxazolone L2 are unambiguously characterized by the single crystal X-ray crystallography. The ligand L1 belongs to orthorhombic system with P2(1)/C space group and the unit cell parameters are a = 8.1552(3) ?, b = 10.1169(4) ?, c = 17.0819(6) ?, α=β=γ= 90° and volume V(A3) = 1409.35(9). The synthesized isoxazolone ligands and their copper(II), zinc(II) and palladium(II) complexes are subjected for anticancer activity against human breast cancer cell lines MDA-MB-231. The coordination of two different chelating ligands (O^O = L1 and L2 isoxazolones) to the metal center are expected to induce both the cell growth inhibition and apoptosis of MDA-MB-231 cancer cells and suggests the potential of this design for the improvement of the metal based drugs.

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Photodissociation dynamics for 2-bromopropene near 234 nm: Ion-imaging study

김현국 김태규*

부산대학교 화학과

We have investigated the photodissociation dynamics of 2-bromopropene near 234 nm. Two-dimensional photofragment ion-imaging technique was used to obtain the spatial distributions of the nascent Br atoms. The [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme was used for state-selective detections of Br ($^2P_{1/2}$) and Br*($^2P_{3/2}$) generated after photolysis of 2-bromopropene at this wavelengths. The measured total translational energy distributions, recoil anisotropic parameters, and the relative quantum yields were used to explore the inside of surface interaction among the potential energy surfaces in detail.

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Real-time Measurements of Excited State Dynamics with Time-resolved Imaging Spectroscopy

우경철 김상규*

한국과학기술원(KAIST) 화학과

Most of the photodissociation reactions involving repulsive excited states occur in ultrafast timescale. Lots of attempts has been made to observe excited state dynamics related to ultrafast dissociation as a femtosecond pump-probe experiment. Researching time-resolved dynamics with a femtosecond laser has been expected to be helpful for the complete understand of conical intersection dynamics. Here, the progress of establishing new experimental set-up for real-time measurements is presented. In this poster, some demonstrational result should be introduced hopefully.

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Facet Dependent Photocatalytic activity of Bismuth Oxychloride

Haider Zeeshan 강영수*

서강대학교 화학과

Crystal facet engineering is a subject of great interest. There is immense potential to reshape and design semiconductors exposed with desired facets. Surface energies, bonding pattern as well as surface activity of facets are quite different from each other. Bismuth oxychloride (BiOCl), a p type semiconductor has been reported to have excellent photocatalytic ability. This study is focused on fabrication and photocatalytic investigations of BiOCl nanocrystals selectively exposed with high energy {001}-facet by hydrothermal route. A variety of experimental techniques were employed for structural characterization. Crystal structure and morphology of {001}-faceted BiOCl was found to be critically dependent on the solvent ratio adopted during hydrothermal treatment. {001}-facet exposed BiOCl exhibited improved photocatalytic activity.

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Tully's surface hopping nonadiabatic molecular dynamics of large molecule bond breaking system with spin-flip time dependent density functional theory

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서울대학교 화학부 [1]경북대학교 화학과

Generally, the molecular dynamics (MD) of an adiabatic process is described by one Born Oppenheimer (BO) potential surface. When there is a crossing of different BO potential surfaces which is called conical intersection, it is necessary to find a new way to describe nuclear motions which involves more than one BO potential surfaces. Because it become known that conical intersection lead to rapid radiationless decay. In 1990, John C. Tully suggest fewest switches surface hopping algorithm to carry out MD simulations of processes which involve electronic transitions. In this algorithm, the time dependent electronic Schrodinger equation (SE) is solved to obtain forces acting on nuclears and hopping probability. The nuclear motions are propagated by the classical mechanical equation. Commonly, multi-configurational self-consistent field (MCSCF) method is used to the solve electronic SE in Tully's algorithm. However, MCSCF is too heavy method to study excited states of large molecule system. Recently, Vlasta Bonai-Koutecky suggest a way to do with time-dependent density functional theory (TDDFT) numerically. TDDFT is single-reference ab initio method which is fit to calculate excited states of large molecule. In single-reference ab initio method, the spin-flip (SF) formalism is proposed to describe the bond-breaking problem. Through this poster, I would like to discuss potential of SF-TDDFT formalism in Tully's surface hopping nonadiabatic molecular dynamics of large molecule bond breaking system.

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High SERS-activity in Films of Ag Nanorod?Nanoparticle Assembly Structure

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Silver nanorod-nanoparticle assembly structures were fabricated and their morphological and optical properties were investigated for applications in surface-enhanced Raman spectroscopy (SERS). For the fabrication of the nano-assembly structure, silver nanorod (AgNR) arrays, fabricated via oblique-angle deposition by thermal evaporation, were functionalized by (alpha,omega)-alkanedithiols to which silver nanoparticles (AgNPs) were linked. The morphology of this conjugated system and its SERS-activity were characterized by scanning electron microscopy (SEM) and micro-Raman spectroscopy followed by benzenethiol-functionalization, respectively. Typical values of the diameter and length of the AgNRs are ~70 nm and ~900 nm, respectively. And, the average diameter of the AgNPs was ~ 70 nm. Population densities of these AgNPs linked to AgNR arrays were found to vary between 20 and 130 per ?m^2 with the variation of dithiol chain lengths, where the dithiol with smallest chain length is found to link higher number of AgNPs; the reason behind this behavior was explored. From the SERS characterization, very significant increase in the enhancement factor (E.F.) of the Ag NR-NP assembly film was observed over that of bare AgNR array, to which 'hot spots' generated at the NR-NP junctures are attributed. This hot spot effect in the aforementioned assembly structure is unique since it elevates the overall E.F. by > 5 times from the huge value (~10^8) of bare AgNR array. This conjugated nano-assembly structure film was found to be reproducible and will pave the way for high sensitive analyte detection, where the hydrophobic interaction with the alkane chains of dithiols located at the 'hot spots' between AgNR and AgNP will play an important role.

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Comparative study on the gas-phase heats of formation

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Prediction of various physicochemical properties of not-yet-synthesized molecules is a prerequisite for further development of new molecules. Heat of formation is an important property for this purpose. When experimental data is not available, the best way is to compute energy (and enthalpy) using computational packages. Politzer and coworkers estimated heats of formation of organic molecules using BP86/6-31G(d,p) optimized structures and some correction terms involving hybridization states of atoms. The average absolute error (AAE) and standard deviation (SD) were 3 and 4 kcal/mol, respectively. Here, we developed parameters for low-cost computational methods - B3LYP/6-31G(d), AM1 and PM3. We obtained better results for R^2 and SD (0.995 and 2.8 kcal/mol) using B3LYP parameters. Among semi-empirical methods, parameters derived from PM3 can be applied to a routine work for fast prediction of heats of formation of unknown molecules.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Studies on the Reaction of dilithio-1,3-butadiene

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The formation reaction from silyl 1,4-dilithio-1,3-butadiene to lithio silole is investigated theoretically at the CCSD level of theory with 6-31+G(d) basis set in the gas phase. The solvent effects is considered by using IEFPCM in diethyl ether. Without HMPA catalyst, the reaction cannot occur due to a higher activation barrier. Assuming that the HMPA catalyst can dissociate the Li^+ cation(s), the reaction can proceed with small activation barrier both in the gas phase and in solvent.

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Theoretical Studies on the Bimolecular Nucleophilic Substitution Reactions for Benzene Sulphonates with Pyridines

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The kinetics and mechanism of the pyridinolysis (XC_5H_4N) of isothiocyano benzene sulphonates [(Y-$C_6H_4O)S(=O)_2(NCS)$] in acetonitrile are investigated computationally at 25.0 °C using Gaussian 09 package in acetonitrile solvent. According to the literature and several experimental evidences, concerted or a stepwise mechanistic route during the expulsion of isothiocyanate (NCS) leaving group from the intermediate or TS are possible, where positive and negative ρ_X, and β_X values imply the characteristics of the nucleophilic attack. Physical and thermodynamic parameters as well as molecular orbital analysis indicate the concerted back-side nucleophilic attack of pyridines and leaving group (${}^{?}$NCS) departure strategies. In addition, the steric effects of the ligands can play an important role in determining the rates of the reactions.

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DFT study of molecular hydrogen physisorption on graphene

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Over the past few decades, there has been extensive research to seek a solution for the issue of global warming caused from use of fossil fuels. One of the most challenging studies in this realm would be the development on exploitable hydrogen energy, since the hydrogen could be used as a clean and recyclable energy source in fuel cell. In this work, to investigate the physisorption properties more accurately, detailed DFT calculation on various poly-aromatic hydrocarbons (PAHs) as model systems for graphene sheets have been carried out. Several DFT methods including dispersion correction were applied to obtain the binding energy. The basis functions were used DNP(Double Numerical plus Polarization), TNP(Triple Numerical plus polarization), and DNP+(Double Numerical plus polarization). All the calculations were performed by using the material studio DMol^3 code.

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Real-time observation of upconverting nanoparticles in nuclear by cell division

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Upconverting nanoparticles (UCNPs) have been explored as primary vehicle for gene delivery because of their unique properties such as photostability and low toxicity. So far, most studies have shown that UCNPs are in the cytoplasmic and perinuclear regions and aren't situated within a nucleus. Because it does not have a sufficiently small size as to pass through the nuclear pore. In this study, we observed whether UCNPs enter into the nucleus during the cell division or not. Because the nuclear membrane break down during cell division and then UCNPs can traverse through nuclear membrane. We used a epi-fluorescence microscope with 980-nm excitation. It is great interested in biological application such as nuclear-targeted therapy by delivering drug into cancer cell.

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Observation of the photoinduced exciplex formation between the triplet copper(Ⅱ) tetraphenylporphyrin and the hetrocyclic solvent

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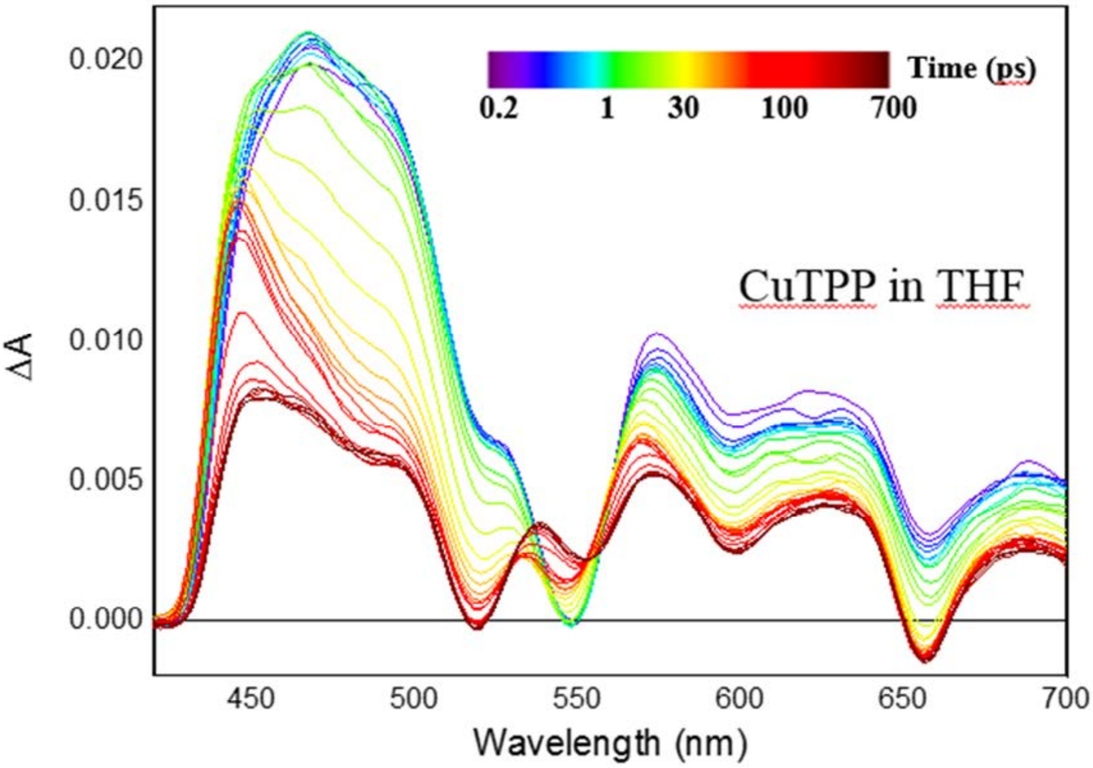
한국과학기술원(KAIST) 화학과

Photorelaxation dynamics of copper (Ⅱ) tetraphenylporphyrin (CuTPP) have been studied with ps and ns transient absorption spectroscopy. Excited complex between the triplet CuTPP and the heterocyclic solvent is the transient species to controversially assign the charge transfer (CT) state or the (d,d*) state. We observed the absorption changes of the exciplex formation of CuTPP with some solvents including N- or O-atoms with broadband femto-TA spectroscopy. The transition metalloporphyrin shows the solvent dependence of the spectra on the contrary to H_2TPP's one being excited at the wavelength of 400 nm. While there are relatively slow dynamics of CuTPP with non-coordinating solvents such as benzene and toluene, the temporal profiles of CuTPP in pyridine, THF, benzonitrile, and 1,4-dioxane have the photodecay process and the derivative-like shape spectra span the range from 500 to 600 nm including slightly red shift at that position in process of time. These variation could occurs as a result of forming the transient exciplex species from a five-coordinating complex. Also, there is no significant changes in piperidine due to predominantly the ground state coordinating complexes explaining them in reference. Presently, we have analyzed these whole spectra for setting the reasonable spectrotemporal models.


Time (ps)
0.2
1
30
100
700
CuTPP in THF
ΔA
0.020
0.015
0.010
0.005
0.000
450
500
550
600
650
700
Wavelength (nm)

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Related between Reaction Rate and Reaction Probability in Monte Carlo Simulations

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Even though the imperfect trap problems have a large variety of applications in physics, chemistry, and biology, it is not easy to relate the experimental reaction rate to the reaction probability in computer simulations since the relationship between the two is ambiguous yet. By comparing theoretical and simulation results, we try to establish the simple relationship between two parameters in one, two, and three regular dimensions. This can increase greatly the versatility of the lattice-based Monte Carlo simulation methods to be straightforwardly applied to more realistic diffusion-reaction systems.

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Monte Carlo simulation studies on the anisotropic diffusion-influenced reaction system

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동아대학교 화학과

Even if the latticed-based Monte Carlo simulation method is one of the simplest numerical experiments for diffusion-reaction systems, the anisotropic systems are not easy to be simulated. We find that anisotropy can be controlled by changing the probability ratio of the stay to the movement in two or three dimensional simulations. We confirm the accuracy of Monte Carlo methods by reproducing the theoretical predictions in isotropic diffusion-reaction systems. Simulation results are easily obtained and compared in anisotropic systems where theoretical predictions are absent.

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Resistive switching characteristics of semiconductor nanowires and nanobelts using conductive atomic force microscopy

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고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자 [2]호서대학교 그린에너지공학과

The resistive switching (RS) characteristics of 1-dimensional nanostructures have been widely studied, as this property is considered promising for nonvolatile memory applications. In this paper, the RS properties of various semiconductor nanowires and nanobelts were investigated using a conductive atomic force microscopy (C-AFM) system. The I-V curves obtained by placing a C-AFM tip as a movable contact on single-crystalline CdS, CdSe, PbS, PbSe, and ZnO nanowires (or nanobelts), are characteristic of reversible bipolar RS behaviors for all devices. The conduction mechanism underlying the RS behaviors of CdS nanobelts is shown to follow a trap-controlled space-charge-limited conduction model. The results suggest that C-AFM can be used to characterize the spatial distribution of conducting channels in 1-dimensional nanostructures.

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Measurement of aromatic molecular ion mobility for separation by High E-field

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Conventional IMS (ion mobility spectrometer) with linear low field is widely used in portable chemical agent detector. Detector should be quickly, accuracy, high selectivity and high sensitivity. To do this, we may regard the ongoing shift of interest from conventional IMS to FAIMS (Field Asymmetric waveform Ion Mobility Spectrometry). Because FAIMS is one of the powerful portable detectors for chemical agents. Our study is focused on nonlinear effect of ion mobility in high electric field. Because the ion mobility itself control the characteristics of FAIMS device.

We have been developed the experimental set up for the measurement of ion mobility, especially, its variation in high field. First we decided benzene, toluene as a sample and then simple electrodes like FAIMS were constructed. Their ionization part used a dye laser to construct the REMPI system. This can simplify whole measurement system. It can simply define the starting time of sample ions, and what they are. Through the experimental set up, we observed ion mobility of nonlinear region in high field. These results would be established simulation of ion mobility in high field. Then it should be applied to optimized asymmetric waveform of FAIMS. The measurement system of ion mobility for the FAIMS device and their mobility values will be presented.

Key word : Ion mobility, FAIMS, nonlinear region in high field, REMPI

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CRASY: Correlated Rotational Alignment Spectroscopy of Acetylacetone Tautomers

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CRASY is a novel type of spectroscopy which correlates high-resolution rotational spectra with femtosecond time-resolved mass or electron spectra. CRASY provides the information of molecular composition, photochemical dynamics, electronic structure, and nuclear structure in a single optical experiment. Therefore, we can identify each of components in impure samples. First, we will look at the mechanism of photochemical reactions in acetylaceton tautomers. CRASY is sufficiently sensitive to identify minority compounds, for instance the minor tautomer acetylaceton. Photochemistry reaction of acetylaceton may be relevant for atmospheric chemistry.

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니켈 이온을 도입한 수산화인회석의 합성 및 물성 연구

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경상대학교 화학과

수산화인회석은 뼈와 무기물의 주성분으로서 칼슘과 인산염으로 구성된다. 본 실험에는 다양한 염기 조건 (2, 5, 10 M NaOH) 하에서 수열합성법 (Hydrothermal method)를 이용하여 합성하였다. 합성된 샘플들은 XRD 분석을 통하여 수산화인회석임을 확인하였으며, 염기 조건을 조절하는 것으로 일정한 모양과 크기를 제어할 수 있다는 것을 확인하였다. 합성된 수산화인회석의 표면에 니켈 이온을 이온 교환 반응을 통하여 도입하였으며, 도입된 표면을 TEM 이미지 관찰을 통하여 분석하였다.

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수산화인회석의 표면에 도입된 은 나노 구조체의 합성 및 물성 연구

표은지 권기영*

경상대학교 화학과

본 연구에서 지지체로 사용된 수산화인회석(Hydroxyapatite)은 칼슘과 인산염으로 구성된 무기물이다. 다양한 농도의 염기조건 (2, 5, 10 M NaOH)하에서 서로 다른 형태의 수산화인회석을 수열합성법 (Hydrothermal method)을 이용하여 합성하였다. 합성된 각각의 수산화인회석은 XRD 분석을 통하여 결정성을 확인하였으며 TEM 이미지 분석 결과 ,일정한 모양과 크기를 형성하는 것을 확인하였다. 합성된 수산화인회석의 표면에 은 나노 입자를 서로 다른 조건 하에서 이온 교환 반응을 통하여 도입하였다. 일정한 조건 하에서 합성된 은 나노 구조체는 XRD 분석을 통하여 은 입자의 존재를 확인하였으며, 도입된 표면에 TEM 이미지 분석을 수행한 결과 은 나노 구조체의 크기를 제어할 수 있다는 것을 확인하였다.

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Highly Sensitive and Selectively Deposited Gold Nanoparticles on the Reduced Graphene Oxide for the SERS Application

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UNIST Chemistry [1]울산과학기술대학교(UNIST) 친환경 에너지 공학부

Surface enhanced Raman scattering (SERS) is the enhancement of the Raman signal by several orders of magnitude via the electromagnetic enhancement or the chemical enhancement of metal nanostructures. In addition, graphene also has a Raman enhancement by its novel property that is referred to graphene enhanced Raman scattering (GERS). In this, we combined electromagnetic enhancement of the gold nanoparticles which has a selectivity onto the sp^2 carbon surface and the GERS effect of patterned reduced graphene oxide (prGO) for the highly sensitive and stable SERS platform. Our SERS substrate can be applied to the diagnostic SERS device and also enables the selective and dense attachment of metal nanoparticles on the graphene surface.

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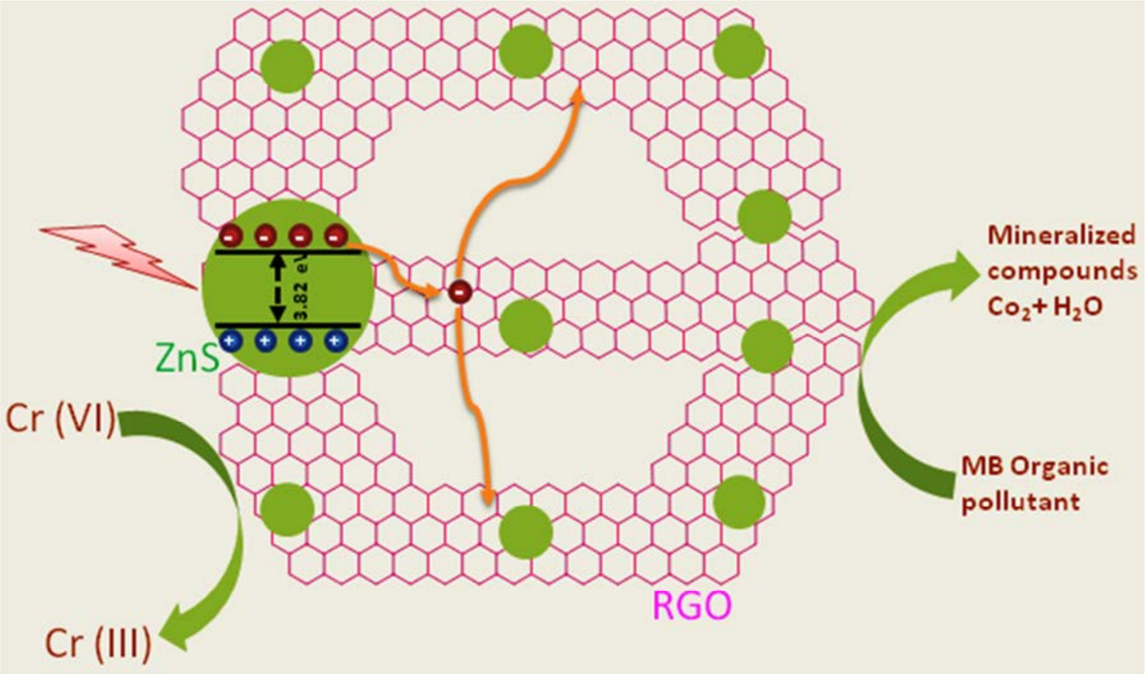
Self-assembled Macro Porous ZnS-Graphene Aerogels for Photocatalytic Degradation of Contaminants in Water

이승희 **devulapalliamaranathareddy** 최지하 마로리 김태규*

부산대학교 화학과

A facile, green protocol for synthesis of self-assembled 3D porous ZnS-graphene aerogels (ZnS-GAs) using vitamin-C to obtain a 3D network of supramolecular hybrid nanostructured materials was developed. Structural, morphological, and optical measurements demonstrate that the ZnS-GAs nanostructures have good crystallinity, and the graphene nanosheets are densely decorated by ZnS nanostructures. The photocatalytic properties of ZnS-GAs were assessed based on photocatalytic degradation of methylene blue (MB) and Cr(VI) under simulated sunlight irradiation. Superior photocatalytic performance was achieved with the ZnS-GAs compared to bare ZnS. This enhancement is ascribed to efficient charge transfer from ZnS to the graphene sheets. Overall, the present work provides new insight into the green synthesis of 3D ZnS-GAs, and the developed composites are highly active photocatalysts with stable cycling that can be exploited in environmentally friendly applications.

Photocatalytic-performance of 3D Porous ZnS-graphene aerosols


Mineralized compounds
Co₂+ H₂O
ZnS
3.82 eV
Cr (VI)
Cr (III)
MB Organic pollutant
RGO

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P3HT Oxidation on Bare and TiO_2-covered ZnO Ripple Structures Evaluated by Photoelectron Spectroscopy

김대한 정명근 박은지 한상욱 이주하 김보라 김승연 박기정 김일희 김영독*

성균관대학교 화학과

P3HT layers with thicknesses of ~5 nm were deposited on bare and TiO_2-covered ZnO ripple structures. The TiO_2 layer with a thickness less than 5 nm was deposited on the the wet-chemically prepared ZnO ripples using atomic layer deposition. Under humid air and visible light illumination, the oxidation behaviors of P3HT on these surfaces were studied using photoelectron spectroscopy. It was found that P3HT on TiO_2/ZnO oxidizes more easily than that on bare ZnO ripples. Using a model substrate of a flat ZnO surface in combination with angle-resolved photoelectron spectroscopy, we found that oxidation of P3HT occurs at the surface of the topmost layer of P3HT, not at the P3HT/oxide interfaces, even though P3HT oxidation is strongly influenced by the interface structure. It is suggested that the lifetime of electron-hole pairs can be strongly influenced by the interface structure, which can also affect the oxidation behavior of P3HT.

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장기저장된 폴리우레탄계 복합화약의 특성 분석

이소정 조은소리 권국태 김진석[1,*]

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부

고가의 정밀유도무기는 실전 배치되면, 오랜 기간 동안 개봉하지 않고 운용된다. 유도무기 내부에 있는 화학물질로 구성된 화약은 시간에 따라서 점점 특성이 변하게 되며, 특히 고분자 물질로 구성된 복합화약의 경우 고분자의 분자량이 변하여 복합화약의 기계적특성이 점점 변하고, 이에 따라서 화약의 각종 특성이 변하게 된다. 화약의 주요 특성으로는 성능특성, 민감도특성 및 열적특성을 대표적으로 들 수 있다. 본 연구에서는 약 35 년 이상 장기 저장된 공대지 유도미사일 내부의 주조형복합화약 3 종에 대하여 구성성분, 민감도 특성 및 열적특성을 비교분석한 연구결과다. 3 종의 화약 중 1 종은 고분자의 노화가 많이 진행되었음을 확인 할 수 있었고, 속감도에서도 민감한 결과를 나타내었다.

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A Structural Understanding of the Amyloid Off-Pathway Assembly Mediated by Metal Ions

이신정 김준곤*

포항공과대학교(POSTECH) 화학과

.Human islet amyloid polypeptides (hIAPP) is one of amyloidogenic proteins which form insoluble β-fibrils via cytoxic aggregation. Particularly, hIAPP is related with the type II diabetes mellitus (T2DM), and it is also known to interact with T2DM-relevant metal ions such as Zn(II) and Cu(II). Herein, we observe that Zn(II) and Cu(II) have the inhibitory effects on hIAPP fibrillation and that they rather facilitate compact oligomer formation. We further investigate the conformational properties of hIAPP associated with these metal ions and suggest an oligomeric assembly pathway also. Similar as other oligomers of amyloid proteins, the metal-mediates oligomers of hIAPP are cytotoxic to cells, but they have distinguished characteristics in the aspect that these metal-associated oligomers are off-pathway not intermediates existing prior to mature fibrils. As the metal-mediated oligomers are off-pathway, these oligomers can give more deteriorative effects persistently. Our understanding of off-pathway oligomerization of metal-associated hIAPP will give insights for design and discovery of therapeutic compounds to target amyloidogenic toxic species.

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Fabrication of Modified Electrodes Based on Au_{25} Nanoclusters for Electrochemical Sensing Applications

장미 이동일*

연세대학교 화학과

Thiolate protected Au_{25} nanoclusters (NCs) have been the focus of intense research because they exhibit unique electrochemical and optical properties with excellent stability. Previous studies revealed that Au_{25} NCs showed excellent electrocatalytic activity toward the oxidation of dopamine, ascorbic acid and uric acid. Au_{25} NCs with these electrochemical properties can be utilized in a variety of electrochemical applications. In this study, we examined several matrices for the immobilization of Au_{25} NCs on electrode. Sol-gel technology has been commonly used for the encapsulation of a variety of materials including gold nanoparticles. Au_{25} NCs were immobilized into (3-mercaptopropyl)-trimethoxysilane (MPTMOS) network via thiol linkers to form Au_{25} sol-gel electrode (Au_{25}SGE). Cyclic voltammograms of Au_{25}SGE exhibited stable, well-defined and reversible redox peaks of Au_{25} NCs. In addition, enzyme sol-gel electrodes prepared by immobilizing glucose oxidase (GOx) on Au_{25}SGE showed electrocatalytic activity toward the oxidation of glucose. In another study, we explored the possibility of using cationic polymers, for example chitosan and polyethylenimine (PEI), to immobilize Au_{25} NCs. Whereas the redox peaks of Au_{25} NCs in chitosan were not well-resolved, they became clearly resolved by the addition of an ionic liquid, for example 1-decyl-3-methylimidazolium tetrafluoroborate ($DMImBF_4$). The electrochemical sensing properties of Au_{25} NCs immobilized in these matrices are also presented.

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Fluorescent-free Immunoassay on Nanobiochip by Wavelength Dependent-enhanced Dark Field Microscopy

이승아 박근영[1] 주소영 강성호*

경희대학교 응용화학과 [1]경희대학교 화학과

Highly sensitive fluorescent-free detection on gold-nanopatterned sandwich immunoassay chips was investigated by a wavelength dependent-plasmon resonance scattering (PRS) technique. Individual silver nanoparticle (SNP) conjugated-target protein molecules on the nanobiochip were selectively detected by the wavelength dependent-enhanced dark field illumination. With the enhanced dark field spectral imaging technique, we observed label-free cardiac troponin I as a model target molecule on 100 nm and 500 nm gold spots by monitoring changes in the plasmonic resonance based on wavelength dependence. Quantitative analysis as a function of increasing PRS intensity was possible in the range of 85 aM - 35 fM through enhanced dark field microscopy. We also showed that the PRS signals from the SNPs (blue color) and the gold spot (yellow color) could be clearly distinguished by using the color camera. The wavelength dependent-enhanced dark field illumination method allows us to selectively detect target biomolecules at the single-molecule level for next generation biochips.

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Prediction of vapor pressure and phase transition enthalpy of energetic plasticizer

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

In the system of melt castable explosives, thermal properties are very important. Because of this reason, analysis of explosives and plasticizers is needed.Recently, studies of energetic plasticizers are very active. And calculation or determination of thermal properties of these energetic plasticizers is also needed.TGA(Thermal Gravimetric Analysis) method is easy to measure and handle.From TGA data, in this presentation we will show calculation of vapor pressure and phase transition enthalpy.They can be calculated using derivation of ideal gas equation and Clausius-Clapeyron equation.Benzoic acid was used as standard material for taking important two constants. And using those constants, we could calculate vapor pressure and phase transition enthalpy of energetic plasticizers.

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Novel One-Capillary Dual-Wavelength Nonaqueous Capillary Electrophoresis for Simultaneous Analysis of Various Synthetic Organic Dyes

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경희대학교 화학과 [1]경희대학교 응용화학과

Dual-wavelength nonaqueous capillary electrophoresis (DW-NACE) was developed for simultaneous analysis of seven synthetic organic dyes [i.e., crystal violet (CV), methyl violet blue (MVB), methyl violet B base (MVB), rhodamine 6G (R6G), rhodamine B Base (RBB), nile blue A (NBA), and methylene blue (MB)] at different emission wavelengths in a single-capillary. All synthetic organic dyes were simultaneously injected, detected, and quantitatively analyzed using two lasers (543 nm laser and 635 nm laser) within 15 min in the dynamic ranges as follow: CV, MVB, MBB (0.5 - 50 μM), R6G (0.05 - 5 nM), MB (0.02 - 10 pM), NBA (0.006 - 10 pM), and RBB (0.4 - 1000 fM). In particular, the limit of detection (LOD, $S/N = 3$) in the RBB was 0.4 fM, which was 2 x 10^5 times lower than the LOD obtained from previous nonaqueous micellar electrokinetic chromatography methods. This novel method shows the feasibility of fast high-throughput screening of various synthetic organic dyes.

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Sub-diffraction limited resolution of nanoparticles by wavelength-modulation plasmonic scattering nanoscopy

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경희대학교 화학과 [1]경희대학교 응용화학과

Sub-diffraction limited resolution of Nanoparticles (NPs) was achieved with wavelength-dependent enhanced dark-field (EDF) illumination. Diffraction limited and color blended adjacent EDF images of gold nanoparticles (GNPs), gold nanorods (GNRs), and silver nanoparticles (SNPs) were modulated at their specific localized surface plasmon resonance wavelengths. The point spread functions of NPs were approximated as symmetric two-dimensional (2D) Gaussian functions and fitted with least-square algorithm to resolve the central coordinates (x, y). The Cram?r-Rao lower bound (CRLB) based localization precisions of GNPs, GNRs, and SNPs were measured as 2.5 nm, 5.0 nm, and 2.9 nm, respectively. According to the resolved coordinates of NPs and the corresponding localization precisions, sub-diffraction limited images were rendered. This novel method was applied in a live single cell and provided remarkable sub-diffraction limited images of NPs.

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Evaluation of UV-curing behaviors for acrylate polymer by real-time FT-IR

박재홍 남궁현*

(주)코오롱 중앙기술원 분석평가센터

Real-time FT-IR spectroscopy enables us to monitor the change of functional groups involving in the polymerization. By detecting the conversion of monomers into polymer as well as unreacted groups in curing polymer, the curing behaviors could be readily observed and characterized. We have developed the optimal FT-IR system consists of an ATR, a mercury xenon UV-lamp, and a FT-IR spectrometer. With the real-time FT-IR spectroscopy, we investigated the characteristics of the curing kinetics of the UV-cuable acrylate. It is found that the proper vibrational band indicating curing process of the acrylate was determined at the 810 cm^{-1}, out of plane, C-H bending in $H_2C=CH-$ group. The curing kinetics of the polymerization was phenomenologically described as a compressed exponential function without physical interpretation. Using this empirical modeling, UV-curing behaviors of the acrylate resin were evaluated with varying photo-initiator concentration. Analysis on the curing behaviors allows us to specify relationship of photo-initiator concentration, curing rate of the polymer, and amount of residual with various UV-curing environments.

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Time-dependent Metabolomics of Traditional Wheat Nuruk Starter Fermentation

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The preliminary metabolomics of traditional wheat Nuruk starter fermentation with the lapse of time was investigated for the primary metabolites including sugars and sugar alcohols, amino acids, several organic acids and fatty acids. In the experiments, two kind of traditional wheat Nuruk starter samples cast in disc-shape were prepared in accordance with the traditional method but just varying fermentation conditions. the one (named as TN-1) was incubated at 36 oC for 30 days and the other (TN-2) at 45 oC for 10 days followed by 35 oC for 20 days. Two commercial Nuruk Starters were used for the metabolomic comparison. The time-dependent Nuruk samples were collected at 0, 3rd, 6th, 10th, 20th, 30th day after start of fermentation. The metabolomic study was performed using GC/MS. For the preparation of the final samples applied to GC/MS analysis, 80% ethanolic extracts of Nuruk samples were derivatized as oximarized and/or silylated ones by further two in-situ chemical modification, i.e. oximation (MeONH2.HCl/pyridine) and silylation (N-methyl-N-(trimethylsilyl)trifluoroacetamide-1% trimethylchlorosilane, 37 oC). The general features is that the variation of metabolites in two traditional Nuruks is not observed, even with the lapse of time. However, the variation of the amount of each metabolite compared in two Nuruk samples is notable. Comparing with the commercial Nuruk Starters (C-1 and C-2), the same tendency in the kind of chemical species metabolized in fermentation was exhibited, but it’s notable that in commercial Nuruk samples the amount in phosphoric acid and sugar alcohols such as xylitol and mannitol is apparently higher than two TN Nuruk samples. However, the variation tendency of the amounts of each metabolite is metabolite-specific fashion.

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Electrocatalytic Conversion of Carbon dioxide Using Atomically Precise Metal Nanoclusters Modified Electrodes

최우준 이동일*

연세대학교 화학과

Conversion of carbon dioxide (CO_2) an unintended byproduct from energy generation and fuel consumption has become the most important worldwide issue. Hence, efficient conversion of CO_2 to valuable chemicals such as syngas, CO, formate and methanol remains one of the challenges for CO_2 utilization. Of the diverse approaches of CO_2 conversion, electrocatalytic reduction of CO_2 has received much attention because it can be easily designed for a continuous process at room temperature. However, the electrode materials such Cu and Ag currently employed in the electrocatalytic reduction of CO_2 exhibit large overpotential and low current density, which makes it difficult to develop carbon neutral process from electrocatalytic methods. In this poster, we report that atomically precise metal nanoclusters for example, $Au_{25}(SR)_{18}$ where SR is thiolate, can be effectively used as homogeneous and heterogeneous catalysts. CO_2 reduction potential was found to be -2.0 V vs. NHE at a glassy carbon electrode in CH_2Cl_2, which decreased significantly in the presence of Au_{25} nanoclusters and more overpotential decreasing was observed by introducing an ionic liquid as co-catalysts. Various types of nanoclusters prepared by doping with foreign metals such as Pt, Pd and Cu offer special advantages in the development of electrocatalysts. The preparation and effects of doping in the electrocatalytic reduction reaction are presented. Au_{25}-based modified electrodes were also found to be an efficient heterogeneous catalyst for the reduction of CO_2. The electroreduction of CO_2 was found to start at -1.2V at glassy carbon electrode in aqueous media and positively shifted to -0.9 V at the modified electrode, indicating the electrocatalytic effect of Au_{25} nanoclusters.

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Electrochemical Sensing Platform Based on Large-Area Gold Nanostructures with Ultraclean and Ultraflat Surface

성유리 김봉수*

한국과학기술원(KAIST) 화학과

Sensitive and selective detection of DNA has attracted great attention since DNA biomarkers are highly related to the onset and progression of disease state. Numerous methods developed for DNA detection, however, still require complex procedures, dedicated equipment, and expert knowledge for analysis. In light of these challenges to overcome, electrochemical sensing methods have become one of the most promising candidate approaches owing to its speed, simplicity and cost-effectiveness. Here, we constructed a new electrochemical sensing platform using large-area gold nanostructures with perfectly clean crystal surfaces which provided biocompatible platform substrate for DNA immobilization. Long-range DNA structures were self-assembled on the gold substrate and methylene blue, electrostatically bound to DNA structures, was used as a redox indicator. We expect that electrochemical signals are increased due to wide and well-arranged self-assembly monolayers of DNA complex on ultraflat and ultraclean gold nanostructures.

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Ultrasensitive detection of disease biomarker by Au nanoplate-Au nanoparticle platform

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Developing the robust sensor platform for the quantitative measurement of target biomarker is desired in cancer diagnosis and therapy. Many researchers have explored the sensitive and reproducible detection. Especially, surface-enhanced Raman scattering (SERS) has been considered as a highly sensitive and robust analysis technique for biomolecule detection. Herein, we newly designed Au nanoplate-Au nanoparticle platform for biomarker sensor. Due to the combination of ultraplat Au nanoplate and nanoparticles, a large number of hot-spots are provided at the surface of Au nanoplate. Ultrasensitive and highly-reproducible sensing was possible by using our novel SERS platform. We anticipate that our Au nanoplate-Au nanoparticle SERS sensor has the great potential in practical cancer diagnosis.

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Determination of radiochemical purity using luminescence imaging

하영수 유정수*

경북대학교 의과대학 분자의학교실

The quantification of radiochemical purity is usually determined by radio-TLC (Thin Layer Chromatography) scanner or radio-HPLC (High-Performance Liquid Chromatography) methods. Radio-TLC scanner method is a relatively simple technique for determining radiochemical purity, which takes few minutes to perform. However, the resolution between closely located spots are limited, and basically radio-TLC scanner generates one-dimensional information from two-dimensional TLC plates. Radio-HPLC method provides better resolution and accurate quantification data but is more complicated method than radio-TLC method; it takes longer time than radio-TLC method and needs expensive chromatograhpic column, and skills for handling HPLC instrument. Here we report a new method of radiochemical purity determination, which utilizes 'Cerenkov radiation' emitted from the radionuclides. We scanned various different TLC plates spotted with radioactivities using a luminescence imaging instrument containing high sensitive CCD (charged-coupled device) detector. All imaging data were quantified and compared with those of conventionally used methods. This new method for the measurement of radiochemical purity is simple, easy to handle but providing accurate quantification data in short time.

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Optimization of chromatographic conditions for analysis of amino acids using hydrophilic interaction column

김희원 차은주[1] 김소희[2] 문명희 이재익[2,*]

연세대학교 화학과 [1]고려대학교 화학과 [2]한국과학기술연구원(KIST) 도핑콘트롤센터

Amino acids play an important biological role in various disease biomarker such as inborn errors of metabolism, parkinsonism, and diabetes. The analytical methods for determination of amino acid have been consistently developed during the past 50 years. However, these methods show difficulty to routinely analysis of amino acids because of zwitterion. The pretreatment of amino acids in these developed methods is usually involved protein precipitation, derivatization and control of pH. The direct process of preparation (e.g. protein precipitation) is very simple and fast. And the indirect process is performed with derivatization for measurement of amino acids. In this study, we optimized the chromatographic conditions for analysis of amino acids using hydrophilic interaction column. The salt concentrations, acid modifiers, composition of mobile phase and oven temperatures have been optimized for the best chromatographic peak shape and sensitivity by direct process. This work was supported in part by Korea Research Institute of Standards and Science and in part by an intramural grant from Korea Institute of Science and Technology.

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Optimization and Application of APCI Hydrogen?Deuterium Exchange Mass Spectrometry (HDX MS) for the Speciation of Nitrogen Compounds

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A systematic study was performed to investigate the utility of atmospheric pressure chemical ionization hydrogen?deuterium exchange mass spectrometry (APCI HDX MS) to identify the structures of nitrogen-containing aromatic compounds. First, experiments were performed to determine the optimized experimental conditions, with dichloromethane and CH3OD found to be good cosolvents for APCI HDX. In addition, a positive correlation between the heated capillary temperature and the observed HDX signal was observed, and it was suggested that the HDX reaction occurred when molecules were contained in the solvent cluster. Second, 20 standard nitrogen-containing compounds were analyzed to investigate whether speciation could be determined based on the different types of ions produced from nitrogen-containing compounds with various functional groups. The number of exchanges occurring within the compounds correlated well with the number of active hydrogen atoms attached to nitrogen, and it was confirmed that APCI HDX MS could be used to determine speciation. The results obtained by APCI HDX MS were combined with the subsequent investigation of the double bond equivalence distribution and indicated that resins of shale oil extract contained mostly pyridine type nitrogen compounds. This study confirmed that APCI HDX MS can be added to previously reported chemical ionization, electrospray ionization, and atmospheric pressure photo ionization-based HDX methods, which can be used for structural elucidation by mass spectrometry.

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Global phosphopeptide enrichment by grating phospho-specific antibodies into online mHFER-nanoLC-ESI-MS/MS

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Phosphoprotein, one of post translational modifications, is involved in cellular processes such as cell proliferation, cell signaling, and apoptosis. Mass spectrometry in phosphoproteomics is commonly utilized due to accuracy, sensitivity, and precision. However, phosphoproteins in MS analysis have several limitations due to low abundant and low ionization efficiency caused by negatively charge ion of phosphates in general MS analysis with a positive acquisition mode. Although conventional enrichments (e.g., SCX, IMAC, and TiO_2) in phosphoproteome has been widely used, a large amount of proteins (above 500 ug) is inevitably required for next shotgun analysis. Herein, we introduce a new strategy for enrichment of targeted phosphopeptides whereby that enables the identification of phosphopeptides and their sites of phosphorylation with the smallest sample amount (~1 ug). To this end, we newly developed the concept of coupling online microbore hollow fiber enzyme reactor (mHFER) with phospho-sepcific antibodies (pAbs) to selectively enrich targeted phosphopeptides from protein complex mixture. In pAbs-based online phosphopeptide enrichment with mHFER, tryptic peptides obtained from MCF7 were mixed with pAbs, and then followed by the mixture was injected into online mHFER-nanoLC-ESI-FT orbitrap-MS/MS. The peptides having no-affinity with pAbs were washed out during flow-through in the mHFER (10 kDa in MW cutoff), and the remaining phosphopeptides eluted subsequentially from mHFER by tryptic digestion were subjected to online shotgun analysis. As a result, we found that pAbs-based online mHFER is highly selective, precise, and suitable for phosphopeptide enrichment, compared to that of conventional mothods.

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Analytical method for simultaneous assay for the detection of human butyrylcholinesterase and albumin adducts to exposure to nerve agents

이진영

국방과학연구소 5본부 3부

Organophosphorus (OP) nerve agents inhibit the activity of cholinesterases by phosphylation of the active site serine-198. In addition, sarine (GB), soman (GD) and tabun(GA) have been shown to phosphylate a tyrosine-411 residue in albumin. Organophosphate-inhibited butyrylcholinesterase (BuChE) in human plasma is the most persistent and abundant source for biomonitoring of exposure to organophosphate anticholinesterases.Basically, three approaches have been explored to detect exposure to an organophosphorus nerve agents, fluoride reactivation, enzyme digestion for BuChE and Albumin. To purify the each BuChE and Albumin from the human plasma, another affinity column was needed and plasma samples were consumed respectively. This work is time-consuming and a labor intensive process.We developed new sample treatment and simultaneous analytical method for the detection of human butyrylcholinesterase and albumin adducts to exposure to nerve agents.

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Application of isotope-coded carbamidomethylation for absolute quantification of human serum BNP-32 using a nanoLC-ESI-MS/MS

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Brain natriuretic peptide-32 (BNP-32) is widely known as an essential biomarker in congestive heart failure (CHF). N-terminal proBNP, a precursor form of BNP-32, is more abundant than that of cardiac troponin T, when exposed to the extraordinary left ventricle-ejection fraction (LV-EF) caused by CHF. In spite of determination of BNP-32 in human serum is essential for precise determination of CHF, it is still challenges, due to its low abundance in human serum (100 pg/mL) and higher variation in measuring targeted BNP-32 using an immunoassay. Here, we applied a novel and simple isotope labeling method, named as isotope-coded carbamidomethylation (iCCM), to the quantification of the human BNP-32. In iCCM, two aliquots of BNP-32, having two cysteine residues, was denatured with a reducing buffer (50 mM ammonium bicarbonate contained with 10 mM dithiothreitol) and then alkylated separately with each of iodoacetamide (IAA) as carbamidomethylation (CM) and its isotope (IAA-13C2, D2), thereby leading to the mass difference of 8 Da between CM- and iCCM-labeled BNP-32. To evaluate the efficiency of iCCM approach, the CM- and iCCM-labeled BNP-32 standards were pooled at five different mixing ratios and then introduced into nanoLC-ESI-MS/MS. As a result, the mixing ratios of CM-/iCCM-peptides were dramatically matched with their expected ratios with good linearity (R2=0.9999). The developed iCCM strategy is an alternative tool for quantification and early diagnosis of BNP-32 in CHF patients.

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Top-down and bottom-up lipidomic analysis of lipoproteins from rabbits by FlFFF and mass spectrometry

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Lipidomic analysis from lipoproteins requires separation of high-density lipoproteins (HDL) and low-density lipoproteins(LDL), followed by mass spectrometry (MS). In a separation technique of flow field-flow fractionation (FlFFF), particles attain different equilibrium heights based on their sizes and smaller particles at the higher equilibrium height elute faster than larger particles, having a higher velocity in the flow-driven laminar flow. As the size of HDL is smaller than that of LDL, separation of lipoproteins from plasma is easily achieved by FlFFF in their intact forms. The bottom-up lipidomic analysis of lipoproteins is carried out by FlFFF for fractionation of lipoproteins, lipid extraction, and analysis by liquid-chromatography-mass spectrometry (LC-MS). Although bottom-up method can provide an extensive library of lipids, it requires tediously long preparation or analysis time, which is extremely inconvenient when the sample set is large. For analysis of targeted lipids from lipoproteins, top-down approach of on-line FlFFF-MS can shorten the analysis time as neither of off-line FlFFF nor lipid extraction is required and still provides highly accurate analysis. In this study, a comprehensive lipidomic analysis of lipoproteins from pooled serum samples of rabbits with metabolic conditions were investigated by the bottom-up approach using multiplexed hollow fiber FlFFF (MxHF5) for separation and collection of lipoproteins, followed by nanoflow LC-ESI-MS/MS for lipid analysis. Based on the result from bottom-up method, lipid species showing significant differences between groups of rabbits were selected and quantified by individual samples in top-down chip-type asymmetrical FlFFF-ESI-MS/MS.

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Evaluating the Effect of Cross-linking Agent Content and Polymerization Methods on Molecular Weight and Structure of Branched Cationic Polyacrylamide Copolymer by Frit-inlet Asymmetrical Flow Field-Flow Fractionation &Multi-angle Light Scattering

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연세대학교 화학과

Polyacrylamide (PAM) consists of acrylamide monomers, which form long-chain polymers by free radical polymerization, and it is widely used as flocculant in waste water treatment and oil removals. For higher efficiency in flocculation, molecular weights, structures, and charge densities of PAM must be taken into consideration. For negatively charged particles in waste water, branched cationic PAM has been reported to be more efficient flocculant than linear one as branched one has lower viscosity and higher solubility than linear polymers. In this research, effect of different amount of crosslinking agent and different kinds of polymerization methods on absolute molecular weight and structure of branched cationic PAM copolymers were investigated. Different amount of crosslinking agent determines the number of branches per polymer molecule, which eventually affects the structure and molecular weight. As the amount of crosslinking agent increases, polymers are predicted to be more compact in sizes. Two different polymerization methods, solution and emulsion polymerization, affect the chain length of polymer, which changes the molecular weight and RMS radius of the copolymer. Changes in molecular weight and RMS radius by the content of crosslinking agent and different polymerization methods were analyzed by frit-inlet asymmetrical flow field-flow fractionation (FIAF4)-multi-angle light scattering (MALS).

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Lipid Profiling of Diabetic Rat Muscle tissues under Physical Exercises using Nanoflow LC-ESI-MS/MS

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연세대학교 화학과

Lipids are responsible for various biological functions such as constituents of cell membrane and participants in cell signaling, and they are relevant to the development of various human diseases such as diabetes. As diabetes develop, general lipids profile is likely to alter from that of healthy control. Exercise has been reported as one of the major factors that alters the lipids profile in many types of diseases. Thus, lipidomic research on the change in the abundance of lipid species induced by exercise is important in revealing the correlation between diabetes and exercise.In this research, the gastrocnemius and soleus muscles of skeletal muscles from the lower leg were selected to investigate the effect of exercise on healthy controls and diabetic models. While gastrocnemius is mainly composed of white muscle that contracts lower leg rapidly and powerfully by anaerobic bursts of activity, and soleus is a red muscle that contracts for longer period of time with little force by aerobic bursts of activity. Lipids in gastrocnemius and soleus skeletal muscles from four groups of rats - healthy controls, healthy controls under exercise, diabetic models, and diabetic models under exercise - were investigated to discover the lipid species showing significant differences between healthy and diabetic rats, and to evaluate how exercise changes the profile of lipids from healthy and diabetic rats. Lipids in two different muscles were extracted from pooled samples in each group using the modified Folch method with MTBE/MeOH, and characterized by nanoflow liquid chromatography electrospray-ionization tandem mass spectrometry (nLC-ESI-MS/MS). A total of 245 and 252 lipid species from gastrocnemius and soleus muscles, respectively, were identified and analyzed quantitatively.

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Effect of Incubating Microbial Species in Freshwater on Dissolved Organic Matters by Flow Field-Flow Fractionation

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Dissolved organic matters (DOM) and particulate organic matters (POM) are organic substances that are generated by microbial metabolism in the environment and are widely distributed in soil and freshwater. There have been a number of studies that adopted various methods to analyze and characterize organic matters. Among different kinds of organic matters, biodegradable organic matters (BOM) are fraction of organic matters that are ingested and metabolized by microbial species. In this study, asymmetrical flow field-flow fractionation (AF4) was utilized to analyze biodegradable DOM (BDOM) and POM (BPOM) in forest stream, agricultural stream, and Bamseom in Korea and characterize the change in organic matters caused by incubating microbial species in each sample. Since humic and fulvic substances, which best represent the organic matters in most of the freshwater, are sensitive to change in ionic strength of the carrier solution used in AF4, it is important to optimize the condition of the carrier solution to obtain reproducible result. Also the retention of organic matters during analysis is affected by the type of membrane material used. In this experiment, by examining the result of changing ionic strength of carrier solution and membrane material, the best carrier solution and membrane material for fractionation were selected.Two different signals, protein-like and humic-like signals, were selected to characterize two types of fluorophores in each sample. After the fractogram of each sample is obtained, peak areas of before- and after-incubation samples are compared to see the degree of degradation of each kind of organic matters by the microbial species.

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High Speed Subcellular Organelle Fractionation by Flow Field-Flow Fractionation

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Subcellular organelles have their own specific roles in cells. When organelles malfunction in cells, activities of proteins in cells can be affected, causing organelle related diseases. Researches on discovering biomarkers of disease by separating organelles have attracted increased attention in biological research fields. Therefore, in subcellular organelle studies, fractionation of organelle is a fundamental and crucial stepUsually, separation of subcellular organelles is conducted by centrifugal methods but even though procedures are relatively simple and easy to carry out, the methods can be time-consuming as they require additional purification processes due to the low efficiency in purification. Besides centrifugal methods, fractionation of subcellular organelles can be conducted by fluorescence activated sorting or affinity purification methods. However, these methods usually require relatively complex preprocessing steps. Flow field-flow fractionation (FlFFF) is an elution method based on size-separation. In this study, FlFFF was attempted to fractionate the various cell organelles in a short period of times without any complex pre-processing steps. Separation of organelle was carried out in a steric mode of FFF and completed within 15 minutes. Organelles in each fraction were confirmed with different methods of scanning electron microscope (SEM) for observe and compare the particle sizes and western blotting to identify organelle markers. Lastly, by using nanoflow liquid chromatography and tandem mass spectrometry, subcellular proteins from each fraction was analyzed.

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Profiling of phosphoproteome from respiratory syncytial virus-inducedsera using phospho-specific antibodies in combination with online mHFER nLC-ESI-FT orbitrap-MS/MS

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Respiratory syncytial virus (RSV) is a major pathogen of infants and young children, and its infection annually results more than 300,000 deaths worldwide. Although the proteomic study for treatment of disease caused by RSV has been reported, discovering biomarker of RSV is not fully evaluated. To unveil a biomarker from RSV-induced samples, we carried out the profiling of phosphoproteome in RSV-induced sera. Phosphoprotein, one of post translational modifications, is relevant to many human diseases and bioresponses. In order to profile phosphoproteome from RSV-induced sera, phospho-specific antibodies (pAbs) with online microbore hollow fiber enzyme reactor (mHFER, M.W. cut off 10 kDa) was utilized for phosphopeptides enrichment. RSV-induced mouse sera (3days and 7days) and control (0 day) were digested with trypsin and proteolytic peptides from each mouse serum (0day, 3days, 7days) were reacted with pAbs for 1 hour at 4℃. The resulting mixture was introduced into online mHFER-nLC-ESI-MS/MS. Both of ordinary peptides and phosphopeptides having no affinity with pAbs will be first eluted during flow-through run, and the remaining phosphopeptides in mHFER were simultaneously released by trypsin. Consequently, phosphopeptide enrichment utilizing pAbs-based online-mHFER facilitates for understanding cell signaling in RSV infection pathway and contributing development of therapeutic agent.

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Enantiomer separation of acidic chiral compounds on a quinine-silica hybrid monolith by capillary electrochromatography

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영남대학교 화학과

An organic-silica hybrid capillary monolithic column was prepared by a ‘one-pot’ process in a fused silica capillary with weak anion-exchanger, tert-butylcarbamoylquinine as chiral selector. The column was employed for electrochromatographic enantioresolution of acidic chiral compounds using mobile phases consisting of acetonitrile and methanol as organic solvents, and acetic acid and triethylamine as background electrolyte. The influences of several experimental parameters (electrolyte concentration, acetic acid?triethylamine ratio and acetonitrile?methanol ratio) were evaluated in order to obtain improved enantioselectivity and efficiency as well as short run times for the enantiomeric separation of acidic chiral compounds.

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Highly active graphene based Ni-Pd binary alloyed catalysts for electrooxidation of ethanol in an alkaline media

Mohammad Shamsuddin 전승원*

전남대학교 화학과

Highly active graphene (G)-supported NixPd100-x binary alloyed catalysts (BACs) were prepared with the variation of Ni and Pd metals loading, through a facile chemical reduction method and used as an anode catalyst for ethanol oxidation reaction (EOR). The X-ray diffraction reveals that the NixPd100-x/G catalysts were homogeneously alloyed and Ni was present with the oxidized form. The transmission electron microscopy images also suggest the alloyed formation with different shapes of metal nanoparticles (NPs). The electrochemical properties of the catalysts were evaluated using cyclic voltammetry (CV) and chronoamperometry (CA) in 1 M KOH electrolyte. The higher catalytic activity for EOR was observed in Ni50Pd50/G. Among all NixPd100-x/G BACs, the Ni50Pd50/G catalyst showed highest onset potential (?0.8 V) with long term stability. The overall parameters of EOR study were determined that the Ni50Pd50/G was more favorable in various ethanol concentration and scan rate.

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An amerometric biosensor for Virus Proteins

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In this presentation, we demonstrate a sandwich assay platform involving aptamer-protein-antibody complex for the electrochemical detection of virus protein onto a gold nanoparticle modified electrode surface. Our attempt was to achieve viral protein (e.g. H5N1) sensing through the measurement of associated current resulting from the enzymatic reaction between alkaline phosphatase conjugated to anti-H5N1 adsorbed onto aptamer/H5N1 surface complexes and the substrate, 4-amino phenyl phosphate (APP).Cyclic and differential voltammetry methods were used to characterize the detection method.

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Separation of differently sized gold nanorods using gel electrophoresis

김수희 이혜진[1,*]

경북대학교 자연과학대학/화학과 [1]경북대학교 화학과

본 포스터에서는 불균일하게 크기가 분포되어 있는 금 나노로드 콜로이드 용액으로부터 균일한 크기의 나노로드를 젤 영동법으로 분리하기 위해 젤 매트리스 및 계면활성제 농도를 변화시켜 분리법을 최적화시키고자 하였다. 이와 함께, 항체로 코팅된 금나노로드 입자를 크기별로 분리하는데 최적화된 방법을 적용하였다. 젤 영동 분리 실험 결과를 전자투과현미경(TEM) 이미지와 UV-vis 분광법을 이용하여 확인하였다.

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Structural characterization of MAS NMR as a cathode material for lithium ion battery

안지은 김민지 하지원 이영일*

울산대학교 화학과

$LiCoO_2$ is generally used as the cathode material, however, it has the thermal instability, poor rate performance, and the toxicity and high cost. As alternative $LiCoO_2$, $xLi_2M'O_3*(1-x)LiMO_2$ electrode materials (M′= Mn, Ti and M = Mn, Ni, Co) have attracted much attention due to its high rate performance and improved safety. In this work, structural investigations of $LiNi_{0.8}Co_{0.1}Mn_{0.1}$, $LiNi_{0.8}Co_{0.15}Mn_{0.05}$, $LiCo_xAl_yO_2$ cathode materials has been performed by ^7Li , ^{27}Al and ^{59}Co MAS NMR.

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Characterization of bleached human hair by FT-IR microspectroscopy and Chemical imaging

<u>장원형</u> 유수련[1,*] 권오선 신관우[2,*]

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

The FT-IR imaging method enables chemical imaging by combining the spectral and spatial information. The chemical images consist of chemical information from all pixels covering the measuring areas at the same time. It also useful method of analysis for human hair, with the ability to analyze the central core, cortex, of cross sectioned hair. We studied bleaching of the hair, and checked chemical effects as a function of position in the hair cross section. Many researchers observed the surface of hair using SEM, and now it is well known that cuticle layers lift and break. The transformation due to breakage of a specific chemical group was observed and spatially characterized. In this study, the products from disulfide oxidation of the amino acid cystine are sulfonic acid of cystine, cystine monoxide, and cystine dioxide. We observed the cystine monoxide band from the products of disulfide oxidation of the amino acid cystine that is also associated with hair damaging. By spectrally mapping infrared functional groups, the images of the damaged location can be obtained from bleached hairs.

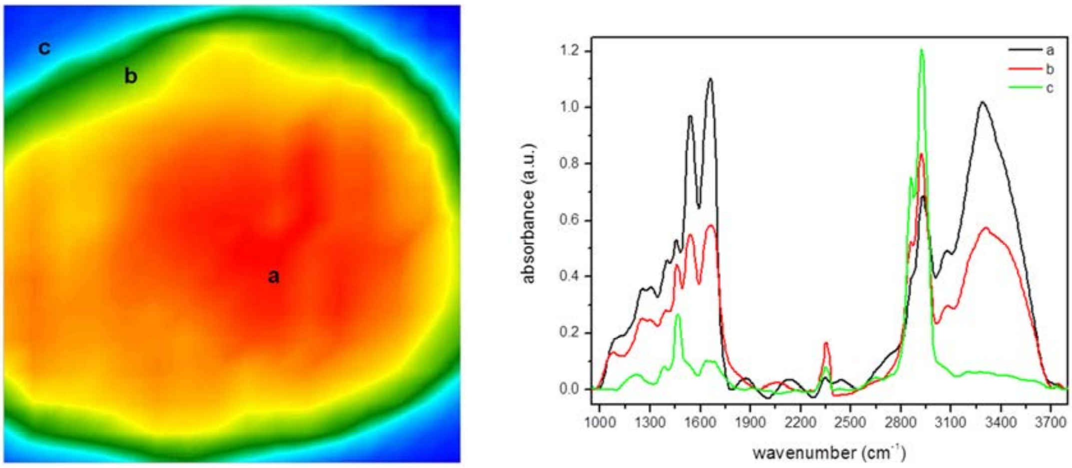

Figure 1. Chemical image and FT-IR spectra of cross-sectioned human hair.

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The Development of Combined System with Parabolic IR Emitter and Pyroelelctric sensor within Bandpass Filter for Open Path Remote Analysis

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한국건설기술연구원 화재안전연구센터 [1]동덕여자대학교 약학대학

화재 시 화염과 더불어 독성 가스가 발생하며 이 가스를 현장에서 분석할 때 여러 가지 방식이 사용되고 있다. 기존 방식은 발생가스를 직접 샘플링하여 실험실에서 측정하는 방법이 주로 사용되었으나, 샘플링 등의 절차에서 발생되는 분석오류를 줄이기 위해 현장에서 샘플링없이 직접 측정하는 방식이 요구되고 있다. 화재 현장의 경우 화재 위험 반경에 때문에 근접 분석이 어려워 원거리에서 측정하여야하며, 현재 사용하는 원거리 분석 장치(Passive Open Path FT-IR)의 장비 크기 및 이동 문제로 현장 접근성에 어려운 단점이 있다. 따라서 원거리 분석을 용이하게 하기 위해 센서의 크기를 최소화하고 측정자의 위험을 최소화하기 위해, 무선 통신을 통하여 가스를 모니터링하도록 개발하였다. 원거리 측정을 위하여 고 감도 Pyroelelctric sensor 와 Silicon nitride 소재로 한 Parabolic 적외선 광원으로 구성하였으며, 무선 통신은 blue-tooth 통신으로 구성하였다. 이러한 장비를 사용하여 CO 등 화재 관련 데이터를 정량 분석한 결과 상관계수(R2)가 0.9 이상의 높은 선형성을 확인하여 원거리 측정의 가능성을 입증하였다.

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Fabrication and evaluation of erythromycin-incorporated zirconia hybrid monolith for enantioseparation of basic analytes using capillary electrochromatography

dixitshuchi 박정학*

영남대학교 화학과

Erythromycin (ERY), a macrolide antibiotic, has been successfully employed as a chiral selector in high-performance liquid chromatography and capillary electrophoresis due to its unique structural features and functionalities that allow multiple interactions (electrostatic, inclusion, hydrogen bonding etc.) with analytes having widely different structures. Nevertheless, a comprehensive survey of literature reveals no reports on application of ERY as CS in capillary electrochromatography (CEC) until date. The present work was therefore designed to address the said void by fabrication and evaluation of chiral discriminating abilities of erythromycin-incorporated zirconia hybrid monolith (ERY-ZHM) using CEC. The monolith was prepared by a single-step in-situ sol-gel approach using triethoxysilylpropylcarbamate derivative of ERY (TEOSPC-ERY) as a co-precursor to form a porous zirconia network inside a fused-silica capillary. A sol solution consisting of 5×10-3 M of polyethylene glycol, 1 M water, 2 M acetic acid and 0.06/0.94 ratio of TEOSPC-ERY/zirconium butoxide resulted in homogeneous monolith having well defined through-pores and tightly anchored to the capillary wall. Baseline resolutions were observed on thus-prepared column for eight basic chiral drugs (i.e., propranolol, atenolol, metoprolol, citalopram, indapamide, cetirizine, atropine and sertraline) in mobile phase consisting of 10/90 MeCN/TEAA (10mM, pH 8) at applied voltage of 10 kV and temperature 25ºC. The RSD values for retention time and resolution were less than 2.0% and 2.5%, respectively, for separation of propranolol enantiomers under optimized conditions while using three columns prepared from three different sol-gel batches. This indicates excellent reproducibility of the simple and single-step approach for preparation of ERY-HZM reported in the present work.

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Simultaneous Analysis of NSAIDs in Aqueous Sample by Dispersive Liquid-Liquid Microextraction (DLLME) and LC/MS

박소연 명승운*

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Dispersive liquid-liquid microextraction (DLLME) may be utilized as a green chemistry approach to reduce the consumption of hazardous organic solvents in the chemical analysis. A simple and efficient sample preparation method was developed using DLLME prior to LC/MS analysis for simultaneous extraction and determination of trace amounts of Non-Steroidial Anti-Inflammatory Drugs (NSAIDs) including indoprofen, ketoprofen, naproxen, diclofenac, ibuprofen, mefenamic acid, tolfenamic acid from an aqueous sample. Optimal dispersive solvent and extraction solvent were chosen acetonitrile and chloroform, respectively. Simultaneous chromatographic separation of seven NSAIDs by HPLC/MS system was achieved on an Eclipse XDB-C18 (2.0 mm i.d. × 150 mm length, 5 ㎛ particle size) column using isocratic elution with 0.1 % formic acid and methanol (30:70).

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Chemical Speciation Applied Supercritical Fluid Chromatography-atmospheric Pressure Photon Ionization Hydrogen/Deuterium Exchange (HDX) Mass Spectrometry for Structural Anaylsis

조윤주 김성환*

경북대학교 화학과

For comprehensive complicated mixture, structural identification is a very important for mass spectrometry analysis of poly aromatic hydrocarbon compounds. Hydrogen/Deuterium Exchange (HDX) technique has been used for structual interpretation in proteins, peptides, metabolites, antibiotics and petroleomics. However, HDX technique is limited because expensive deuterium solvent is used a lot and hence coupling to high performance liquid chromatography (HPLC) has been limited. In this study, HDX tendency of 21 standard compounds including polar heteroatoms at the molecular level was identified by combination of HDX in the process of atmospheric pressure photo ionization (APPI) and Supercritical fluid chromatography-Mass Spectrometry (SFC-MS). SFC utilizes supercritical carbon dioxide, methanol as mobile phase and offers a faster runtime in comparison with HPLC which is used aprotic solvents. In other words, mobile phase only a little of deuterated methanol is needed when HDX is applied to SFC. 0.3 mL of CH3OD for deuterium exchange was just used during all chemicals was eluted in 9 minutes. Overall, HDX SFC-MS was successfully applied to nitrogen-containing compounds preliminary to analysis of heavy crude oils for structual elucidation. Therfore, these results are examples of using powerful separation technique and we expect that this developed technique will be carried out to study crude oils and metabolites where a many unknown compounds have to be determined.

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Electrochemical and HPLC analysis of anticancer drugs

한혜연 이혜진[1,*]

경북대학교 화학 [1]경북대학교 화학과

본 포스터는 서로 섞이지 않는 두 전해질 (수용성 액체/유기성 액체) 계면에서 항암제가 전이하는 반응에 따라 전류 값의 변화를 측정하는데 기초를 둔 항암제 검출용 전기화학 센서 개발에 관한 연구 결과를 나타냈다. 수용성 액체와 유기성 액체 사이에 계면을 형성하고 전압을 걸어주었을 때, 물에 존재하는 약물 이온이 유기용액으로 전이하는 정도에 따라 전류의 변화가 일어나는 것을 순환전압전류법과 시차펄스 전위법을 사용하여 분석하였다. 또한, 항암제를 검출한 전기화학적 데이터와 HPLC 로 분석한 결과를 비교분석하였다.

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The Quantification and Characterization of N-linked Glycans by Capillary Electrophoresis UV-Visble Spectroscopy and Capillary Electrophoresis Mass Spectrometry

서현경 정다솜 이용일 임재민*

창원대학교 화학과

Glycosylation is attaching the oligosaccharides to proteins or peptides by post-translational modification processing. Various investigations concerning quantitative glycan analysis have been performed because of the importance of the oligosaccharide moieties on glycoproteins that affect a wide range of protein functions such as cellular recognition processes.Presently, capillary electrophoresis (CE) has become an accepted technique for the analysis of the biomolecules. The biomolecules can be separated by CE with high speed and resolution. In this study, the quantitative analysis of N-linked glycans of the glycoprotein has performed in UV-Visble spectroscopy with 2-amino benzamide (2-AB) labeling techniques. The structural analysis of N-linked glycans was characterised by capillary electrophoresis tandem mass spectrometry (CE-MS/MS)Key WordsCapillary electrophoresis, Mass spectrometry, UV-Visble spectroscopy, 2-AB labeling and N-linked glycan

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Carboxyl Modification of Peptides with Linear Aliphatic Diamines for Increasing Charge States

김상진 김한별 서현경 이용일 신동수 임재민*

창원대학교 화학과

Mass spectrometry has been used usually in protein identification. Especially mass spectrometry played a significant role in the analysis of peptides sequence, as well as posttranslational modification (PTM) analysis. However, analysis of PTMs, such as phosphorylation and glycosylation, is difficult with collision-induced dissociation (CID) by the loss of modification residues. The CID and electron-transfer dissociation (ETD) are complementary each other to interpret the PTMs. But ETD is particularly ineffective for the dissociation of tryptic peptide in doubly and singly charge states.In this study, we have tested carboxyl modification of peptides as a method for increasing the charge states of peptides in electrospray ionization with tandem mass spectrometry (ESI-MS/MS). The carboxyl-reactive crosslinker reagent 1-[Bis(dimethylamino)methylene]-1H-1,2,3-triazolo[4,5-b]pyridinium 3-oxid hexafluorophosphate (HATU) is used to crosslink the carboxylic acid group of the peptide angiotensin II and the tryptic digested albumin peptides to linear aliphatic diamines such as ethane-1,2-diamine, butane-1,4-diamine, and hexane-1,6-diamine.As a result, the carboxyl modified peptides increased the most abundant charge state compared to native peptides. The longer crosslinkers effectively increased the most abundant charge state because of the reduction of the charge repulsion in the peptides.Key WordsPeptide, Carboxyl modification, ETD, Mass spectrometry, HATU, and Linear aliphatic diamines

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An EWOD (electrowetting-on-dielectrics) platform for detection of chemical and biological warfares

장인애 권오선 신관우[1] 오한빈[*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Electrowetting-on-dielectrics (EWOD) devices actuate droplets of volumes up to several microliters using the principle of modulating the intersurfacial tension between an electrode coated with a dielectric layer and a liquid droplet. In this study, we have sought to perform sample preparation for MALDI-TOF detection of chemical and biological warfares using EWOD technology. In this study, electrodes were patterned on the paper with a conducting material and then its surface was coated with a dielectric layer of parylene-C and covered with a Teflon AF thin film to increase hydrophobicity on the surface of the chip. Application of voltage potential to the electrodes reduces the solid-liquid interfacial tension, so resulting in movement of a droplet through a series of electrodes. This result is expected to help one achieve the automation of the detection of chemical warfares. In the poster-session, the detailed experimental setup and the results will be presented.

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MALDI-TOF Quantitative Analysis of Polymeric guanidine-containing Biocide ingredients in commercial products

배정은 장인애 김은희 오한빈*

서강대학교 화학과

Guanidine-containing polymeric ingredients, such as polyhexamethylene guanidine (PHMG) and poly hexamethylene biguanidine (PHMB), possess antiseptic, antibacterial activity and therefore are able to prevent the growth of bacterial, mold, and any microbe. Due to this reason, these biocidal ingredients are used in commercial products such as wet wipes, humidifier disinfectants, contact lens cleansers, and cosmetic removers. Recently, it was reported that long-term exposure to guanidine-containing polymeric biocides can cause pulmonary disease when it is inhaled in a form of droplets. For this reason, the necessity to qualitatively and quantitatively analyze these compounds has been addressed. In the present study, we developed a sample purification and enrichment procedure for the analysis of these PHMG and PHMB, and the pre-processed sample was analyzed using MALDI-TOF mass spectrometry. And, we proved for quantitative analysis of PHMG and PHMB by applying the internal standard method. We have tested several internal standards which were chosen based on the similarity to PHMG; internal standard using 13C-guanidine substituted PHMG shows different distribution in comparison with normal PHMG which can overcome the peak overlapping. The developed method is expected to provide a useful protocol for the quantitative analysis of guanidine-containing polymeric biocides use in commercial consumer products.

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TEMPO-assisted FRIPS MS analysis of a peptide with three or more disulfide bonds

김은희 오한빈*

서강대학교 화학과

We characterized the small proteins of insulin (51 amino acids, 5,733 Da) using FRIPS (free radical initiated peptide sequencing) mass spectrometry. Insulin consists of two segments, A-chain and B-chain, which are linked together by a multiple disulfide bonds, TEMPO-assisted FRIPS MS approach is reported to selectively cleave the disulfide bond. However, it is not reported yet whether or not it is applicable for peptides/proteins with multiple disulfide bonds. In the present study, we applied the TEMPO-assisted FRIPS approach to the insulin to see how multiple disulfide bonds affects the fragmentation behavior of peptides with multiple disulfide bonds. In our preliminary results, it was found that with TEMPO-assisted FRIPS can provide more detailed structural information of insulin without the reduction of disulfide bonds than the conventional CID could do. In the symposium, we will discuss the potential use future direction of the current research.

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Radical-based peptide fragmentation MS

류이슬 오한빈*

서강대학교 화학과

The bottom-up MS approach is most widely applied to identify and characterize proteins. However, there exists a weakness that the sequence coverage is rather low. To achieve a better sequence coverage, the middle-down MS approach has been suggested as a complementary tool, which is run in parallel with the bottom-up MS. With this information, we have sought to extend the TEMPO-assisted FRIPS (free radical initiated peptide sequencing) MS approach to the middle-down MS of proteins. As a preliminary study, first, we have explored the possibility of characterizing a relatively large peptide of melittin of ~3 kDa using TEMPO-assisted FRIPS MS, which showed extensive backbone fragmentations. Motivated at the promising results for melittin analysis, we applied the FRIPS methods to peptides produced by Lys-N digestion of BSA. As Lys-N cleaves at N-terminal side of lysine amino acid, it is expected that a longer peptide sequence can be obtained compared with the trypsin digestion that are mostly used in the bottom-up method. For the longer peptides, it was revealed that extensive a, c, x, and z-type fragments were generated in FRIPS MS. Further details of our study will be presented in the symposium.

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Colloidal Carbon Black Nanoparticles & Graphene Oxide Embedded Thin Sol-Gel Film for Dye Molecule Analysis of Handwriting Inks by Laser Desorption/Ionization Mass Spectrometry

방승훈* **차상원[1]** **이광빈[1]** **조성민[2]**

국방부조사본부 과학수사연구소 [1]한국외국어대학교 화학과 [2]서울대학교 화학부

Colloidal carbon black nanoparticles were used as a matrix for matrix-assisted laser desorption/ionization(MALDI) analysis of Handwriting ink dye mollecules. For the application of the analysis method of forged document using the surface-assisted laser desorption/ionization(SALDI) similar to MALDI, we conducted a research to use the Spraying Method of Carbon Black nanoparticles to enhance the detection sensitivity of dyes such as Methyl volet, Crystal violet,Rhodamine B and other 12 dyes on paper and real inks on paper of handwriting. This research focused on the chemical properties of the OMR card marker as a Carbon Black colorant. Through material analysis of these colorant and real-application test, we selected the collidal Carbon Black ink from the appropriate manufacturer. And we investigated the good concentration needed for optimum condition when applying the Carbon Black colorant. Depending on the organic dye, the optimum detection sensitivity appeared within the range of 1 μg/mL - 100 μg/mL. Through the comparison of results, we found this method to be more reliable than the Matrix agents such as HABA(2-(4-Hydroxyphenylazo)benzoid Acid). On the other hand, Graphene oxide (GO) has been widely used more recently for a matrix of laser desorption/ionization (LDI) mass spectrometry of small molecules because GO has relatively lower matrix noise than conventional MALDI matrixes such as DHBA(2,5-dihydroxybenzoic acid). However, use of carbon-based materials is not desirable for time-of-flight (TOF) mass spectrometers since carbon nanomaterials stick to TOF electronics and therefore cause the instability of the MS operation. In order to overcome this issue, we applied GO embedded sol-gel film substrates for LDI MS of extracted ink dye samples of handwriting. Our results showed that the GO sol-gel film matrix substrate produced a much lower background noise than the aqueous GO particle matrix. This suggests that ablated carbon materials were significantly

reduced when using the sol-gel film substrates. In addition, GO-embedded sol-gel film produced very clear and intense profiles of synthentic ink dye molecules in the region of m/z 0 - 1000

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Synthesis of CNFs electroplated Co-Ni and Co-Cu on C-fiber textiles for anode material of Li secondary batteries

장건호 이상훈 이창섭*

계명대학교 화학과

In this study, we have synthetic carbon nanofibers(CNFs) on Co-Ni and Co-Cu catalysts electroplated on carbon fiber(C-fiber) textiles by thermal chemical vapor deposition(CVD) and applied the CNFs to an anode material of Li secondary batteries. C-fiber textiles were oxidized with nitric acid before electroplating of Co-Ni and Co-Cu catalysts. The oxidation process created the hydroxyl group on the C-fiber textiles, and the hydroxyl group was used as an active site for the catalysts electroplating. After being electroplated, the catalysts were dried in an oven heated to 40℃, and maintained for 30 min. Ethylene as a carbon source was flowed into the quartz tubular furnace heated to 700℃, and maintained for 1 h to synthesize CNFs. The characteristics of carbon nanofibers were analyzed by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The as-synthetic CNFs onto C-fiber textile were directly employed as an anode material without any binder. The electrochemical characteristics of CNFs as an anode of Li secondary battery were investigated using coin cell. The electrochemical performances were carried out by using a battery tester.

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Characterization of CuZn Nanofibers Prepared by Electrospinning

정은강 강용철* 강유진 박주연

부경대학교 화학과

The copper-zinc (CuZn) nanofiber was obtained by electrospinning method. CuZn/PVP (polyvinylpyrrolidone) precursor solution was made by zinc acetate, copper sulfate, and distilled water. PVP was used as control method of precursor solution viscosity. The electrospinning method was set with three parts; syringe, collector, and power supply. The distance between syringe needle and collector was 16 cm and the high voltage was applied on the tip was 18.1 kV. And the obtained CuZn/PVP nanocomposite was annealed at 353K to remove the distilled water and then clacinated at 973K for removal of PVP. The obtained CuZn nanofibers were characterized by X-ray photoelectron spectroscopy (XPS) for investigation of chemical properties, scanning electron microscopy (SEM) for morphologies of nanofiber, and X-ray diffraction (XRD) to characterize the crystallinity and the phase of CuZn nanofibers.

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Fabrication of CuSn thin films with various rf powers

강유진 박주연 정은강 강용철*

부경대학교 화학과

CuSn thin films were fabricated by rf magnetron co-sputtering method with Cu and Sn metal targets with a variety of rf powers. CuSn thin films were characterized by a surface profiler (alpha step), X-ray photoelectron spectroscopy (XPS), X-ray induced Auger electron spectroscopy (XAES), and contact angle measurement. The results of surface profiler showed that the thickness of CuSn thin films increased as rf power increased. From the survey XPS spectra, the Cu and Sn peaks were observed. Therefore, we could conclude CuSn thin films were successfully deposited on the Si(100) substrate. The oxidation state and chemical environment of Cu and Sn were investigated with high resolution Cu 2p, Cu LMM, and Sn 3d XPS spectra. Using contact angle measurement, surface free energy (SFE) and wettability of the CuSn thin films were studied with distilled water (DW) and ethylene glycol (EG).

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Ion-pairing reversed phase chromatography with inductively coupled plasma atomic emission spectrometry for the elemental speciation of As

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목포대학교 화학과

The toxic and biological effects of arsenic species vary with the different chemical forms in a sample. In the past study, two kinds of separator columns were used for the separation of arsenic species in a seaweed, and the separation chromatograms were completely different for the five arsenic species. Anion separator column (AS-7 column) could not separate the five arsenic species while the other column (PRP-X100 column) separated them in a seaweed. The two columns could separate five arsenic species in standard solutions. The matrix in a seaweed made an adverse effect on the separation of the arsenic species when the AS-7 column was used.In this work, ion-pairing reversed phase column was investigated for the arsenic speciation in a seaweed. The different chemical species of As elements were separated by ion-pairing reversed phase chromatography, then, the separated species are selectively detected by inductively coupled plasma atomic emission spectrometry.

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Detection of Salmonella bacteria using nanoparticles based on immunoassay

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Food-borne pathogenic bacteria have posed a serious risk to human health and caused food poisoning in many countries. Therefore detection of bacteria is very important to prevent these threats to human health. For this reason, various methods have been developed for the detection of bacteria in foods. In particular, Salmonella is one of the most frequently occurring pathogens in food that threats people's health. In this work, we used surface-modified nanoparticles for the immunoassay to detect Salmonella bacteria. For the extraction of bacteria from sample, metal (Cd) dopped magnetic nanoparticles (MNPs) were used, while Gd dopped silica nanoparticles (Gd-SNPs) were used as a detection probe for the ratiometric measurement of the tagged particles. The ratiometric method compensated for the particle loss happened in the magnetic separation, suppressing signal fluctuation. Furthermore, a membrane filtering is also used to reduce the background of nonspecific reaction. For demonstration, salmonella bacteria was detected by immunoassay using inductively coupled plasma mass spectroscopy (ICP-MS). The calibration curves with the linear regression of 0.9716 and the detection limit (LOD) of 7.33*10^2 cells/ml were obtained for demonstration.

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Detection of Streptomycin in honey by laser induced fluorescence microscopy(LIFM)

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Streptomycin (STR), an aminoglycoside antimicrobial agent produced by Streptomyces griseus, has been used in veterinary medicine and animal husbandry particularly for treatment of bacterial infections. However, it is known that STR may cause ototoxicity, allergic reaction, Neophrotoxicity, neuromuscular paralysis and resistant bacteria, and the residues of STR in animal food-stuff present a potential hazard to humans. For this reason, variety methods have been developed for the detection of streptomycin in foods. But, more sensitive and rapid method is still required for human health. In this work, we developed a method combining nanoparticles with immunoassay to detect streptomycin by laser induced fluorescence microscopy (LIFM). From the calibration curve, a linear correlation coefficient of 0.9621 (R2) and the detection limits (3σ) of 38.8 ppt were obtained. The cross-reactivity test with other antibiotics showed low interferences except for dihydrostreptomycin (56.86%).

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Micro-headspace in-tube microextraction coupled with capillary electrophoresis

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서울대학교 화학부

In conventional headspace (HS) extraction, analytes evaporated from a sample donor phase in a sealed vessel can be enriched to an acceptor phase often in a liquid form or a sorbent coated on a fiber. The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus an acceptor of small volume is preferred and a single acceptor drop of small volume hanging to the capillary tip has been used in HS extraction for capillary electrophoresis (CE) [1]. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME)/CE using a liquid plug inside a separation capillary as an acceptor in place of the drop [2]. Here, we present micro-headspace (?HS) ITME/CE, a simple but easy way of conducting HS extraction of a small volume sample for subsequent CE analysis. Instead of using a sealed vessel to prepare a HS, a ?HS of a volume much smaller than 1 ?L was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor. Futhermore, ?HS-ITME-CE was performed using the acceptor plug remained in the capillary. Due to the small volumes of the ?HS and acceptor plug, it was possible even for a small volume donor to retain a high ratio of the donor and acceptor volumes for high enrichment factors. All steps of ?HS-ITME-CE were carried out automatically using a commercial CE instrument without any modification. Therefore not only the sample volume could be dramatically reduced, but also the need for a special apparatus was eliminated.

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Stable aqueous dispersions of reduced graphene oxides using a water-soluble pyrene derivative with a zwitterionic arm

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경희대학교 화학과

Here, we report a pyrene derivative, 3-((pyren-3-yl)methyl)imidazolium-1-propionate (PImP), with a zwitterionic arm, imidazolium-1-propionate, which stabilized reduced graphene oxides (RGOs) in aqueous solutions. Stabilized RGOs were obtained by reducing graphene oxides chemically in the presence of PImP. The resulting RGO-PImP composites were characterized using UV-vis spectrophotometry, fluorometry, and atomic force microscopy, which confirmed the stabilization of RGO with PImP via noncovalent π-π interaction between RGO and the pyrene moiety of PImP. The stabilized RGO-PImP composites were also applied to functionalize indium tin oxide (ITO) surface for enhanced electrochemiluminescence (ECL) of luminol/H_2O_2, which was utilized further for sensitive ECL-based cholesterol assays.

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Surface nanostructure analysis of diblock copolymer films according to the solvent annealing and thermal annealing using AFM and TOF-SIMS

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Diblock copolymers coated on the Si wafer were prepared by different solvent annealing and thermal annealing conditions. The morphology of diblock copolymer film was changed according to the annealing solvent, temperature, and concentration. In this study, diblock copolymers such as poly(deuterated styrene-b-methyl methacrylate) (dPS-b-PMMA), poly(deuterated styrene-b-ethyl hexylacrylate) (dPS-b-PEHA), poly(deuterated styrene-b-tertbutylacrylate) (dPS-b-PtBuA), deuterated polystyrene-b-isooctylacrylate (dPS-IsoOctA) and deuterated polystyrene-b-trimethyl hexylacrylate (dPS-TMHA) were used to investigate microphase separation in copolymer films. Diblock copolymer films were annealed in different solvents such as acetone, THF, CS2 to observe microphase separation. Atomic Force Microscopy (AFM) and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) were used to obtain the nanostructural information of the diblock copolymers. The AFM results provided information about the surface morphology, microphase-separated structure according to the solvent and copolymer concentration. The TOF-SIMS results provided the composition information for lamellar structure of the diblock copolymer films after solvent annealing or thermal annealing.

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Reduced Graphene Oxide Film on Pt DEN-Grafted ITO for Enhanced Electrochemiluminescence of Luminol/H_2O_2

임효정 김주훈*

경희대학교 화학과

Here, we report assembly of reduced graphene oxide (RGO) films on indium tin oxide (ITO) surfaces modified with dendrimer-encapsulated Pt nanoparticles (Pt DENs), which we denote as RGO/Pt DEN/ITO, for enhanced electrochemiluminescence (ECL) of luminol/H_2O_2. Specifically, we synthesized Pt DENs using amine-terminated polyamidoamine dendrimers, and immobilized the Pt DENs on ITO surfaces via electrografting of the amine-terminated dendrimers encapsulating Pt nanoparticles. We then assembled graphene oxide (GO) nanosheets onto the Pt DEN-grafted ITO surfaces via EDC/NHS chemistry, and reduced the assembled GO film chemically. The resulting RGO/Pt DEN/ITO exhibited highly catalyzed electrochemical redox reactions of luminol/H_2O_2, which leads to significantly enhanced ECL of luminol in the presence of H_2O_2 and thus sensitive luminol ECL-based assays for detection of H_2O_2

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Surface properties of fluorine-containing carbon thin films deposited by two different plasma polymerization techniques

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Plasma polymerization is nowadays considered as a promising and versatile technique allowing the deposition of plasma polymer films with functional properties on surface without affection the intrinsic properties of the substrates. In this study, the surface properties of the plasma polymer films were investigated as a function of experimental parameters. Different fluorocarbon thin films were deposited on Si substrates using two different plasma polymerization methods: inductively coupled plasma (ICP) and capacitively coupled plasma (CCP). Fluorine-containing hydrophobic thin films were obtained by ICP and CCP with a mixture of fluorocarbon precursors C2F6, C3F8, or c-C4F8 and acetylene (C2H2). Different process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, and processing time were used to generate various fluorocarbon thin films. Surface properties of fluorocarbon films such as the hydrophobic properties, surface hardness, adhesion ability and wear behavior were evaluated. The water contact angle results showed that the ICP plasma polymer film with c-C4F8 had more hydrophobic surface than other polymer films. The CCP plasma polymer films had higher pencil hardness and better friction properties than the ICP plasma polymer films. Peel test results indicated that the CCP technique provided more adhesion strengths of plasma polymer film than that the ICP technique. In addition, the adhesion strengths of fluorocarbon thin films were improved by the pretreatment methods such as plasma and plasma source ion implantation (PSII).

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Analysis of gel-containing butadiene rubber using ThFFF-MALS-DLS-RI and size-exclusion chromatography

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한남대학교 화학과

Rubber has a significant role in tire industry, which tries to attain a better compromise between the wear and rolling resistance, and ice and wet grip properties of tire tread compounds. Butadiene rubber (BR) is used widely in tire tread compounds, hoses, and conveyor belts. Molecular weight (MW) and gel content are important parameters of rubbers as they influence the physical, mechanical, and rheological properties of the polymers. Small difference in low or high MW fractions can result in significant differences in the end use properties. Thus the molecular weight distribution (MWD) of a rubber is one of important parameters in quality control, monitoring of product stability, reclaiming off-spec material, and development of new materials.Thermal field-flow fractionation (ThFFF) is a polymer separation technique, where a separation is controlled by the thermal diffusion coefficient, D_T, a basic transport parameter describing the movement of a matter under a temperature gradient. ThFFF is useful for MW-based separation and molecular characterization of various types of polymers. ThFFF channel is open (unpacked), and is particularly useful for separation of polymers of high MW that are susceptible to shear degradation or those containing microgel. ThFFF can provide separation of microgel particles from soluble components.ThFFF coupled with a multi-angle light scattering (MALS) and a concentration detector such as refractive index (RI) or UV/VIS detector yields the molar mass, hydrodynamic diameter (R_h) and root-mean-square (*rms*) radius (R_g) of each ThFFF slice, and thus the conformational information of the molecules. MALS yields the absolute molar mass and molecular conformation of samples without reference to molar mass standards. Dynamic Light Scattering (DLS) can estimate hydrodynamic diameter of particles in nano to micron size from the light scattering intensity of the particles. In this study, we determine molecular weight and size of various commercial BR materials using ThFFF-MALS-DLS-RI and compare the results with those from size-exclusion chromatography (SEC).

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Optimization of electroactive polymer modified biosensors

김은미 이혜진*

경북대학교 화학과

본 포스터에서는, 탄소 기반 전극을 이용한 바이오센서의 경우 생물질 검출용의 탐침용 리간드 물질(항체 또는 앱타머)을 전극 표면에 도입하기 위해 탄소 표면을 전처리하거나 또는 여러번의 화학적 처리 과정을 사용해야하는 단점을 보완하기 위해 전기적 활성을 갖는 도파민고분자로 코팅한 결과를 나타내고자 하였다. 탄소 기반 센서 표면에 도파민 도입 및 생물질 리간드 고정과 이들을 도입한 바이오센서의 전기화학적 활성에 대해 순환전압전류법과 시차펄스전위법을 이용하여 분석한 결과를 나타내었다.

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Development of acid sensor based on Chitosan-graft-Polyaniline copolymer film

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성균관대학교 화학과

Polyaniline(PANI) is a conducting polymer, shows a change of electrical conductivity with protonic acid doping process. Therefore PANI can be used for acid sensor. But PANI could not be utilized so much, because of its poor solubility. So we introduce Chitosan(CS) to improve its processibility. Because CS itself has good mechanical and solubility properties. In this study we have chemically synthesized CS-g-PANI copolymer by using ammonium persulfate. The product was characterized by UV-vis, FT-IR, Scanning Electron Microscope(SEM), X-ray diffraction(XRD). Electrical resistance of CS-g-PANI copolymer is observed using a 4-point probe. Resistance of copolymer film was decreased up to 1/500 by comparing with the value obtained before acid doping. Consequently, CS-g-PANI copolymer film could be used for the acid sensor. This work was supported by the Component and Material Technology Development Program (No.10046641, Development of Electronic Ink and Coating Material for Leak Monitoring of the Hazardous Chemicals) funded by the Ministry of Trade, industry & Energy (MOTIE, Korea)

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Synthesis of new crosslinked polyacrylate composite microgels

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Microgels are lightly cross-linked polymer networks (hydrogels) with an ability to swell and deswell in response to changes in their environment and they are unique materials because of their valuable applications as superadsorbents. The purpose of this study was to develop a facile method for the preparation of new polyacrylate composite gels (PACGs) with a motivation to use them as adsorbents. The polymer PACGs syntheses were performed via radical polymerization of different monomers and crosslinker -N,N'-methylenebisacrylamide in aqueous solution using ammonium persulfate as an initiator in the presence of a surfactant and superadsorbtion improving additives. The PACGs were characterized using Fourier transform-infrared (FT-IR) spectroscopy, thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). The PACGs showed very high adsorption efficiency and adsorption capability for the cationic dyes and metal ions and were promising to act as toxic substance adsorbents

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An aldehyde sensitive colorimetric chemosensor for determination of fruit ripeness

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A naked-eye detective chemosensor have received much attention in a variety of application fields due to the simplicity, favorable performance, selectivity, and low cost. In agricultural food and other related fields, chemosensor, supplying consumers with communication as a marketing tool, offers to consumer with the great easy of use and time-saving convenience for the final purchasing decision. Apple is one of the representative climacteric fruits, emitting the characteristic aroma including the variety of volatile organic materials, such as aldehyde, acetate and alcohol etc during the storage. To fabricate an aldehyde sensitive colorimetric indicator (ACI), Methyl red was dissolved in methanol (1.2 mM) and adsorbed on the papers. The colorimetric sensor mechanism arises from intermolecular hydrogen bond between azo group in methyl red and oxygen of aldehydes. The colorimetric response of ACIs and the apple quality were investigated with the variation of a storage time. As increasing the exposure time of apple aroma, the color of ACI was changed from yellow to red. The color change profile of ACI was analyzed by the RGB value. In order to investigate the quality of apple, components analysis and sensory test consisted of 5 investigation items (appearance, sweetness, sourness, crunchiness, and over all acceptance) were conducted with the different storage-period apples. The characteristic component changes were the diminishment of Phenolics and Flavonoid. These results in relation to the sensory test and color change indicate that ACI fabricated by doping Methyl red is to apply a fruit ripeness sensor as well as an aldehyde detective sensor.

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Preparation of polyaniline/titanium dioxide core-shell hybrid nanomaterials

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Combination of polyaniline (PANI) and transition metal oxide in the nanoscale range may result in hybrid materials which present improved features, such as electrochemical, mechanical or thermal behavior, or novel properties not observed for the isolated components. This paper reports the preparation and characterization of a novel hybrid nanomaterial of PANI and nanostructures of titanium dioxide (TiO_2) in the core-shell nanoarchitecture. Core?shell TiO_2@PANI hybrid materials with previously nanostructured TiO_2 residing in the core regions with PANI residing in the shell regions were prepared. The morphologies, microstructures, and optical properties of the pristine TiO_2 and TiO_2@PANI hybrid materials were characterize. by scanning electron microscopy (SEM) x-ray diffraction (XRD), fourier transfer infrared spectroscopy (FTIR) and UV-visible spectroscopy. The photocatalytic properties of the TiO_2@PANI nanoarchitectures have also been evaluated. Results show that the enhancement in the photocatalytic activity was attributed to the synergetic effect and also the chemical bonding leads to the interfacial charge transfer effect between TiO_2-PANI interfaces

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Selectivity Comparison Studies for Calcium Ion Sensing at Liquid/gel Interfaces

김민지 이혜진*

경북대학교 화학과

본 포스터는 서로 혼합할 수 없는 않은 수용성 액체/ 유기 젤 계면에서 전압을 주사할 때 수용액 안에 존재하는 칼슘 이온이 젤안에 도포된 선택적 이온운반체에 의해 이동하는 반응에 따라 전류값이 변화함을 측정하는 센서 개발에 대해 나타내었다. 이를 이용하여 칼슘이온을 검출할 때 선택성을 증대시키기 위해 두 가지 이온운반체 (예: calcium ionophore Ⅱ와 calcium ionophore A23187)를 사용하였는데, 이들 각 운반체의 칼슘 이온 선택성에 대해 순환전압전류법과 시차펄스전압전류법을 이용하여 조사하고 그 결과를 비교 분석하였다.

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Synthesis of a new biocompatible chitosan based nanocomposite gel

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A new chitosan based nanocomposite gel (CNCG) was synthesized through metal-binding reactions between titanium ions, chitosan and a polyaniline derivative. The CNCG was systematically characterized by Fourier transform Infrared spectroscopy (FTIR), Raman spectroscopy, scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). More importantly, the new CNCG could be used as an effective adsorbent for toxic Cr(Ⅵ) ion in water samples. The experimental results from FTIR and XPS measurements indicated that the possible removal mechanism involved: ⅰ) Cr(Ⅵ) adsorption by electrostatic attraction and ⅱ) reduction of Cr(Ⅵ) to less toxic Cr(Ⅲ) and ⅲ) re-adsorption of Cr(Ⅲ) into the gel. It is expected that CNCG can be a promising adsorbent for the treatment of Cr(Ⅵ) in real water samples.

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NMR Structural Analysis of Antimicrobial peptides, LPcin analogs with Enhanced Activities in aligned samples

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Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of bovine proteose-peptone PP3. LPcin analogs were designed and modified to enhance antibacterial activity using mutation, sequence shuffling for better amphipathic characteristics. It helps to improve interacting with bacterial membranes. Three candidates with enhanced antibacterial activity were selected among 12LPcin analogs, the name of LPcin-YK1, LPcin-YK2 and LPcin-YK3 respectively. LPcin-YK1 and LPcin-YK3 has shorter amino acids at C-terminus, LPcin-YK2 has same number of amino acids but several amino acids were substituted for better amphipathic characteristics. To understand the correlation between their structures and antibacterial mechanism, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using various biophysical techniques.We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with many biophysical techniques such as Ni-NTA affinity chromatography, dialysis, CNBr chemical cleavage and reversed-phase semi-prep.HPLC. To verify the purified peptides, we performed Tris-tricine PAGE, MALDI-TOF MS and CD spectrometry. In order to investigate the structures and dynamics, we use various 1D and 2D NMR techniques using micelle and especially bicelle samples to the closest anionic membrane environments.In here, we will present not only the optimization of high-yield expression and purification, but also solution and solid-state NMR experiments to elucidate the correlation between structure and antimicrobial activity. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra and PISA Wheel pattern were also underway.

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인-질소 클러스터 화합물의 질량분광 실험연구(Mass Spectrometric Stydy on Phosphrorus Nitride Clusters)

배광태 고은미 조수경*

국방과학연구소 국방고등기술원

고에너지물질 연구 분야에서는 고질소 함유 화합물을 개발하는 작업에 많은 노력을 기울이고 있다. 이들은 자체적으로도 많은 활용성이 있지만, 폴리질소를 합성하는 전구체로 활용할 수 있어 이들 물질의 합성 뿐 만 아니라 분해 매카니즘을 확인하는 작업도 매우 중요하다. 본 연구에서는 폴리질소계 화합물을 합성 할 수 있는 방안으로 인-질소 클러스터 화합물을 레이저로 이온화하여 질소만으로 구성되는 분해물을 형상하는 매커니즘을 조사하였다. 비행시간 질량분광기에 인-질소 클러스터 화합물에 대한 MALDI 및 LDI 실험을 수행하였으며, 실험 조건에 따른 분해 패턴을 분석하였다.

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Asymmetrical flow field-flow fractionation (AsFlFFF) coupled with light scattering for separation and characterization of egg yolk plasma

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In this study, the capability of asymmetrical flow field-flow fractionation (AsFlFFF or AF4) coupled online with two light scattering detectors (quasi-elastic light scattering (QELS) and multiangle light scattering (MALS) was evaluated for separation and characterization of egg yolk plasma. The system also includes a UV/VIS and a fluorescence (FS) detector as a concentration detector, which makes the system called as ‘AF4-UV/VIS-QELS-MALS-FS’. AF4 provided a size-based separation of the major components of the egg yolk plasma such as free proteins, low density lipoproteins (LDL) and their aggregates. AF4 is known to be gentle, allowing separation without degradation of the sample components. Free proteins were completely separated from LDL by a programmed AF4 run, where the cross-flow was gradually reduced during a run. For each component, QELS and MALS yielded hydrodynamic radius (R_h) and radius of gyration (R_g), respectively, allowing determination of the conformation (e.g., shape) based on R_g/R_h. The R_g/R_h data were confirmed by Cryo-transmission electron microscopy (Cryo-TEM) images of collected AF4 fractions. The R_g/R_h results indicated that LDL has a homogeneous spherical shape, while larger aggregates have swollen microgel-type structure. Elution of LDL was confirmed by staining with Nile red, a fluorescent dye. Collected fractions of free proteins were further characterized using a sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE). Results suggested that the absence of Ca^{2+} leads to aggregation, while the presence of Ca^{2+} leads to binding of proteins. The effect of heating and enzymatic treatment on egg yolk plasma was also investigated. The results suggest that LDL undergoes a ‘clusters-fusion-gelatin’ process under a heating treatment at 65°C, while an enzymatic treatment with phospholipase A2 (PLA2) significantly enhances the heat stability of LDL. It was shown that AF4-UV/VIS-QELS-MALS-FS is a gentle and useful tool for analysis of egg yolk plasma.

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Development of home-built solid-state NMR probes for specific purposes

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The solid-state NMR spectroscopy has been widely used for various insoluble materials like industrial polymers and biological samples. Also, solid-state NMR analysis of membrane protein on a membrane-like environments, such as lipid bilayer and bicelle, is especially valuable for their structure and function relationship. However, most of biological proteins on lipid bilayers have high dielectric property due to containing large amounts of lipids, water, and salts as well as probe efficiency are decreased cause of their electrical properties of lossy samples. Therefore, specific probe with high efficiency is required to study biological samples by using solid-state NMR. Also solid-state NMR methodologies for structural study of membrane protein in bicelle could be used for the in-situ analysis of liquid crystalline materials in LCD panels as well as Li materials in Li ion batteries. Here, we present the optimized design, construction and efficiency of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil for structural study of membrane protein in bicelle. The 1H-15N 2D SAMPI-4 spectra from a single crystal and membrane proteins oriented in bicelles were successfully obtained by using these solid-state NMR probes. We also present the development of a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a solenoidal coil for analysis of industrial materials. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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고분자소재의 효율적인 열전도도 및 비열 분석 접근방법

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단열소재, 방열소재 등의 물질이 전도에 의해 열을 전달할 수 있는 능력을 나타내는 열전도도, 비열 분석에 있어서 다양한 소재 특성 및 방향성, 시료의 크기에 따라서 적합한 분석 솔루션에 대해서 분석하였다. 방향성에 따라서는 Isotropy 고분자의 경우, silicone rubber 를, anisotropy 의 경우는 CFRP (carbon fiber reinforced plastics)를 사용하였고, lazer flash, hot wire, hot disk 로 분석하여 열전도도를 비교 하였다. 또한 Ain/BN Composite Materials 과 pyroceram, sapphire 등 reference sample 과의 시료형태에 따라 DSC, LFA 로 비열 측정하였을 때 그 양상을 확인하였다. 그 결과, 열전도도, 비열 분석에 있어 분석기기에 따라서 약간의 결과 차이는 있으나, 시료의 방향성과 시료크기에 따라서 보다 효율적으로 분석접근 하여 오차를 줄일 수 있는 방법을 제공할 수 있게 되었다.

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Characterization of Fe_2O_3 nanoparticle coated with humic acid using Field-Flow Fractionation (FFF) and related techniques

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Nanoparticles (NP) in environment (water, soil and sea-sediment) that have risk element to human and environment is a problem worldwide. Recently, magnetic particles such as Fe_2O_3 NP has become an interest in the field of environment because of its potential efficiency in the treatment of contaminated soil or groundwater. In application of those nanoparticles, it is important to analyze the particle size and its distribution for characterization and quantification of NP. NPs in aqueous system usually have broad size distributions and, even exist as aggregates. In order to have nanoparticles well dispersed in an aqueous system, a surfactant is added or the particles are coated with charged polymers. However, these methods have some disadvantages as the additives or surface modification process may be expensive and may be toxic.Recently the 'Green coating' attracts interest in the environment field, where the nanoparticles are coated with dissolved organic matter (DOM) such as humic acid (HA). HA is a dark-colored organic material that can be extracted from soil by dilute alkali and other reagents and that is insoluble in dilute acid. The merits of 'Green coating' is that it is environmentally friendly, inexpensive and nontoxic.Field-Flow Fractionation (FFF) is a family of separation techniques that are capable of providing separation and characterization of macromolecules or particles ranging in size from nanometer up to micrometer.In this study, HA-coated Fe_2O_3 nanoparticles were prepared, and then were analyzed using FFF and related techniques to determine the particle size distribution and to study the particle dispersion, HA-adsorption, and stability of the HA-coated particles.

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Effect of Surfactant on retention behaviors of polystyrene latex beads in asymmetrical flow field-flow fractionation: Effective boundary slip model approach

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Field-flow fractionation (FFF) is a family of separation techniques that can provide separation and characterization of various types of particulates and polymeric macromolecules. It has been shown that FFF is useful for separation of particles ranging in size from a few nm up to about 100 μm. Flow field-flow fractionation (FlFFF) is considered to be the most universal among the members of FFF. No-slip boundary condition (BC) model has been applied with great success to model many macroscopic fluid flow experiment which would be insensitive to partial-slip BC. When we applied FFF experiments, No-slip BC have some limitation. No-slip BC cannot account for the characteristic flow properties with sufficient accuracy, particularly for systems with channel walls having very weak interaction with the carrier fluid itself or interactions between the particles and the channel wall (or membrane surface). Compared to the standard retention theory and experiment, the most crucial limitation is perhaps due to the wall effect attributed to the interactions existing between the particles and the channel wall. Therefore, for a successful application of the SRT, an effective means is required that enables as little as possible overall wall effect so that the particles follow the presumed ideal retention behavior. For example, an introduction of appropriate additives (surfactants, pH controllers, salts) into standard particles systems is one of the most frequently practiced prescriptions to control the retention or elution behavior of the particles in asymmetrical FlFFF (AF4) operations.In this study, we investigated the effects of surfactant and ionic strength on the retention behaviors of polystyrene (PS) latex beads of 20-100 nm in diameter.

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전자소재의 cyclosiloxane 및 아웃가스 분석법 연구개발

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전자소재와 화학제품에서 발생하는 가스 및 VOC(Volatile organic compounds) 는 제조기기나 최종제품(특히 전자제품)의 트러블이나, 악취의 원인이 되기도 하고, 유해성분이 인체에 영향을 미치기 때문에 전자소재의 아웃가스(outgas, 또는 발생가스) 분석에 대한 중요성이 근래에 들어 더욱 부각되고 있다. 아웃가스(outgas)는 용제뿐만 아니라 전반적인 저분자 유기물질을 함유하고 있는 것으로, TD(Thermal Desorber)-GC/MS 와 HS(Headspace)-GC/MS 를 이용하여, 특정온대에서 열을 가해 발생되는 기체성분을 트랩에 포집한 후, GC/MS 에 주입하여 검출되는 성분의 정성 또는 정량 분석이 가능한 분석법으로, 에폭시, 실리콘 등의 다양한 전자소재의 아웃가스 분석에 적용 가능한 분석법을 연구하였다.

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Carbon cloth supported Au nanodendrite matrix as a electrochemical and SERS-based sensing platform

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A three dimensional (3D) Au nanodendrite matrix constructed on a carbon cloth by simple electrochemical deposition has been demonstrated. It is unbreakable, rugged and easy to use for analysis due to the flexibility of carbon cloth. Initially, its analytical usage was demonstrated for electrochemical detection of Hg (II) in an ultra-low concentration range. Due to the large surface of 3D Au nanodendrite, the Hg concentration of 1 ppb is clearly detectable. Further, its potential as a SERS substrate was evaluated. For the purpose, 1 nM 2-naphthalenethiol was applied on the substrate and the corresponding SERS spectra were acquired. The spectral feature of 2-naphthalenethiol was clearly observed and the SERS intensity was maintained even with repeating folding of the substrate. In overall, the carbon cloth supported Au nanodendrite has several advantages as a sensing platform such as good substrate-to-substrate reproducibility, mechanical flexibility and low cost in preparation

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Combination of capsaicin-templated molecularly imprinted polymer and Raman spectroscopy for identification of geographical origins of red pepper powder

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Red pepper powder is one of the most consumed foods in Korea, so it has been largely imported from other countries, mainly China. As generally known, the contents of capsaicin in domestic and imported red pepper powders are different, so their measurement could allow the determination of geographical origins. This study aims to develop a simple analytical method for identifying geographical origins of red pepper powders. It intends to measure capsaicin content semi-quantitatively by combining capsaicin-templated molecularly imprinted polymers (MIPs) containing capsaicin-specific recognition sites and Raman spectroscopy for direct measurement of captured capsaicin. We synthesized the MIP for *N*-vanillylnonanamide, a synthesized capsaicin as a template. For the preparation, 4-vinyl pyridine, azobisisobutyronitrile (AIBN) and ethylene glycol dimethacrylate (EGDMA) were used as a functional monomer, a cross-linker and an initiator for thermal polymerization, respectively. The performance of MIP in the capture of capsaicin, and Raman spectral features before and after the capture were examined.

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Electrochemical Immunoassay for detecting Hippuric acid (HA) on the Carbon included Screen Printed Nickel Electrode(SPNE)

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Hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring of exposure to toluene is very important in occupational health care. In this work, we are using electrochemical immunoassay system that several advantages such as simple instrumentation, relatively low cost, miniaturization, portability, disposability and fully automation. The system was comprised with immobilization of Fe-HA on the Carbon included SPNE. We made electrode that marked Fe-HA on the carbon included SPNE. The surface morphology of the immobilized Fe-HA on the carbon included SPNE was examined by scanning electron microscopy (SEM). Hippuric acid (HA) has been detected competitively on the interaction of free HA and pentacyanoferrate-(4-aminomethylpyridine-hippuric acid) (Fe-HA) to its antibody on the Carbon included SPNE. This system generated electric signals proportional to free HA concentration. The electrical signal was measured by Cyclic voltammetry(CV) technique. The resulting currents were linearly related with the concentration of HA. The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.

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Development of indicator solution for the measurement of pH from the fat and oils

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CDR-Foodlab device has been used for checking the pH value in Fat and Oil. To operate CDR-Foodlab device, we need to use the kit with indicator solution. However the indicator solution, which received from company, is expensive. So to make similar product with indicator solution of company, we used various indicator. The components of indicator solution of company were analyzed by UV, IR and GC-MS. We chose various indicator compared with indicator solution of company. To check the pH value in a CDR-Foodlab device, we prepared the standard pH solution of 1 to 13. B sample was matched with indicator solution of company. It will be used as a reagent which can replace the existing that is cheap and accurate. 본연구는 2014 년도 교육부 대학특성화사업(CKⅡ) 사업비중 일부 지원받아 수행되었음.

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Synthesis and Electrochemical performance of SiO_2-Carbon Nanofibers composite as anode material for lithium secondary battery

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In this study, Carbon nanofibers (CNFs) and SiO_2-Carbon nanofiber (CNF) composites were synthesized and applied as anode materials of lithium secondary batteries. Carbon nanofibers and SiO_2-CNF composites were grown via chemical vapor deposition (CVD) method with iron-copper catalysts and silica-covered Ni foam as collectors. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 600 ℃, and maintained for 10 min to synthesize CNFs and SiO_2-CNF composites. The morphologies, compositions and crystal quality of the prepared CNFs and SiO_2-CNF composites were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of CNFs and SiO_2-CNF composites as an anode of Li secondary battery were investigated using three-electrode cell. The as-deposited CNFs and SiO_2-CNF composites on Ni foam were directly employed as an working electrode without any binder, and lithium foil was used as the counter and reference electrode. Glass fiber separator was used as the separator membrane. 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. The galvanostatic charge/discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. Acknowledgement : This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO. 2012026209).

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Dynamic Nuclear Polarization: Sensitivity Enhancement for Multi-molecular Magnetic Resonance Imaging Agents

정기진 고혜지 공경현 이영복*

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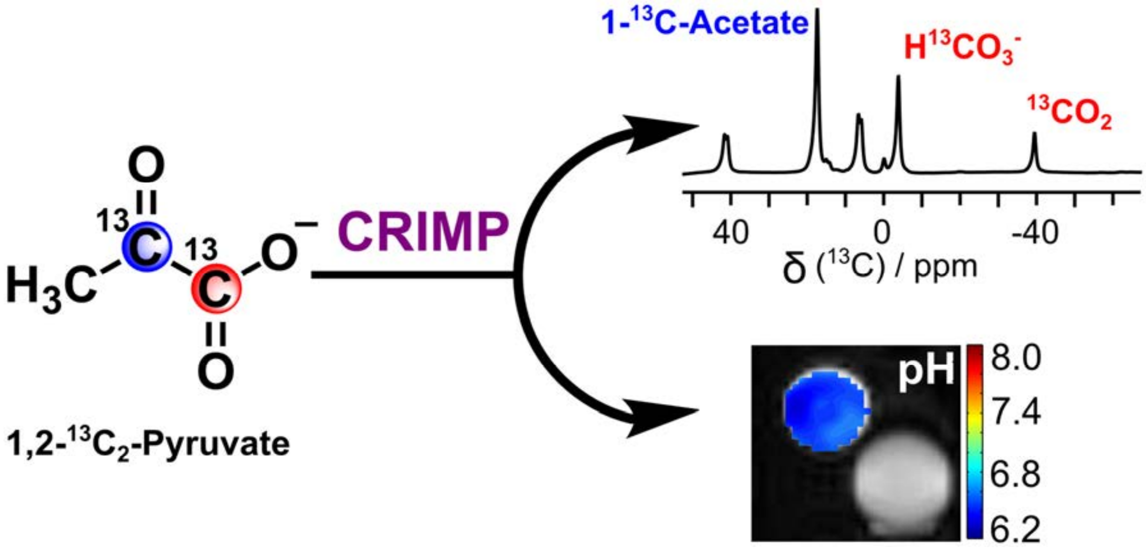
Here we present a novel hyperpolarization method, Chemical Reaction-Induced Multi-molecular Polarization (CRIMP), which could be applied to the study of several *in vivo* processes simultaneously including glycolysis, TCA cycle, fatty acid synthesis and pH mapping. Through the use of non-enzymatic decarboxylation, we generate four hyperpolarized imaging agents from hyperpolarized 1,2-^{13}C pyruvic acid. The CRIMP method is a simple versatile chemical method that can be done without any physical changes to the dissolution pathway or to the polarizer. Many new techniques in the literature including cross polarization, microwave frequency modulation, generating a faster dissolution or injection setup and increasing the magnetic field from dissolution to scanner are all physical methods used to increase hyperpolarization percentages or to increase the T_1 value of hyperpolarized imaging compounds. The new method can potentially be applied to study several in vivo metabolic pathways and multiple biochemical reactions concurrently in real-time.


1,2-$^{13}C_2$-Pyruvate
CRIMP
1-^{13}C-Acetate
$H^{13}CO_3^-$
$^{13}CO_2$
40
0
-40
δ (^{13}C) / ppm
pH
8.0
7.4
6.8
6.2

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Challenge in Identification of Proteins; Immobilized Trypsin Column

노주형 유병수[1] 조원련*

원광대학교 바이오나노화학부 [1]원광대학교 생명나노화학부

Although trypsin digestion has a long history in protein identification, there is no outstanding trypsin column in proteomics. This study shows an efficient, fast, economical, reproducible, and reusable trypsin column with biopolymers. Biopolymer I synthesized and immobilized to porous silica gel. Then trypsin is immobilized to this modified silica gel and trypsin column is packed in an empty PEEK column. HSA and human transferrin are digested as standard proteins in trypsin column and compared with solution digestion mode. This study examines trypsin columns made with biopolymers for biological usage.

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A Method for Recognizing Specific Glycans Associated with Glycoproteins in the Interactome

신지훈 정미선 조원련*

원광대학교 바이오나노화학부

This poster explores the possibility that affinity interactions and protein-protein interactions (PPIs) can occur simultaneously during lectin affinity chromatography and be exploited in proteomic studies of the interactome. Fifty seven glycoproteins were identified by serial affinity chromatography with human plasma, some of proteoforms were resolved by displacement chromatography. MetaCore was used to elucidate the interactions of the identified proteins and to obtain the corresponding interaction map. The presented results suggest that lectin affinity chromatography can be used to study disease interactomes.

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Lectin Affinity Chromatography explains Sample Displacement Chromatography (SDC)

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원광대학교 바이오나노화학 [1]원광대학교 바이오나노화학부 [2]원광대학교 생명나노화학부

One of the limitations of lectin affinity chromatography is that it is difficult to differentiation between glycoforms. The work presented in this poster examines the potential for displacement phenomena to play a role in glycoprotein fractionation through sample displacement chromatography (SDC). The same glycoprotein was also found to be bound non-sequentially in the column set. For the first time it has been demonstrated that overloading lectin columns clearly leads to SDC with concomitant fractionating glycoprotein proteoforms based on their lectin binding affinity.

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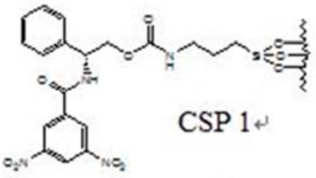
Synthesis and application of (R)-phenylglycinol and (S)-leucinol derived chiral stationary phases to chiral separation

이정미 유정재 김현영[1] 류재정[2,*]

경북대학교 화학과 [1]경북대학교 일반대학원 과학교육학과 [2]경북대학교 화학교육과

(R)-Phenylglycinol and (S)-leucinol 3,5-dinitrobenzoyl(DNB) derived chiral stationary phases(CSP1~2) were used for the separation of various chiral analytes.[1-3] Very recently, four new (R)-phenylglycinol and (S)-leucinol derived CSPs(CSP3~6) were synthesized and the results of separation for fourteen chiral analytes were reported.[4] In this study, two (R)-phenylglycinol and (S)-leucinol derived CSPs(CSP 7 and CSP 8) were newly prepared with *N*-3,5-bis(trifluoromethyl)benzoyl chloride and 2- theonyl chloride instead of previously used acyl chlorides. In addition, new 26 chiral analytes were used for testing the newly prepared CSPs(CSP 7 and CSP 8) and previously reported CSPs(CSP1~6), and the chromatographic results were compared to each other.References 1. S. H., Im; J. J., Ryoo. Chirality 2002, 14, 329. 2. J. J. Ryoo; S. H., Im.; K. P., Lee. Microchemical J. 1999, 63, 128. 3. J. J., Ryoo; T. H., Kim; S. H., Im; Y. H., Jeong; J. Y., Park; S. H., Choi; K. P., Lee; J. H. Park. J. Chromatogr. A 2003, 987, 429. 4. J. M. Lee; D. H. Ryoo; J. J. Yu; J. J. Ryoo. The 114th General Meeting of the Korean Chemical Society, Gwanju, 2014.10.15~17, Abstract book p.848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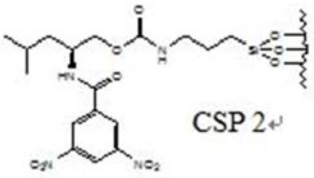
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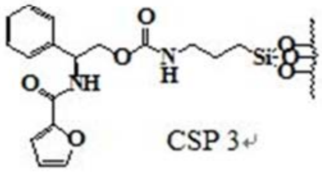
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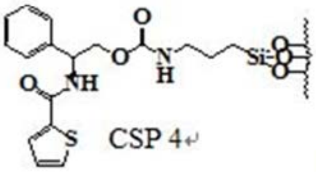
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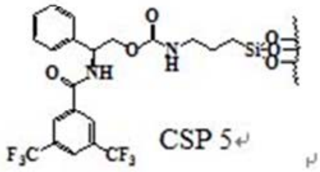
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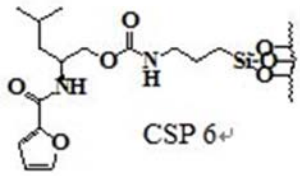
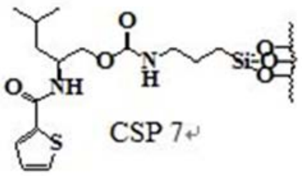
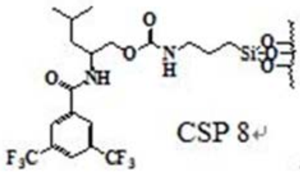

CSP 6


CSP 7


CSP 8

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Proton-Coupled Electron Transfer Reactions of Metal Nanoparticles Anchored on Metal Oxide Surface

이용진 이동일*

연세대학교 화학과

Noble metal nanoparticles (metal = Au, Ag, Pd, and Pt) anchored on the surface of semiconductor nanoparticles show catalytic activities for the reduction of azobenzene and CO_2. In azobenzene photocatalytic reduction, the ZnO composite coated with Pd nanoparticles showed the highest reduction activity, followed by Pt, Au and Ag, but the catalytic activity of bare ZnO was found to be negligible. Through the product analysis of the photocatalytic reactions, it was found that azobenzene was reduced to hydrazobenzene via proton-coupled electron transfer reaction. This tendency of metal effect can be elucidated by the proton binding tendency of metals in the composites that controls the proton-coupled electron transfer reaction. Another proton-coupled electron transfer reaction, namely reduction of carbon dioxide, is also performed. In this case, CO_2 reduction experiments were conducted with metal/TiO_2 composite colloids under light (> 320 nm) in aqueous solution (pH 1). The products of CO_2 reduction were analyzed by GC-MS from the headspace and solution of the catalysis reactor and were found to be propane and acetaldehyde.

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Paper Cone Spray Ionization Mass Spectrometry: Simple and Efficient Methods for Solid Sample Analysis

김푸름 차상원*

한국외국어대학교 화학과

The use of the ambient ionization mass spectrometry (MS) have been expanded enormously because of its relatively simple interface and also because of its raw sample analysis capability. Paper spray ionization (PSI) method is the extractive ambient ionization technique that utilizes a triangular shape filer paper as a sampling base as well as an electrospray tip. Active applications of PSI MS include drug monitoring from dried blood spots, food contaminant analysis, and metabolite fingerprinting. In this study, we developed a PSI-based solid sample analysis platform, called paper cone spray ionization (PCSI). Major difference between PSI and PCSI is paper geometry: PCSI uses a triangular pyramid shape or circular cone shape paper base instead of planar triangular shape one. Therefore, a paper base of PCSI can act as a solid sample container and a liquid-solid extraction chamber, as well as an electrospray tip. Analysis of various solid samples and viscous liquid samples such as food powders, animal tissues, and petroleum will be demonstrated in this presentation.

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Differentiation of Ganglioside Isomers by MALDI TOF/TOF Mass Spectrometry

박우진 이동건 차상원*

한국외국어대학교 화학과

Gangliosides, acidic glycosphingolipids, have various structural isomers of which sialic acid residue positions are different from each other. Most abundant ganglioside isomers in biological systems are GD1a and GD1b, gangliosides with two sialic acids. In this study, we developed an effective matrix-assisted laser desorption/ionization (MALDI) mass spectrometry (MS) protocol for differentiating GD1a and GD1b isomers. For this purpose, we employed 5-methoxysalicylic acid (5-MSA) as a MALDI matrix because our recent study showed that this matrix induced minimal in-source fragmentation in the ionization of the labile gangliosides, GD1a. In addition, we incorporated salt additives of which cation charge state was +2 in the MALDI sample preparation because this cation could still carry +1 charge after charge neutralization of carboxyl anion group in a sialic acid residue and therefore more information-rich fragment ions could be generated in tandem MS experiments. Our results showed that relative intensities of isomer specific fragment ions were greatly enhanced in tandem mass spectra of GD1a and GD1b by employing doubly-charged cation such as calcium ion instead of singly-charged cation such as potassium ion.

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Sol-Gel Encapsulation Method for Nitrite-Sensitive Membranes Doped with Tetraoctylammonium Bromide

김성우 박성배[1,*]

인제대학교 일반대학원 화학과 [1]인제대학교 화학과

An organic-inorganic hybrid sol-gel matrix was used as host for tetraoctylammonium bromide(TOAB) which is a dissociated ion-exchanger for anion detection. The sol-gel precursor was obtained by the reaction of 3-isocyanatopropyltriethoxysilane with 1,4-butanediol. Being mixed with TOAB with an acidic catalyst, the sol-state precursor slowly gelled to give a TOAB-containing membrane. Tributylphosphate(TBP) was used as a plasticizer. The performances of the sol-gel membrane-based electrodes were compared to those of TOAB-based poly(vinyl chloride)(PVC) membrane electrodes. Membranes with an optimum ratio of TOAB:sol-gel precursor (1.0 : 9.2 by weight), showed very stable baseline potential. Response slope toward nitrite was approximately 54mV/decade in between 10^{-4} - $5x10^{-1}$ M at 20℃. Moreover, selectivity toward nitrite over salicylate and other lipophilic anions was significantly improved, deviating from the Hofmeister selectivity pattern which is observed in most dissociated charged carrier-based potentiometric membrane sensors. The selectivity coefficients measured by the separate solution method in 0.05M MES buffer, pH 5.5, were log $k^{pot}_{nitrite,chloride}$ = -0.7, log $k^{pot}_{nitrite,salicylate}$ =0.4, and log $k^{pot}_{nitrite,thiocyanate}$ =1.4.

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Analytical Platform Employing Graphitized Carbon Liquid Chromatography-Mass Spectrometry for Glycomic Characterization of Biotherapeutic Glycoproteins

서나리 안현주*

충남대학교 분석과학기술대학원

Monoclonal antibodies (mAbs) represent one of the largest classes of drugs in development due to their great efficacy for treatment of diseases such as cancers and rheumatic therapies. It has been known that glycosylation of protein therapeutics can radically affect their biological activity, plasma half-life, immunogenicity, and stability. Therefore, analysis of glycosylation is crucial for proper characterization of biotherapeutics in order to ensure the quality, safety, and consistency of the product. However, glycan analysis still remains analytical challenge due to its inherent microheterogeneity and diversity including the large number of isomeric structure. Liquid chromatography coupled with mass spectrometry (LC/MS) has become a key technique for rapid glycan profiling with high sensitivity and structure elucidation using tandem MS (LC/MS/MS). LC separation is essential for glycan isomer analysis because MS alone does not distinguish isomeric glycans with same mass. Hydrophilic interaction chromatography (HILIC) and porous graphitized carbon (PGC) combined with LC/MS are widely used for glycan separation. In this study, we have evaluated the chromatographic performance of HILIC and PGC including isomer separation, sensitivity, and quantitation for native and 2-AB labeled N-glycans, respectively. All peaks eluted from LC were further assigned by triple quad (QQQ) MS. We found that higher sensitivity was obtained from 2AB labeled glycans separated by HILIC column while this approach requires additional sample steps including glycan labeling and desalting. On the other hand PGC is a powerful tool in separating isomers of native glycans including neutral and acidic species with minimum sample preparation. Our analytical platform can be used to provide a reference for the column choice and optimized separation conditions for glycan analysis of biopharmaceutical glycoproteins.

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Highly Sensitive Detection of Estradiol in Human Serum Using SERS-based Competitive Immunoassay

WANGRUI 주재범[1,*]

한양대학교 바이오나노학과 [1]한양대학교 생명나노공학과

Estradiol (E2) is a biologically active sex steroid hormone that serves as important diagnostic marker in serum of premenopausal and postmenopausal women and in men. Therefore, it is very meaningful to establish highly sensitive and rapid methods for the detection of E2 in human serum. In the past decades, several technologies, including high performance liquid chromatography-mass spectrometry (HPLC-MS), gas chromatography-mass spectrometry (GC-MS) and immunoassays have been developed for the measurement of E2. However, the chromatography methods have lower sensitivity, and need well-trained personnel. Thus, these methods cannot satisfy with the requirements of routine clinical diagnosis. Surface-enhanced Raman scattering (SERS)-based immunoassay using functional nanoparticles has attracted more and more attention due to its higher sensitivity. Herein, we report a SERS-based competitive immunoassay for highly sensitive detection of E2. The method can be applied to detect E2 with good precision at concentrations as low as 0.1 pg/mL. The proposed method has been successfully applied to the determination of E2 for 30 human sera and showed a good correlation compared with the commercially available chemiluminescent microparticle immunoassay (CMIA) kit with good reproducibility. This method has exhibited great potential in the clinical analysis of E2 in human serum.

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Highly Sensitive Detection of Anthrax Marker using SERS-based Competitive Immunoassay

고주희 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Anthrax is a highly acute disease caused by the bacterium Bacillus anthracis. In this article, we report a highly sensitive detection technique for pathogenic B. anthracis, based on the use of a surface-enhanced Raman scattering (SERS)-active magnetic sensor. Gold nanoparticles (GNPs) and magnetic beads were used as SERS nanotags and supporting substrates, respectively. Here, an SERS-based competitive immunoassay platform is described for the quantitative evaluation of the anthrax marker. Poly-γ-D-glutamic acid (PGA) capsules were used as a target biomarker for the highly sensitive detection of B. anthracis becausePGAis known to be closely associated with the pathogenesis of B. anthracis infection. The SERS-based competitive assay reveals an extraordinarily high sensitivity for PGA with a limit of detection of ~1.0 ng/mL. This work provides a conceptually new immunoassay prototype for fast and sensitive detection of PGA markers.

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Surface characterization of molybdenum chalcogenide thin films with various oxygen gas ratios

박주연 강용철*

부경대학교 화학과

Molybdenum chalcogenide (MoO_xS_y) thin films were synthesized by rf magnetron sputtering in ultra high vacuum (UHV) chamber. To control the characteristics of the films, MoO_xS_y thin films were obtained at various mixing gas ratios of argon and oxygen gases. MoO_xS_y thin films were characterized with alpha step, X-ray photoelectron spectroscopy (XPS), ultra violet photoelectron spectroscopy (UPS), contact angle, and 4 point measurement. The thickness of MoO_xS_y thin films was decreased with increasing the oxygen gas ratios. The oxidation states of Mo and S were studied with high resolution Mo 3d and S 2p XPS spectra. The work function of thin films was calculated by UPS and it is increased with increasing the oxygen gas ratio. The conductivity is dramatically increased at 1.0 sccm of O_2 gas flow rate. The contact angle of films were analyzed by water and ethylene glycol.

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Plasmon assisted fluoro-immunoassay for influenza virus sensing system using Au NPs decorated MWCNT

오상진 김정효[1] 이재범[2,*]

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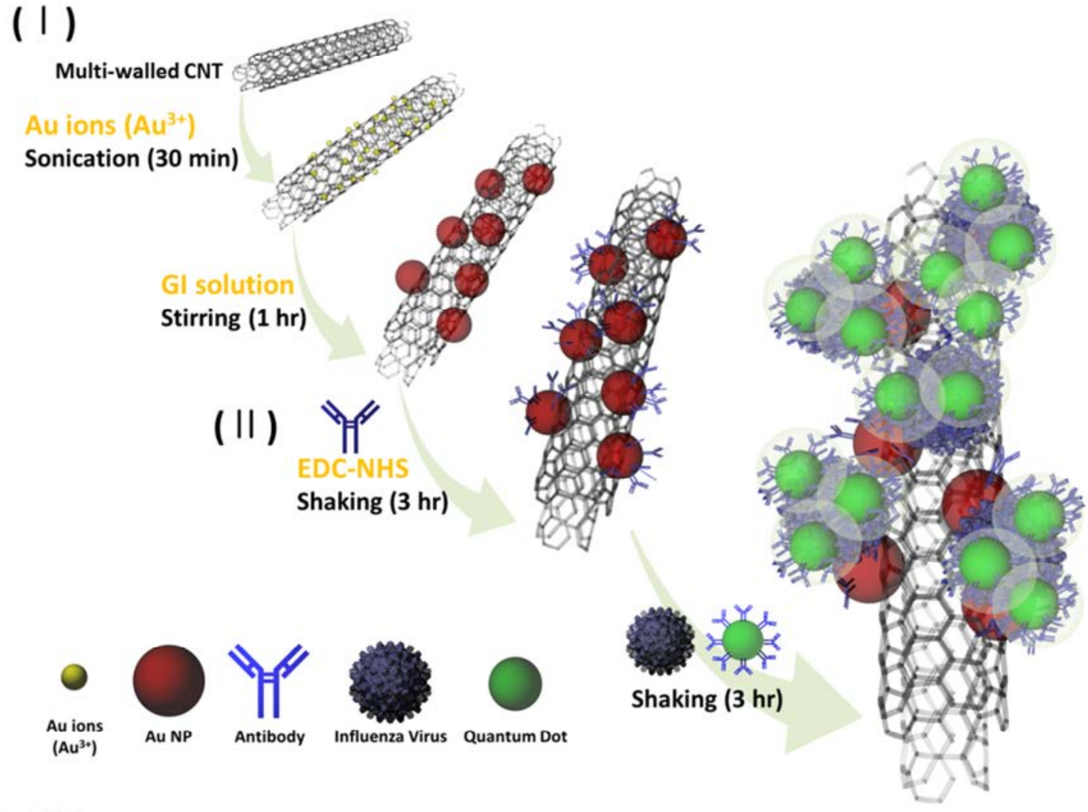
Recently, many carbon based nanomaterials have been interested because of their potential property. Among of them, Au nanoparticles (NPs) decorated carbon nanotube (AuCNT) has been spotlighted due to its great functions such as optical, plasmonic and catalytic properties and so on. Here, we have successfully synthesized AuCNT at the room temperature with mild reduction condition. In particular, this AuCNT possesses plasmonic property, so if some fluorescence NPs are located near AuCNT nanostructure, their FL intensity could be enhanced by plasmonic resonance energy transfer (PRET). Therefore we demonstrated the influenza virus detection using this phenomenon, and this sensing system is called as plasmon assisted fluoro-immunoassay (PAFI). To detect the virus, influenza virus antibodies (Abs) were decorated on the surface of AuCNT and CdTe NPs, respectively. Subsequently, different amounts of influenza virus were added into Abs modified nanomaterials environment. In this case, two different nanostructures were bound by virus-antibody reaction. As increased the virus concentration, FL intensity was also increased. It established that the binding ratio between AuCNT and CdTe NPs was determined corresponding to the virus concentration. Moreover, it meant that influenza virus was detected by FL enhancement monitoring. Through our system, 3 types of virus were monitored, and those are influenza virus A/Beijing/262/95 (H1N1), Influenza virus/New Caledonia/20/99IvR116 (H1N1) and Influenza virus A/Yokohama/110/2009 (H3N2). In our novel sensing system case, the minimum detection limitation was 0.1 pg/ml. In addition, the medical sample (Influenza virus A/Yokohama/110/2009 (H3N2)) was monitored in a detection range from 50 to 10,000 PFU/ml with a detection limit of 50 PFU/ml. Furthermore, this system possesses excellent selectivity for influenza virus detection. Therefore, this

system shows high potential for sensing platform and it is extraordinarily valuable not only to detect the influenza virus but also to apply the various disease sensing.



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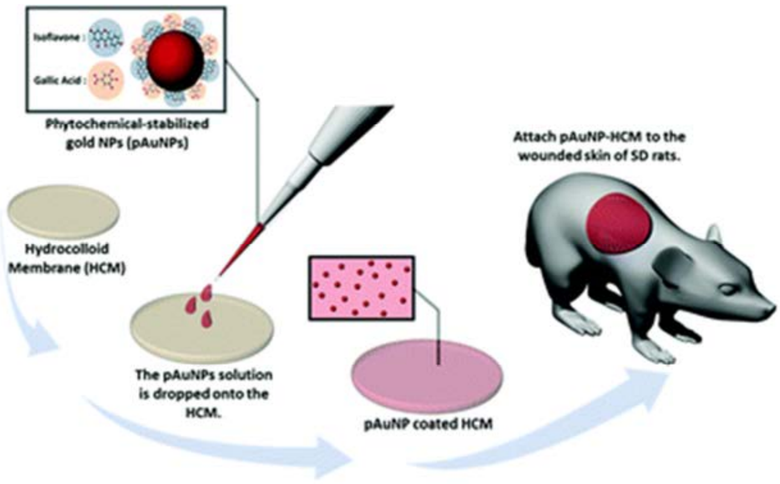
Therapeutic effect of phytochemical-stabilized gold nanoparticles coated on hydrocolloid membrane in cutaneous wound healing

오상진 이재범[1,*]

부산대학교 인지메카트로닉스공학과 [1]부산대학교 나노메디컬공학과

Acute healing of dermatological wound is of importance because of no longer infection as well as the decrease of post-treatment side effects such as hypo-pigmentation or permanent scarring and cosmetic reason. In this article, we report therapeutic effects of pAuNPs that are coated on hydrocolloid membrane (HCM) for curing cutaneous wound skin because both pAuNPs and HCM show excellent biocompatibility and phytochemicals can be an antioxidative agent. The remedial effects of pAuNPs on skin regeneration and angiogenesis were examined in injured skins of Sprague Dawley (SD) rats after the pAuNP-coated hydrocolloid membrane (pAuNP-HCM) was applied for 15 days. The rate of wound closure was about 30 % faster in pAuNP-HCM treated group than that of gauze (GZ) or HCM treated group in first 5 days. Furthermore, wound widths in pAuNP-HCM treated group were significantly decreased in the treatment day 5 ~ 15 after the injury when compared with other groups. Also, significant increase of collagen expression, as well as a decrease of matrix metalloproteinase (MMP) -1 expression and TNG-1beta concentration were observed in the pAuNP-HCM treated group at the day 5. Wound tissue applied with pAuNP-HCM showed enhancement of vascular endothelial growth factor (VEGF), Ang-1 and Ang-2 expression at the day 10. Then, these values were maintained as consistent level until the day 15. Furthermore, notice that the activity of superoxide dismutase (SOD) was significantly increased in skin tissue of the pAuNP-HCM treated group, compared with the GZ or HCM treated group. In conclusion, the pAuNP-HCM may accelerate the process of wound healing in injured skin of SD rats through the synergetic regulation of angiogenesis and connective tissue formation as well as stimulation of anti-oxidant effects.


Isoflavone :
Gallic Acid :
Phytochemical-stabilized gold NPs (pAuNPs)
Hydrocolloid Membrane (HCM)
The pAuNPs solution is dropped onto the HCM.
pAuNP coated HCM
Attach pAuNP-HCM to the wounded skin of SD rats.

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A Microfluidic Chip based Strategy for Biopharmaceutical Glycosyl Modification Analysis

서영숙 안현주*

충남대학교 분석과학기술대학원

Glycosylation plays an important role in ensuring the proper structure and function of most biotherapeutic proteins. However, bioactive glycan modifications add significant complexity to an already-diverse biopharmaceutical glycome. This diversity can greatly complicate glyco-analytical efforts during drug development, production, and regulatory approval. To address this issue, we have developed a novel microfluidic chip capable of online capture, enrichment, and LC separation of phosphoglycans. The chip allows online fractionation of phosphoglycans and non-phosphoglycans onto two different chromatographic runs, with LC gradients and instrumental settings independently optimized for each. Analysis is initiated by injection of glycan mixture onto the two-layer enrichment column. Phosphoglycans are trapped and enriched by the titanium dioxide(TiO_2) layer of the enrichment column, while non-phosphoglycans flow past the TiO_2 layer and are trapped by the PGC layer of the enrichment column. Following enrichment, a water/acetonitrile gradient elutes the non-phosphoglycans from the PGC layer of the enrichment column, which further separates neutral and sialylated glycans. Next, phosphoglycans are eluted from the TiO_2 layer of the enrichment column by injection of a high-pH aqueous elution buffer. We analyzed phosphoglycans selectively by LC/MS chip with a TiO_2-PGC enrichment column. This chip-based strategy for biopharmaceutical glycan analysis increases chromatographic peak capacity, enhances MS sensitivity, and improves glyco-analytical capabilities.

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Observing Platinum Single Nanoparticle Collisions on Copper Ultramicroelectrode by Electrocatalytic Amplification

정승연 권성중*

건국대학교 화학과

Electrocatalytic oxidation of hydrazine occurs at the surface of Pt nanoparticle when it collides onto a Cu ultramicroelectrode (UME). Collision of the single nanoparticle onto a less catalytic electrode surface had observed through a large amplification of the current by electrocatalysis. Pt nanoparticle contacts the electrode, the “blip (or spike)” current response that the current return to the background level was obtained due to the deactivated particles rather than “staircase” response which was described for an Au UME system. The frequency of the current transient was directly proportional to the nanoparticle concentration. And the current transient becomes sharper when the applied potential increases because deactivation rate is rapid. This paper can help us to understand that the interaction between nanoparticles and electrode affects the chemical reaction.

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In Situ Depth Profiling of Plant Metabolites by Nanospray Desorption Ionization (nano-DESI) Mass Spectrometry

이동건 이광빈 전규웅 차상원*

한국외국어대학교 화학과

In nanospray desorption ionization (nano-DESI), one of the extractive ambient ionization methods for mass spectrometry (MS), a steady-state micro-liquid junction formed between two micro-capillaries is used for extracting and dissolving analytes directly from a sample surface at a high spatial resolution. Recently, we have developed nano-DESI MS methods for direct profiling of metabolites from plant tissues in a depth-dependent manner. In the previous study, however, physical removal of plant wax layers was necessary prior to nano-DESI MS analysis, primarily because conventional spraying solvents such as methanol and water could not penetrate the wax layer. In present study, we optimized the nano-DESI spraying solvent system which could allow us to probe metabolites beneath the wax layer without employing any physical removal process. Our results showed that a toluene-containing nano-DESI spraying solvent was the very effective solvent system in terms of spatial resolution of sampling, stability of ion signals, and plant metabolite coverage.

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Synthesis and Characterization of Highly Purified Bimetallic Nanoclusters

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연세대학교 화학과

Bimetallic nanoclusters differ from their homometallic nanoclusters in many ways, which has become a topic of increasing interest in recent years. One major area of interest involves the study of $Au_{25}(SR)_{18}$ nanoclusters with bimetallic compositions such as $Pt_1Au_{24}(SR)_{18}$, $Pd_1Au_{24}(SR)_{18}$, $Ag_{1\sim13}Au_{24\sim12}(SR)_{18}$ and $Cu_{1\sim9}Au_{24\sim16}(SR)_{18}$ nanoclusters, where SR is thiolate ligand. Quantum-size of these nanoclusters induce distinctive quantum confinement effects, which result in unique optical and electrochemical properties. Recently we tried to synthesize highly purified Pt- and Pd-doped Au_{25} nanoclusters and clearly defined their optical, electronic, and catalytic properties. In our synthetic method, a mixture of $Pt_1Au_{24}(C_6S)_{18}$ (or $Pd_1Au_{24}(C_6S)_{18}$) and $Au_{25}(C_6S)_{18}$ was produced via judicious control of reaction conditions and size-focusing process. Relatively short complexation time interrupted the appearance of $Au_{25}(C_6S)_{18}$ and increased the production of bimetallic gold nanoclusters. The reaction product was further purified by selective decomposition of $Au_{25}(C_6S)_{18}$ using H_2O_2 and subsequent solvent extraction, resulting in highly pure $Pd_1Au_{24}(C_6S)_{18}$ and $Pt_1Au_{24}(C_6S)_{18}$ nanoclusters. Successful syntheses of $Pd_1Au_{24}(C_6S)_{18}$ and $Pt_1Au_{24}(C_6S)_{18}$ nanoclusters were confirmed by UV-Vis absorption spectroscopy, mass spectrometry and X-ray photoelectron spectroscopy (XPS) studies.

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Au nanoparticle decorated Graphene sheet for plasmon-enhanced photoluminescence immunoassay platform

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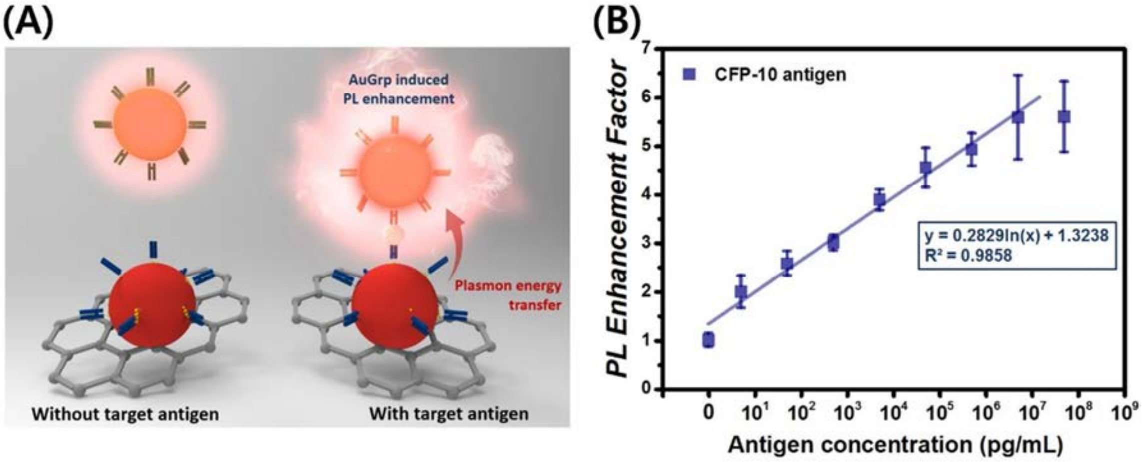
Metal-nanoparticle?functionalized graphene, in particular, graphene sheets containing Au nanoparticles (Au NPs), have generated considerable interest due to their unique optical and electrical characteristics. In this study, we successfully produced graphene sheets decorated with Au NPs (AuGrp) using phytochemicals as reducing agents. During this reaction, Au ions intercalated into the layered graphene flakes and were then reduced into NPs, exfoliating the graphene sheets. The physicochemical properties of the AuGrp nanocomposites were characterized, and the exfoliation process was investigated using a molecular dynamics simulation of Au NPs between graphene sheets. Using antibody (Ab) modified AuGrp sheets and quantum dots, a plasmonic-enhanced photoluminescence immunoassay of tuberculosis (TB) antigen (aG) CFP-10 was demonstrated for a potential application of these materials. The enhancement of photoluminescence (PL) response was monitored depending on the various TB aG concentrations from 5.1 pg/mL to 51 μg/mL, and the detection limit for CFP-10 was 4.5 pg/mL. Furthermore, the selectivity was demonstrated with Ag85 as the other TB aG, and PL enhancement was not observed in this case. Therefore, AuGrp based immunoassay showed the potential for biosensor application.


(A)
AuGrp induced
PL enhancement
Plasmon energy
transfer
Without target antigen
With target antigen
(B)
CFP-10 antigen
y = 0.2829ln(x) + 1.3238
R² = 0.9858
PL Enhancement Factor
0
1
2
3
4
5
6
7
0
10¹
10²
10³
10⁴
10⁵
10⁶
10⁷
10⁸
10⁹
Antigen concentration (pg/mL)

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Label-free Impedimetric Polytetrabenzidene/Dendrimer Nanocomposite Based Highly Sensitive Immunosensor: Femtomolar Detection of Cardiac Troponin I in Serum

Akter Rashida 정봉진 **Md. Aminur Rahman**[*]

충남대학교 분석과학기술대학원

A simple and robust but highly sensitive label-free impedimetric cardiac troponin I (CTI) immunosensor was fabricated using a poly-3, 3, 5, 5-tetramethylbenzidine (PolyTMB)/dendrimer (Den) nanoassemble film as anti-CTI antibody immobilizing platform. PolyTMB was electrochemically grown on a gold (Au) electrode by a potential cycling method. Carboxylic acid functionalized third generation poly(amidoamine) dendrimer (Den) and protein A (PA) was then sequentially covalently attached on the PolyTMB and PolyTMB/Den films, respectively. Anti-CTI antibody was then covalently immobilized on the PolyTMB/Den film with controlled orientation. The surface of the immunosensor was characterized using electrochemical quartz crystal microbalance (EQCM), coulometry, scanning electron microscopy (SEM), Fourier Transform Infrared (FT-IR) spectroscopy. The highly sensitive CTI detection was made by monitoring the impedance changes of the immunosensor surface due the anti-CTI-CTI binding, which affect the PolyTMB redox activity. CTI could be selectively detected at a fg/mL level in human serum samples.

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Effects of morphology of nanostructured surfaces on the viability of HeLa cells

김근오 박현욱 김강영 곽진수 조승익 홍다영[1] 권영욱*

성균관대학교 화학과 [1]성균관대학교 자연과학부 화학과

Interest in the research of mesoporous materials for biomedical studies has increased recently. Therefore, the interaction between nanostructured materials and cells has been studied extensively, but the effect of nanostructured surfaces on the cell viability has received less attention.In this work, we report the viability of HeLa cells on various films such as mesoporous thin films and anodic aluminum oxide (AAO). Mesoporous thin films of various metal oxides (SiO2, TiO2, ZrO2, Al2O3 and Fe2O3) with 10 nm pore size were synthesized by sol-gel process with metal salts and surfactant. In case of Fe2O3 and AAO, we prepared various pore sized films to verify the effect of pore size in cell viability. In order to test the stability of films, films were immerged in a cell culture media for 2 days. And then, we discovered that all films except for SiO2 are stable in a cell culture media. Finally, we observed the viability of cells on various films for 3 days in a cell culture condition. As a result, we found that the cell viability depended on pore sizes as well as types of materials of films.

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Human herpesvirus 8 and Signal transducer and activator of transcription 3

명진종

전북대학교 인수공통전염병연구소

IL-6 is known to play a critical role in two cancers caused by human herpes 8 (HHV-8): Kaposi’s sarcoma (KS) and multicentric Castleman’s disease (MCD). It promotes the proliferation of cancerous cells in lesions affected, creating an inflammatory microenvironment for viral and tumor growth. IL-6 is a canonical activator of Signal Transducer and Activator of Transcription 3 (STAT3), a well-known oncogene. Therefore, it has been postulate that IL-6 activates STAT3 to promote tumorigenesis. However, it is interesting to note that KS and MCD heavily depend on viral lytic replication for the tumorigenesis. Therefore, we hypothesized that STAT3 may be involved in the regulation if KSHV replication. Here we demonstrated that an active form of STAT3 promotes viral replication in both transformed and primary endothelial cells while a dominant-negative STAT3 strongly down-regulates it. We are currently investigating the molecular mechanisms of STAT3-mediated control of HHV-8 infection and replication.

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Interaction of T and endothelials cells through TNFRSF members

명진종

전북대학교 인수공통전염병연구소

Human herpesvirus 8 (HHV-8) is the latest member of the human herpesvirus family. HHV-8 is an oncogenic virus and thus causes various tumors including Kaposi’s sarcoma (KS) and at least two B cell lymphomas. Less than 1 % of HHV-8 carriers develop KS and thus it has been postulated that genetic deficiency may facilitate tumor initiation and growth. In accordance with this notion, only a handful of reports describe KS incidence in children with inborn errors. A pediatric patient with a mutation in one of the exons of the OX40 gene displayed loss of functionality of effector memory CD4+ T cells and has developed KS early in childhood. Therefore we hypothesized that OX40 on T cells may interact with OX40L on endothelial cells. OX40L is known to be abundantly expressed in KS lesions as well. First of all, we demonstrated high levels of OX40 expression on tonsillar T cells and OX40L on endothelial cells upon infection, interaction of which leads to the inhibition of viral replication. Of note, 4-1BB-4-1BBL interactions diminished HHV-8 lytic replication. The regulation of viral replication in B cells required only 4-1BB-4-1BBL interactions, suggesting a cell type-specific mechanism involved. Further in-depth studies are required to delineate the exact role of those interactions in the pathogenesis of virus-induced pathologies.

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Interplay of a pleiotropic cytokine and KSHV: highjack of a host antiviral defense to viral growth advantage

명진종

전북대학교 인수공통전염병연구소

Kaposi's sarcoma-associated herpes virus (KSHV) is aetiologically associated with various human malignancies. In KS lesions, an array of proinflammatory cytokines are found at high levels and they have been shown to promote survival, maintenance, and growth of the tumor element, so-called, spindle cells. In the present study, we have defined the role of a proinflammatory cytokine, interleukin-6 (IL-6). IL-6, is a pleiotropic cytokine and when bound to the IL-6 receptor (IL-6R), it activates gp130, the signal transducing unit of the receptor, which is expressed on most somatic cells in the body. Thus , upon expression, it has a profound effect on many different cell types affecting both cellular and viral processes. We hypothesized that prolonged treatment of IL-6 might change the course of KSHV infection. Indeed, treatment of IL-6, oncostatin M, and ciliary neurotropic factor on induced iSLK.219 cells potentiates viral replication in terms of viral gene expression as well as infectious virion production. Of note, IL-6 stimulated spontaneous lytic replication in tightly latent iSLK.219 cells. Taken together, for the first time in the field, we demonstrated that IL-6 promotes KSHV lytic replication, proposing a rationale to inhibit the action of the cytokine in an effort to control KSHV-related tumors.

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The effect of extein pI values in protein trans-splicing reactions

김다희 권영은*

동국대학교 의생명공학과

Protein trans-splicing (PTS) reaction is self-processing enzymatic 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. Previous works mostly focused on the effect of extein sequences directly flanking the intein and revealed several key residues which are necessary for splicing activity. There are also observations showing that PTS kinetics depend on whole flanking sequences but the reasons are not clearly elucidated yet. As there is an enormous complexity of all possible flanking sequences, we focused on investigating how varying ionic potentials of flanking sequences affect PTS kinetics. For this study, we have chosen *Npu DnaE* intein as a model system as this naturally split-intein mediates fast ($t_{1/2}$ ~ 1 min) PTS in physiological conditions. We prepared multiple pairs of split-inteins that carry exteins of various pI's and analyzed in vitro PTS in different conditions. We observed accelerated reaction rates as the pI's of N intein flanking sequence increased. As for the flanking sequences of C intein, PTS reaction rate increased as pI decreased. This result provides a good guideline in designing an efficient PTS system.

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Synthesis and Characterization of $NaYF_4$:Yb^{3+},Er^{3+} Upconversion Nanoparticles for Biomedical Applications

최승유 박태정*

중앙대학교 화학과

Upconversion nanoparticles (UCNPs) have been studied for a versatile biomedical application such as in vivo imaging with NIR optical detection as a biosensing tool, or delivery of active forms of medicines inside living cells. UCNPs have distinctive characteristics such as bright bioluminescence, high upconversion efficiency, and good colloidal stability. Specifically, UCNPs have been synthesized and analyzed their unique advantages such as photoluminescence, special emission, and low-background fluorescence signal. Thus, UCNPs have many advantages compared with the quantum dots and organic dyes. Here, we report the enhancement of upconversion red emission (Er^{3+} ion) in $NaYF_4$:Yb^{3+},Er^{3+} nanoparticles. We have successfully synthesized $NaYF_4$:Yb^{3+},Er^{3+} UCNPs via solid-state method, which is the thermal decomposition of trifluoroacetate as precursors, organic solvent, at a high boiling point. $NaYF_4$:Yb^{3+},Er^{3+} nanoparticles have emission in the field of near infrared wavelength, cubic shape and nano size. We will further use it for biomedical applications such as in vivo imaging with NIR optical detection onto the solid substrate as a biomolecular diagnosis tool.Keywords: Photoluminescence, Upconversion nanoparticle, Biomedical imagingReferences[1]M. Haase, H. Schafer. Upconversion Nanoparticles. Angew, Chem. Int. Ed., 50 (2011) 5808-5829.[2]H. Chen, F. Yuan, S. Wang, J. Xu, Y. Zhang, L. Wang. Aptamer-based Sensing for Thrombin in Red Region via Fluorescence Resonant Energy Transfer between NaYF4:Yb,Er Upconversion Nanoparticles and Gold Nanorods, Biosens. Bioelectron., 48 (2013) 19-25.

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Label-Free Biosensor System For Food-Poisoning Bacteria Using Magnetic Nanoparticles with Specific Aptamers

최승유 박태정*

중앙대학교 화학과

Food-poisoning bacteria have polluted foods during processing or handling. It can cause illness-like Typhoid and mass recall in the food market. Because people have a great attention to uncooked and well-being food, we should protect contamination and prevent the consumption of contaminated food from food poisoning bacteria. We report an effective platform biosensor system using specific aptamers to detect a target bacterium, *Salmonella typhimurium*. The colorimetric strategies for the detection of *Salmonella* are attractive because they enable rapid sensing with naked-eyes without the need for sophisticated instruments and long analysis time like as PCR (polymerase chain reaction). We just used magnetic nanoparticles (MNPs), colorimetric substrate, and the specific aptamers. Aptamers, which are single-stranded oligonucleotides (DNA or RNA), bind with target molecules with high affinity and specificity compared with antibodies and high stability against biodegradation and denaturation. Due toan enzyme-like activity of MNPs, they can lead to color change with hydrogen peroxide. If MNPs absorb the DNA on their surface, they could shield the enzyme-like activity of MNP. Subsequently, specific aptamers on the MNPs interact with *Salmonella* after adding of *Salmonella* cells into the solution. After separating the MNPs, we saw the color change and UV-VIS spectrum. Considering the inexpensive cost, easy to separation, simple to synthesis and modification, MNPs would be applied to various detection systems. Furthermore, this system for a portable device will be developed *in situ* by time and space.References[1] Min-Ah Woo, Moon Il Kim, Jae Hwan Jung, Ki Soo Park, Tae Seok Seo and Hyun Gyu Park, A Novel Colorimetric Immunoassay Utilizing the Peroxidase, Mimicking Activity of Magnetic Nanoparticles, Int. J. Mol. Sci. 2013, 14, 9999-10014;

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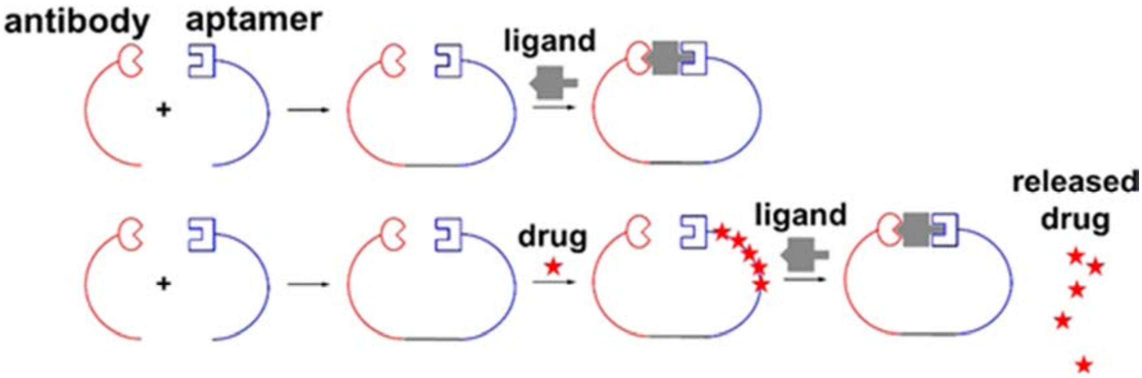
Improved Ligand Binding by Antibody—Aptamer Pincers

강성묵

경희대학교 화학과

To increase the affinities of antibodies or aptamers for their targets, we designed antibody?aptamer pincers(AAPs) or heterodimers for thrombin or human epidermal growth factor 2 (HER2) as a model system. For this purpose, we first conjugated a 15-mer or 29-mer anti-thrombin aptamer, which are well-known to bind to thrombin in two specific epitopes, with an anti-thrombin antibody to enable each binding part of the AAP to simultaneously recognize a different part of the thrombin molecule. The AAP comprising a 15-mer aptamer and an anti-thrombin antibody has an apparent dissociation constant (Kd^{app}) value of 567 pM, and this value is approximately 1/100 of that of the antibody alone or 1/35 of that of the aptamer monomer alone. The AAP comprising a 29-mer aptamer and an anti-thrombin antibody has a much lower Kd^{app} value than that of 15-mer aptamer-conjugated antibody. Furthermore, this concept of the AAP system was employed to HER2-targeted drug delivery system (DDS) based on both antibody and drug-loaded aptamer. Anti-HER2 aptamer was conjugated with anti-HER2 antibody and loaded with doxorubicin, and the resulting AAP-HER2-Dox was found to have approximately 3- and 6-fold highercytotoxicity than drug alone and antibody alone, respectively. Therefore, this novel AAP system constructed by conjugation of the antibody with the aptamer can effectively improve the affinities of the resulting AAPs for their target molecules and the drugloaded AAP system can possibly serve as a platform for targeted DDS against many malignancies.


antibody
aptamer
+
ligand
+
drug
ligand
released drug

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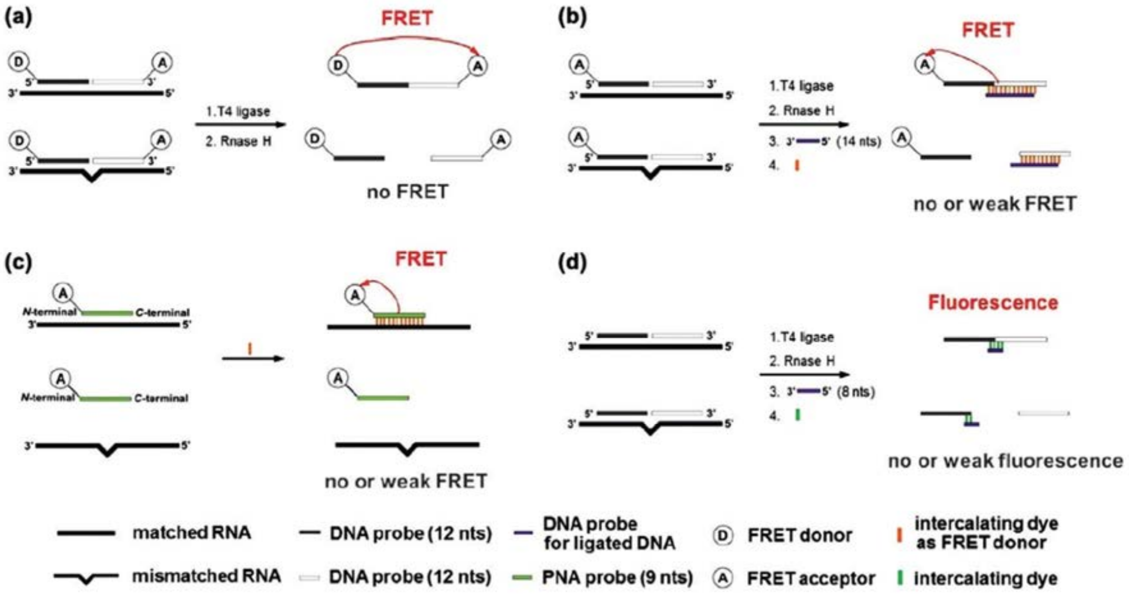
Allele-specific, Hybridization-based, Washing-free Fluorescence Signal Production Platforms for Quantitation of Single-Base Change (C→U) in RNA

박성민

경희대학교 화학과

A single nucleotide polymorphism (SNP) is a single base-pair substitution that commonly constitutes thegenetic variation in individuals. Because of its association with disease susceptibility and drug resistance, SNP detection is of great value in studying the variation in drug responses. Here we report four types of washing-free (i.e., separation-free or sequential addition of reagents) and polymerase chain reaction (PCR)-free fluorescence signal production platforms for quantitative detection of a single-base mismatch in RNA and compare their analytical efficiency. The RNA-templated SNP detection methods in this study are based on the allelespecific hybridization approach and/or on the allele-specific oligonucleotide ligation approach, and have been successfully applied to the quantitation of single-base mutation (C→U) in RNA of the BCR/ABL fusion gene, by endpoint measurements of fluorescence intensity. These methods have several advantages for practical applications, such as direct discrimination of single-base mismatch of the RNA extracted from cells, no requirement of PCR amplification, performance of homogeneous detection, easy design of detection probes, and suitability for large-scale genotyping.


(a)
FRET
D
A
5'
3'
1.T4 ligase
2. Rnase H
no FRET
(b)
FRET
1.T4 ligase
2. Rnase H
3. 3' 5' (14 nts)
4.
no or weak FRET
(c)
N-terminal
C-terminal
FRET
no or weak FRET
(d)
Fluorescence
1.T4 ligase
2. Rnase H
3. 3' 5' (8 nts)
4.
no or weak fluorescence
matched RNA
mismatched RNA
DNA probe (12 nts)
DNA probe (12 nts)
DNA probe for ligated DNA
PNA probe (9 nts)
FRET donor
FRET acceptor
intercalating dye as FRET donor
intercalating dye

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Molecular attraction using CdTe nanostructure and gold nanoparticles thereby biomolecular interaction

김은주 박태정*

중앙대학교 화학과

Eun Ju Kim, Seung Woo Lee, Tae Jung Park*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 156-756, Republic of Korea*E-mail: tjpark@cau.ac.krNovel nanomaterials, such as nanoparticles, nanorods and nanowires, have been attracted considerable attention in chemical and biological applications during the past decade. Cadmium Telluride (CdTe) is an II-IV semiconductor that has been widely used for a variety of applications. The principles of the substrate to improve the sensitivity can be used for more stable detection target of CdTe nanowires (NW). Gold nanoparticles (AuNPs) were specifically performed as a substrate without chemical modification of the antibody bound to the gold surface or bound with gold binding polypeptide (GBP). A novel fusion protein was constructed by genetically combining GBP to avian viral surface antigen (Ala) as a crosslinker for effective affinity against its specific antibodies. The GBP-incorpoerated Ala bound to AuNPs excellently interacted with its antibody and showed changes in absorbance and color, allowing efficient diagnosis. Specific immobilization of GBP-Ala fusion protein onto the gold substrate and its specific interaction with the antibody could be demonstrated. Herein, we demonstrate a conceptually different mehtod to functionalize CdTe NW. A new approach is based on a bifunctional biomolecule with gold-specific binding affinity and correct orientation control as a bioreceptor. The recombinant fusion protein, GBP-Ala, showed specific adsorption on different types of gold nanostructure. A facile functionalization method of CdTe NW using GBP-Ala could be extended to a biomolecular sensing application.

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The sensitive detection of lead ions using sodium thiosulfate-and CTAB-capped gold nanoparticles

김은주 박태정*

중앙대학교 화학과

Eun Joo Kim, Nguyen Le Thao Nguyen, and Tae Jung Park*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 156-756, Korea, Republic of Korea,*Corresponding author. Tel.: +82 2 820 5220, fax: +82 2 825 4736.E-mail address: tjpark@cau.ac.kr (T.J.Park) Environmental pollution has become a serious problem in the world because of the wide and long-term harm. Contamination by heavy metal ions and toxic heavy metals including zinc, copper, nickel, mercury, cadmium, lead cause long-term significant damage to many biological systems as they disrupt biological activities at the cellular level. Lead is one of the most abundant metals on earth, which plays an important role in biological systems and an essential transition metal in the human system. Lead poisoning has been related to several diseases associated with environmental pollution. Therefore, it is essential to detect and remove Pb^{2+} from the aqueous solution. Water-soluble and stable quantum dots (QDs) and cethyltrimetylammonium bromide (CTAB)-capped gold nanoparticles (AuNPs) were applied for the sensitive detection of Pb^{2+}. These CTAB-capped AuNPs were employed to selectively detoxify heavy metal ions such as Pb^{2+} ions. Detailed studies by UV/visible spectroscopy, electron microscopy, and dynamic light scattering, which show competitive binding of Pb^{2+} with the CTAB-capped AuNPs changed the surface properties of the QDs. In the presence of sodium thiosulfate mixture, this system is capable to detect Pb^{2+} with a detection limit as low as 28 nM. This method provides a great potential for the detection of lead ions with simplicity, rapidity, ultrasensitive and excellent selectivity.

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Biosynthesis and characterization of gold nanoparticles mediated with recombinant metal binding

김은주 박태정*

중앙대학교 화학과

Eun Ju Kim, Eun Bee Kim and Tae Jung Park*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 156-756, Korea*E-mail: tjpark@cau.ac.krNanotechonology is a very promising filed of research in nano-science. Although its basic strategy starts with the production of nanomaterials using chemcial and physical approaches, biosyntheis has become an alternatve way of produing them. Biosynthesis is better in ways as it is ecofriendly, cost effective and faster in synthesizing metal nanoparticles compared to other methods. *In vivo* synthesis of gold nanoparticles (AuNPs) using recombinant metal binding proteins (MBPs) is demonstrated here. The rapid formation of stable AuNPs has been found using MBPs in recombinant *Escherichia coli* in aqueous medium at atmospheric condition. The recombinant MBPs were identified to act as a reducing, stabilizing and capping agent. The AuNPs obtained were characterized by UV-visible spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction and FT-IR spectroscopy analysis. TEM analysis revealed that AuNPs were predominantly formed spherical in shape with a size range of 5 - 30 nm. The size and the shape of AuNPs were modulated by varying the concentration ratio of recombinant proteins in the reaction medium. This method showed synthesis of AuNPs within 40 min in diameter suggests that the reaction rate is higher compared to those of the synthesis using other chemical methods. We critically analyzed its great potential as efficient drug carriers for drug delivery system that can be applied in various biomedical fields.

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Effects of nanoparticle-coated graphene oxide on the polymerase chain reaction

김은주 박태정*

중앙대학교 화학과

Eun Ju Kim, Ji Young Park, Ha Young Jung, Seung Hoon Beak, Chan Young Park, and Tae Jung Park*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 156-756, Republic of Korea*E-mail: tjpark@cau.ac.krThe polymerase chain reaction (PCR) has become one of the most important technologies in modern biological and life sciences. PCR can be used to exponentially manufacture a large number of DNA copies from a small amount of DNA molecules in a few minute. However, PCR steps have some limitations like as easily influenced temperature and produce of non-specific DNA fragments. To overcome this limitation, various nanomaterials have been employed to increase the specificity of the PCR reaction. Herein, we report a development of PCR method to effectively avoid nonspecific reactions using inexpensive gold nanoparticles-coated graphene oxide (GO/AuNPs). In particular, as it maintains the equal or higher DNA amplification yields, the reaction time is shortened, and the cooling/heating rates could be increased. The excellent thermal conductivity of the GO/AuNPs should be an important factor in improving the PCR efficiency, which compared with different concentrations of DNA complex, DNA polymerase and different size samples. The results showed a great PCR efficiency and specificity of DNA amplification procedure by employing GO/Au using real-time quantitative PCR (qPCR) and transmission electron microscopy.References[1] Liu, J. Phys. Chem. Chem. Phys. 14, 10485. (2012)[2] H. Li, J. Huang, J. Lv, H. An, X. Zhang, Z. Zhang, C. Fan, J. Hu, Angew. Chem. Int. Ed. 44, 5100. (2005)[3] Yi C, Fong C-C, Chen W, Qi S, Tzang C-H, Lee S-T and Yang M, Nanotechnology. 18 025102 (2007)

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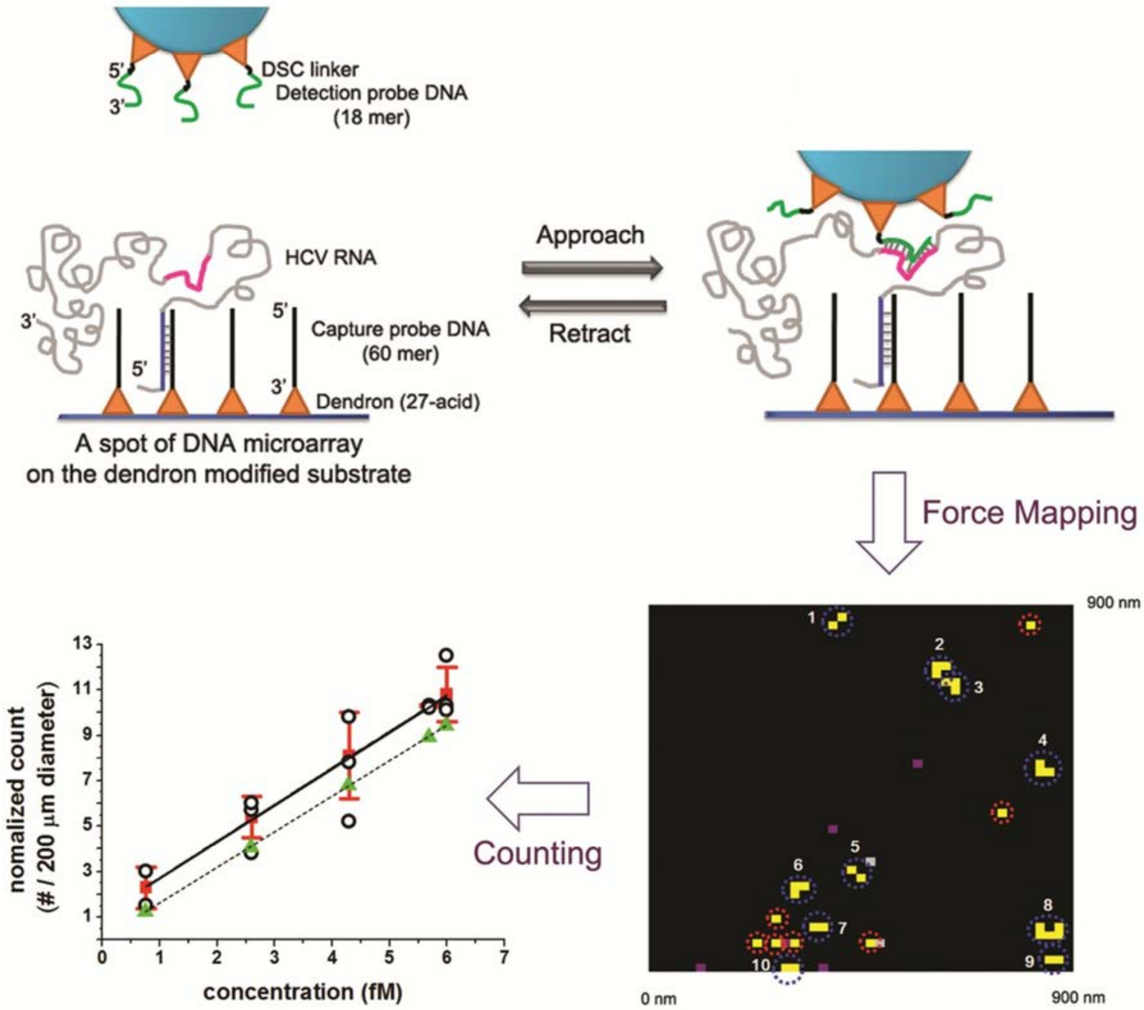
Direct Quantitative Analysis of HCV RNA by Atomic Force Microscopy without Labeling or Amplification

정유진

한국화학연구원 나노바이오융합연구단

Force-based atomic force microscopy (AFM) was used to detect HCV RNA directly and to quantitatively analyze it without the need for reverse transcription or amplification. Capture and detection DNA probes were designed. The former was spotted onto a substrate with a conventional microarrayer, and the latter was immobilized on an AFM probe. To control the spacing between the immobilized DNAs on the surface, dendron self-assembly was employed. Force-distance curves showed that the mean force of the specific unbinding events was 32 ± 5 pN, and the hydrodynamic distance of the captured RNA was 30?60 nm. Adhesion force maps were generated with criteria including the mean force value, probability of obtaining the specific curves, and hydrodynamic distance. The maps for the samples whose concentrations ranged from 0.76 to 6.0 fM showed that cluster number has a linear relationship with RNA concentration, while the difference between the observed number and the calculated one increased at low concentrations.


5'
3'
DSC linker
Detection probe DNA
(18 mer)
HCV RNA
3'
5'
5'
3'
Capture probe DNA
(60 mer)
Dendron (27-acid)
A spot of DNA microarray
on the dendron modified substrate
Approach
Retract
Force Mapping
900 nm
1
2
3
4
5
6
7
8
9
10
0 nm
900 nm
Counting
nomalized count
(# / 200 μm diameter)
13
11
9
7
5
3
1
0
1
2
3
4
5
6
7
concentration (fM)

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A Robust Fluorescence Sensing Strategy based on Graphene Oxide/Gold Nanoparticles

최승유 박태정*

중앙대학교 화학과

A robust signal-on fluorescence sensing strategy was developed to provide specific detections of various target analytes. Especially, fluorescent sensing procedures using fluorescence dyes, such as FITC and FAM, have been a general routine for biological applications including imaging and assays. However, because of the intrinsic signal of dye in the absence of the target, the signal-to-background ratios of fluorescent sensors remains insufficiently high to make the analytical performance. Graphene oxide (GO), a two-dimensional (2D)-layered precursor of graphene preparation, consists of sp^2-bonded carbon with a hexagonal configuration. It is able to adsorb single-stranded DNA (ssDNA) via non-covalent π-π stacking interactions between the graphene and nucleobases. Furthermore, GO is an excellent energy acceptor in fluorescence resonance energy transfer (FRET). The fluorescence resonance of dye-labeled ssDNA onto the GO will be completely quenched. Gold nanoparticles (AuNPs) are one of the most biocompatible substances. Graphene-based AuNPs prepared with molecular level dispersion have been shown to improve sensitivity and specificity of biomolecular sensing much better. In this study, we have used FAM-labeled aptamers that specifically bind to the hyaluronic binding domain of CD44 and demonstrated that fluorescent sensors based on GO/AuNPs would be widely applied in various detection systems.

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Dynamic equilibrium in *E.coli* ACP and identificaion of novel antibiotics against multi-drug resistant gram-negative bacteria

정민철 박영근 김양미*

건국대학교 생명공학과

Acyl carrier protein (ACP) is at the main system responsible for fatty acid biosynthesis and the acyl chain distribution found in membrane lipids. In the presence of divalent cation, apo-*E.coli* ACP (EcACP) shows only one conformation, while holo-ACP shows two sets of resonances, suggesting that two conformers are in dynamic equilibrium. In order to study the secondary structure and thermal stability of EcACP, we measured melting temperatures using circular dichroism (CD) spectroscopy. In order to understand the fundamentals of low thermal stabilities of EcACP, we performed multidimensional heteronuclear NMR experiments and completed the backbone and side chain assignment. We determined the structures of two conformers of EcACP in dynamic equilibrium. The overall structures of two conformers consist of four α-helices connected by three loops with two metal binding sites. The nature of inherent local structural variations in these two conformers of holo-ACP is similar to the nature of structural differences in apo and acylated ACPs. Since multi-drug resistant gram-negative bacterial infections are increasing worldwide thesedays, we tried to discover antimicrobial compounds that have a novel mechanism of action towards new target enzyme, ß-Ketoacyl-acyl carrier protein synthase III (KAS III), a condensing enzyme in bacterial fatty acid synthesis. We identified and optimized novel potent EcKAS III inhibitors with broad-spectrum antimicrobial activity with strong binding affinity to EcKAS III. We will further investigate the potency of this analogs and study the dynamics of EcACP.

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Isolation of RNA aptamers specific to influenza virus NS1 protein

우혜민 정용주[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

Influenza is an infectious disease caused by RNA viruses of the family Orthomyxoviridae, the influenza viruses. Influenza A virus contains 8 segments of (-) ssRNA that encode 13 known proteins. The NS1 of influenza A virus interacts with RIG-I and inhibits the RIG-I-mediated induction of IFN-β. Therefore, inhibition of NS1 may limit further viral infection in the host cells by activation of IFN induction. In this study, we selected a high-affinity RNA aptamers capable of binding to NS1 protein with a dissociation constant of 9.15 nM and 4.91 nM using a SELEX (systematic evolution of ligand by exponential enrichment) procedure. We measured binding affinity of NS1 protein and aptamer by ELISA. The aptamers were incubated with 293T cells expressing NS1 and binding assessed by FACS and Confocal. We revealed that the selected aptamer was successfully able to induce IFN. We suggest that the isolated aptamer in this study are strongly expected to be new molecular drug candidate.

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The optimal condition for ATP hydrolysis of Dengue virus helicase

조진범 김준원[1] 정용주*

국민대학교 생명나노화학과 [1]국민대학교 생명나노화학과

Dengue virus is a viral pathogen that is responsible for causing several diseases in humans. It has been reported that more than 50 million people are infected annually. The virus was transmitted by mosquitoes and ticks. Dengue virus helicase plays a crucial role for viral replication. The main function of dengue virus helicase unwinds the double helical RNA using the energy. We investigated ATPase activity of the helicase with various oligonucleotides. In this study, steady state ATPase analysis analysis showed that poly(U) was more effective than poly(C) or M13 ssDNA. Also, the optimal pH condition for ATP hydrolysis activity was identified as pH 7.0 by pH profiling of activity test. Furthermore, we investigated the helicase activity depending on various divalent metal ions. Rate of the enzyme with Mg^{2+} was 3 times higher than Mn^{2+}. As a result, we established the optimal assay condition for ATP hydrolysis of dengue virus helicase.

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Dictyopteris undulata extract induced apoptosis in human melanoma cells via reactive oxygen species and endoplasmic reticulum stress

김준기 정용주*

국민대학교 생명나노화학과

Extracts derived from various marine brown algae, including *Dictyopteris undulata*, raised apoptosis in cancer cells. The study investigated the hypothesis, which an ethanol extract from *D. undulata* (EE-DU) induces apoptosis in A2058, human melanoma cells via endoplasmic reticulum (ER) stress. EE-DU inhibited A2058 cells proliferation and increased apoptotic body formation, identified by the presence of fragmented nuclei. Moreover, DUE-treated cells showed mitochondrial calcium cation (Ca^{2+}) overloading, increased ER staining, overexpression of ER stress-related protein and cell death modulatory proteins RNA-dependent protein kinase-related ER kinase, phospho-inositol-requiring enzyme 1α, CCAAT/enhancer-binding protein-homologous protein, and phospho-eukaryotic translation initiation factor 2α, accompanied by increased intracellular ROS levels. However, pre-treatment of N-acetyl cysteine, the ROS scavenger, attenuated EE-DU induced apoptosis and ER strss in A2058 cells. These findings suggest that EE-DU treatment triggers apoptosis in human melanoma cells through a mechanism involving ER stress.

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Hydrophobic interaction between F45 and F18 Play Important Role in Structure of *Enterococcus faecalis* Acyl Carrier Protein

박영근 정민철 김양미*

건국대학교 생명공학과

Fatty acid synthesis is essential for cell growth and viability. The Acyl Carrier Protein (ACP) is a key element in the biosynthesis of fatty acids being responsible for the acyl group shuttling and delivery within a series of related enzymes.*Enterococcus faecalis* (*E. faecalis*) is a Gram-positive, commensal bacterium inhabiting the gastrointestinal tracts of humans and other mammals. *E. faecalis* can cause life-threatening infections in humans, especially in the hospital environment. *E. faecalis* can withstand oxidative stress, dry condition, and extremes of temperature and pH. In this study, structures of *Ef*-ACP as well as thermal stabilities of *Ef*-ACP were investigated. CD experiments showed that melting temperature of *Ef*-ACP is 78°C, which is much higher than that of *E.coli* ACP (68°C). We determined the solution structure of *Ef*-ACP. The overall structure consists of four α-helices (helix I (3-17), helix II (39-53), helix III (59-64), helix IV (68-78)) connected by three loops. Phe45 in *Ef*-ACP has stacking interactions with His17 and Phe18, which are essential for the thermal stability of *Ef*-ACP. Stacking interactions between Phe45and and Phe18 contribute to the thermal stability of *Ef*-ACP by stacking interactions and they block the path into the alternate binding cavity of *Ef*-ACP which accommodate the growing acyl chain. Spin relaxation experiments were performed and the dynamics of *Ef*-ACP will be discussed. This study will be helpful to understand the specific recognition mechanisms between *Ef*-ACP and functionally different enzyme partners in fatty acid synthesis pathway.

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Kinetic description of the loop closure in the protein-tyrosine phosphatases of regenerating liver using spin relaxation experiments

박영근 김양미*

건국대학교 생명공학과

Phosphatases of regenerating liver (PRLs) constitute a novel class of small, prenylated phosphatases with oncogenic activity. PRL-3 is particularly important in cancer metastasis and represents a potential, therapeutic target. The flexibility of the WPD loop as well as P-loop of protein tyrosine phosphatases is closely related to their catalytic activity. Using NMR spectroscopy. we studied the structure of vanadate-bound PRL-3, which was generated by addition of sodium orthovanadate to PRL-3. The WPD loop of free PRL-3 extended outside of the active site, forming an open conformation, whereas that of vanadate-bound PRL-3 was directed into the active site by a large movement, resulting in a closed conformation. We suggest that vanadate binding induced structural changes of the WPD loop, P-loop, α4-α6 helices, and polybasic region. Compared to free PRL-3, vanadate-bound PRL-3 has a longer α4 helix, where the catalytic R110 residue coordinates with vanadate in the active site. In addition, the hydrophobic cavity formed by α4-α6 helices with a depth of 14-15 ? can accommodate a farnesyl chain at the truncated prenylation motif of PRL-3, i.e., from R169 to M173. Conformational exchange data obtained from CPMG experiments suggested that the WPD loop moves between open and closed conformations with a closing rate constant kclose of 7 s-1. This intrinsic loop flexibility of PRL-3 may be related to their catalytic rate and may play a role in the substrate recognition.

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Oxidation and coordination properties of ST18, a non-classical zinc finger

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Zinc finger (ZF) domains consist of cysteine and histidine ligands with zinc ions and they are coordinated with tetrahedral geometry (Td) for specific biological activity. ZF domains usually function as transcriptional and translational regulators and bind to DNA and RNA. ZF proteins are classified as classical zinc finger (Cys2His2) and non-classical zinc finger (other than classical ZF) which shows biological variations through enzymatic function. Suppression of Tumorigenecity 18 (ST18) is a non-classical ZF protein and it has six zinc finger domains which show high sequence homology. ZF domain of ST18 coordinates to zinc ion with Cys2His2Cys residues and it generates selective interactions with TNF-α (Tumor necrosis factor-alpha) to inhibit breast cancer. Tandem sequences of ZF domains, ST18-ZF1~2, ZF3~4, ZF5~6, have cloned and expressed successfully in E. coli system. The purified ZF domains are applied to understand the oxidation patterns to identify the oxidized states under hydrogen peroxides. These results provide direct information that reversible disulfide bonds and irreversible further oxidation states. In addition, zinc ion can be replaced with other metal ions such as ferrous and ferric in limited conditions in biological systems. The ITC (Isothermal titration calorimetry) and UV-vis studies will provide its binding affinities. These results will provide how ZF domains of ST18 controls cancer generation and inflammation.

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Improvement of Antifreeze Activity of Recombinant Glaciozyma Ice-binding protein (IBP) by Additives

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Ice-binding protein (IBP) is a protein that binds to ice. IBP can create an gap between melting and freezing points of its aqueous solution, by binding and inhibiting the growth of ice crystals. This property, called thermal hysteresis (TH), has drawn attention from biomedical field because IBP can be used as as a supplement to improve the cryopreservation efficiency of animal cells, blood, stem cells, and tissue.The purpose of this study is to investigate the solutes which can enhance TH activity of Glaciozyma IBP. The Glaciozyma IBP used in this investigation was the 26 kDa of recombinant IBP expressed in P.pastoris. Natural Glaciozyma IBP was used for comparison of TH activity and stability. There were total 18 solutes used in this experiment. Among them, the most effective TH activity enhancer is 2 M ammonium sulfate, which increases the TH values nearly fourfold from 0.2 °C to 0.82 °C. Moreover, Glaciozyma IBP is more thermostable (+ 9 ℃) and does not form aggregation in this solution. However, there is no change of thermostability at 0.25 M of this solute. The results of natural Glaciozyma IBP were similar to the recombinant Glaciozyma IBP while 2 M sucrose is the most effective enhancer. But sucrose provoked aggregates at this concentration on both IBPs. In addition, Trimethylamine N-oxide increased TH activity approximately threefold, and sucrose, D-sorbitol, and ammonium bicarbonate increased TH approximately twofold.From the results presented, selected solutes can be applied to improve the antifreeze activity of IBP, which can be used as an cryoprotectant.

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Docking of Ice-Binding Proteins (IBPs) on Ice Crystal Planes Might Explain their Thermal Hysteresis

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부경대학교 화학과

Many cold-loving organisms produce ice-binding proteins (IBPs) to survive in sub-zero temperatures. IBPs bind to the ice and lower the freezing point non-colligatively, therefore creating gap between melting and freezing points, which is called thermal hysteresis (TH). Based on the TH, IBPs can be classified as moderately active (TH of ~ 1 °C) and hyperactive (TH > 1 °C) IBPs. Previous studies showed that activity was dependent on what planes of ice crystal IBPs binds to. We recently isolated moderately-active LeIBP from Leucosporidium sp. Arctic yeast and hyperactive FfIBP from Antarctic sea ice Flavobacterium frigoris PS1. To evaluate interaction between IBPs and ice crystal planes and to provide insight into the correlation of the ice binding and activity, we carried out molecular docking using Hex program. Docked results with the lowest energy values were examined and analyzed with Shape Complementarity (Sc). High Sc values mean the binding interface between ice crystal planes and IBPs are highly complementary. The Sc values were comparable with TH values. When TH value is higher it must be higher Sc values. The TH activity of FfIBP is tenfold higher than LeIBP. Therefore Sc values of FfIBP were higher than those of LeIBP. The highest Sc values for both LeIBP and FfIBP were from the interaction with secondary ice planes.Keywords: FfIBP, LeIBP, ice crystal plane, AFPs, structures, docking, interaction

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Efficient intracellular delivery of impermeable photosensitizer by DNA tetrahedron and its potential for photodynamic therapy in vivo

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Photodynamic therapy(PDT) is a cytotoxic treatment to kill hazardous cells such as cancer cells and pathogenic bacteria. The cell death was induced by reactive oxygen species(ROS) produced by PDT drugs called photosensitizers(PS). Among various types of PS, methylene blue(MB) has been considered one of the most practical PS since it has decent quantum yield of singlet oxygen generation in the therapeutic window. However, low cellular uptake is a major drawback of MB to be used as a PDT drug. To improve intracellular delivery of MB, we used DNA tetrahedron as a carrier. MB could be loaded on DNA tetrahedron and intracellularly delivered with high uptake efficiency. Evaluation of PDT effect by MB delivered with DNA tetrahedron was initially analyzed at the cellular level. Then, we also demonstrated that the delivery of MB by the DNA nanocarrier could also effective at in vivo level and subsequently lead to enhanced potency compared with free MB.

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Size-controlled DNA nano material

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RCA is a useful method for making DNA-based nanomaterial.However, controlling the size of RCA product precisely is very challenging.This presentation introduces a way to control the size of DNA-based nanomaterial prepared by RCA.

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ECM Delivery to the Cells for Wound Healing Process

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Fibronectin(FN) and collagen(Col) are adhesive proteins that act a crucial role in wound healing. Both proteins directly are repaired by regulating the behaviour of a variety of cell types that are mobilized to the damaged area in order to rebuild the tissue. However, the treatments with FN and Col are limited to wounds of the skin surface. In this study, in order to heal the specific target under the skin, we developed FN and Col delivery system based on liposomes. We attached different vesicles coated with fibronectin on substrates, then put not only on fibroblast but also on various cells. We checked extracellular matrix(ECM) can be delivered to fibroblast and the other cells at specific pH by the trigger. In conclusion, ECM delivery system works successfully at the specific tissue and condition.

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Effects of Lipid Packing on Lipid Flip-Flop Phenomena: A Neutron Reflectivity Study

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The transbilayer movement of phospholipids in cellular membranes, also known as lipid flip-flop or translocation, is an area of significant biological importance. Although in nature lipid translocation is a slow process and is usually controlled by proteins, in a pure lipid system this mechanism can occur spontaneously under certain conditions. Even though lipid flip-flop has been studied for decades but is still far from being understood and well characterized for natural cell membranes as well as for simpler bilayer model systems. Moreover, the packing state of lipid in real system, which is a consequence of multiple factors such as spontaneous curvature of lipid itself, negative charges on headgroup, and protein interaction, is potential to cause defect sites within membrane. These defects play a role as a membrane channel which regulate many biological functions, including of lipid translocation. In this study, we aim at the mechanism of lipid flip-flop phenomenon observed by Neutron reflectivity at molecular level. We would like to investigate the effect of unsaturated lipids, 1) How the dynamics of lipid diffusion process is controlled by the membrane packing; 2) Whether flip-flop can be induced from only one side of the membrane bilayer. By mean of Langmuir-Blodgett/Schaefer deposition methods, it is possible to prepare successive adsorbed layers resulting in a final asymmetric composition. These asymmetric bilayers were characterized by X-ray reflectivity to obtain the information of bilayer quality, complementary with Neutron reflectivity to investigate the absolute composition and the relative location of lipid molecules within the bilayer and at its interfaces.

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Dynamics of Collagen-mediated membrane during apoptotic phosphatidylserine exposure

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Collagens are the extracellular matrix (ECM) as fiber proteins that are located in connective tissue on the extracellular surface which plasma membrane of cells is composed of many kinds of phospholipids and has asymmetric distribution. During the apoptosis of cells, this asymmetry is disrupted by exposure of phosphatidyl-serine(PS) on the plasma membrane of cells. Even though plasma membrane and ECM have critical relationship in biological processes, the dynamics of extracellular matrix during the apoptosis is still not understood. In this paper, we estimated that dynamics of plasma membrane and collagen after disruption of plasma membrane by using mimicking cell system. Apoptotic mimicking cells which are exposure of PS on the membrane induced collagen fibril on the lipid membrane. As thickness of collagen fibril increase, apoptotic mimicking cells changed the structure as function of time. Interestingly, the cholesterol in the lipid membrane induced the structure of blebs on the lipid membrane as thickness of collagen fibril increase. Our models clearly show that the interaction between ECM and exposure of PS during apoptotic process.

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Structural studies of the complexes between factor VIII and low density lipoprotein receptor-related protein: Toward a long-acting factor VIII

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부경대학교 화학과

Low density lipoprotein receptor-related protein (LRP) is a receptor responsible for the clearance of proteases including factor VIII (FVIII) from blood. The binding sites on FVIII for LRP are within its A2, A3, and C2 domains, and these sites interact with clusters II and IV of LRP. Binding of FVIII to LRP might serve to both regulate and clear FVIII. However, given its critical role in endocytosis and cholesterol homeostasis, inhibiting LRP itself has not been considered as a strategy to increase the half life of FVIII. A structure-based understanding at the atomic level of the ligand binding interfaces of FVIII is critical in designing recombinant FVIII with altered binding properties and in developing drugs that will inhibit FVIII-ligand interactions.In this study we cloned, and expressed complementary-type repeats of cluster II of LRP, designated as CR domains, and investigated the interaction between CR domains and VIII using dot blot assay. We successfully cloned, overexpressed, and purified CR34, CR45, CR56, CR67, CR78 domains in E. coli. The purified CR domains were subject to dot blot assay. In the dot blot assay, CR34 and CR45 are highly effective in shielding the FVIII from antibody binding even after 10 minute incubation.

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In vivo synthesis of EuSe nanoparticles and characterization of its related cytotoxicity and contrast agent using T2 mapping

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Biosynthesis of metal nanoparticles can be used in biomedical applications, where they facilitate a drug-delivery system and can be used for a positive targeting of cancer in diagnosis and therapy. We report an *In vivo* biosynthesis of europium selenide (EuSe) nanoparticles by recombinant *Escherichia coli* cells expressing the heavy-metal binding proteins, phytochelatin synthase and metallothionein. These recombinant proteins have a high binding affinity for metal nanoparticles using these favor for metal ions. They are used for *In vivo* biomedical applications such as contrast agents for magnetic resonance imaging (MRI), for cancer or tumor diagnosis and therapy. Herein, we synthesized EuSe nanoparticles and analyzed its magnetic and optical properties. Furthermore, we studied their possibility for contrast agent by T2 relaxation time mapping method. By this study, we can simply check both the cancer diagnosis and therapy at the same time.

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Measuring mechanical properties of cell membrane depending on ECM composition

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In addition to regulating many phenomenon of cells, extracellular matrix(ECM) has important role in providing physical support for cells. Especially, the physical properties of cells determine stiffness of tissue and increased stiffness induced tumorigenesis in organism. However, the relationship between compositions of ECM and stiffness of individual cells is not fully understood. In this paper, we investigated that the ECM compositions highly correlated with elasticity of cells. Comparing various cells having different ECM compositions can offer evidence that ECM composition is related to elasticity of cells. And, comparing real cells with ECM incorporating GUV, which is mimicking real cells, can support this correlation. Micropipette aspiration provided the method for measuring physical properties of membrane of various cells and vesicles such as elasticity.

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Intracellular stimulus responsive non-covalent peptide gatekeepers in hallow mesoporous silica platform for targeted drug delivery

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Among the drug delivery carriers, gatekeepers in mesoporous silica nanoparticles have received much attention in multifunctional targeted drug delivery system due to their tunable pore morphology, high specific surface area, easy surface modification/ bioconjugation for targeting and physiochemical stability. One among them was hollow mesoporous silica nanoparticles. Since they can host the therapeutic compounds that are easily degraded in the hostile biological environment; delivered per se without encapsulation and their void cores can serve as a extra reservoirs for the drug storage. In the present work, we develop a biocompatible and stable carrier for anticancer drug delivery using the noncovalent peptide gatekeeper technique. The drug loaded nanoparticles were wrapped with glutathione s-transferase Z domain peptide. Further this peptide can be decorated with several types of antibody and epibodies to target the cancer cells. Upon its internalization, the drug can be released inside the cell due to the increased intracellular glutathione concentration.Keywords: Glutathione; GST-Z domain; Epibody; Antibody; peptide gatekeepers; mesoporous silica nanoparticles.

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Generation of ssDNA aptamers for detection of gram negative pathogenic bacteria

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Infections caused by pathogenic bacteria pose severe medical issues due to their contagion and lethality. Therefore, development of novel methods for sensitive and specific detection of infectious bacteria is very important for health and safety of humans, animals, and even plants.Herein we report development of aptamers as pathogenic bacteria detection tools. We selected ssDNA aptamers that can detect gram negative bacteria by a toggle-cell-SELEX approach. During the SELEX, randomized single-stranded DNA (ssDNA) library was incubated with Escherichia coli DH5a, Escherichia coli K12, and Serratia marcescens in alternating rounds. SELEX was performed for 12 rounds and the final ssDNA pool was found to have high affinity to all the three target bacteria. After sequencing of ssDNA pools, we examined binding affinity of individual aptamers against various kinds of bacteria with real-time quantitative PCR, fluorescence microscopy, and bio-layer interferometry assay. Through real-time quantitative PCR, we discovered sequences which have high binding affinity against E.coli DH5a, E.coli K12, Serratia marcescens and even E.coli O157:H7. We plan to use these aptamers as biosensors for colorimetric, fluorescence, and impedimetric detection of pathogenic gram negative bacteria.

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Guanidine modified polyethyleneimine-g-polyethylene glycol nanocarriers for long interfering RNA (liRNA) based advanced anticancer therapy

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Combination therapy involving the synergism between different therapeutic approaches seems to be a promising strategy in anticancer treatment. Immunostimulatory long interfering RNA (liRNA) structures capable of executing specific RNA interference (RNAi) mediated gene silencing tasks seem to be potential candidates for a combination approach. Apart from their therapeutic efficacy, the unique structural format of liRNA candidates facilitates better association with cationic polymers and significantly improves their intracellular delivery. In this study, we have developed a biocompatible cationic delivery platform based on low molecular weight branched polyethyleneimine-grafted-polyethylene glycol (bPEI-g-PEG) for advanced liRNA based anticancer therapy. With simple guanidine (GU) modification, the bPEI-g-PEG platform could induce a strong RNAi mediated response in cancer cells, without induction of any obvious toxicity. Moreover, liRNA complexed with GU-bPEI-g-PEG which targets expression of Survivin gene sensitized cancer cells for effective chemotherapy. A combination strategy involving immunostimulatory RNAi mediators with conventional chemotherapeutic drugs seems to be an effective approach in advanced anticancer treatment.

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Development of chemically modified cell penetrating asymmetric siRNA (cp-asiRNA) for enhancing intracellular delivery and RNAi response

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Small interfering RNA (siRNA) is a class of double-stranded RNA molecules that mediate target gene silencing in a sequence-specific manner and can be designed to target genes for therapeutic applications. Current siRNA therapeutics, however, have drawbacks such as off-target effect, instability and poor delivery efficacy. To overcome these limitations, we previously developed novel siRNA structural variants including cell penetrating asymmetric siRNA (cp-asiRNA) structures which could enter into cells and trigger RNAi without transfection reagent in many cell lines. In this study, we present further optimized cp-asiRNA structures. Alternated molecular patterns were applied and we observed that the renewed cp-asiRNA structures retained enhanced gene silencing activity. We also present the application of well-known CPP, Melittin, with facilitating endosomal escape property to our cp-asiRNA and a chemical library screening for further optimization of cp-asiRNA gene silencing activity. We confirmed that Melittin-mediated enhanced RNAi activity is also applicable to cp-asiRNA. For chemical library screening, thousands compounds were analyzed and we obtained compounds which enhance cp-asiRNA activity. Further characterization and optimization of the compounds are in progress. We expect that our results will provide a clear insight into the potential of cp-asiRNA for diverse applications including RNAi therapeutics.

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Structure-Activity Relationship Study on Cellular Internalization of Nucleic Acid Tetrahedron

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Due to the unique feature of sequence-driven self-assembly, a variety of nanostructures has been constructed using DNA as a building block. Interestingly, DNA-based tetrahedron has shown to internalize into cells without any need of delivery vehicles, which makes it potentially useful as a drug delivery vehicle. However, in terms of functionality, DNA tetrahedron has the limitation because double-stranded DNA has no biological function such as gene silencing. In contrast, double-stranded RNA such as small interfering RNA (siRNA) can mediate specific target gene silencing by utilizing RNA interference mechanism. Therefore, we hypothesized that RNA tetrahedron can not only to maintain the self-delivery property of DNA tetrahedron, but also to execute biological activity such as gene silencing. Toward this goal, we first optimized the condition for self-delivery of nucleic acid tetrahedron and investigated the driving force of self-delivery mediated by nucleic acid tetrahedron. Our study will provide a clear insight into the potential of nucleic acid tetrahedron for diverse applications including RNAi-based therapeutics.

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Near-infrared fluorescent sensors for detection of hydrogen sulfide in aqueous solution

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Near-Infrared (NIR) fluorescent sensors have emerged as promising molecular tools for imaging biomolecules in living systems. However, NIR fluorescent sensors are very challenging to be developed. Herein, we report new type of NIR fluorescent sensors (L^1 and L^2) for hydrogen sulfide in aqueous solution. $L^1$and L^2exhibit NIR fluorescence enhancement response to hydrogen sulfide selectively over other physiological species.

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Naphthalimide-based fluorescent probes for detection of hydrogen sulfide in aqueous solution

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Hydrogen sulfide (H_2S) is an important biological messenger but few biologically-compatible methods are available for its detection in organic mix solvent. Herein, we report two bright fluorescent probes L^1 and L^2 that are selective for H_2S over cysteine, glutathione, homocysteine and other reactive sulfur, nitrogen, and oxygen species in aqueous solution(PBS buffer, pH7.4). Based on previous reports of using H_2S to reduce RN_3 to the parent amine moiety, we sought to exploit this chemistry for H_2S sensing. By masking a fluorogenic amine as azido group, mild reduction with H_2S regenerates the parent amine and results in fluorescence turn-on.

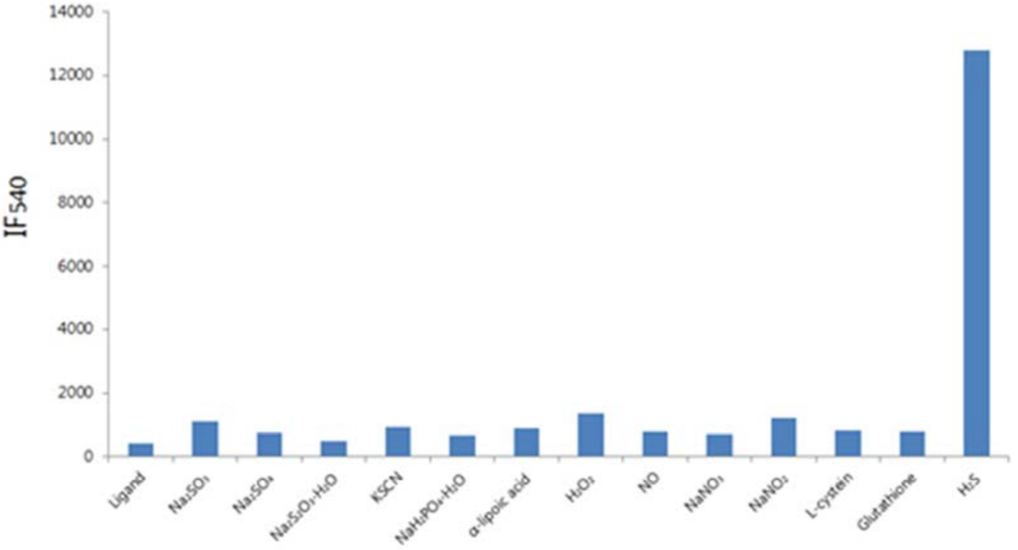

Figure 1. Fluorescence responses of Ligand(10μM) towards sulfur containing inorganic ions($S_2O_3^{-}$, SO_4^{2-}, SO_3^{2-} ,SCN^{-}, 1mM), inorganic salt (NaH_2PO_4, 1mM), organosulfur compound(α-lipoic acid), reactive oxygen species(H_2O_2, 1mM), reactive nitrogen species(NO, NO_3 , NO_2 , 1mM), thiols (L-cvs 1mM, Glutathione 10mM) and H_2S(100μM) in PBS buffer (pH7.4, 5% DMSO) at 37℃ for 30min. Excitation at 435nm.

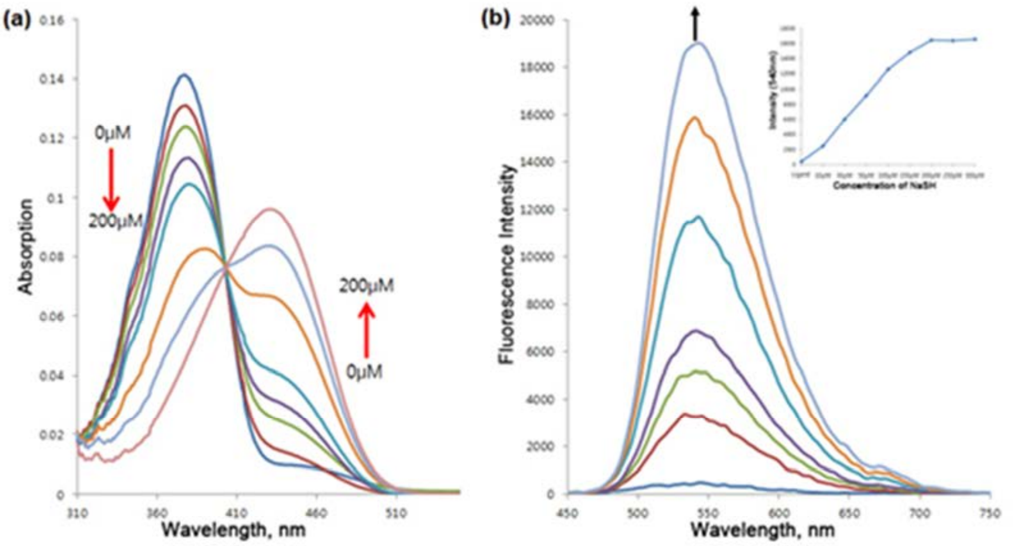

Figure 2. (a) Absorption spectra of **L** (10μM) in the presence of various concentration of NaSH (0-200μM) in PBS buffer(5%DMSO, pH=7.4) at 37℃ for 30min. (b) Fluorescence spectra of **L** (10μM in the presence of various concentration of NaSH (0-300μM) in PBS buffer(5%DMSO, pH=7.4) at 37℃ for 30min. Excitation at 435nm.

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Hydrophobic drug delivery platform with polymer gatekeepers in mesoporous silica nanostructures

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Among small therapeutic molecules which have been developed as an anticancer agent, many of potential active molecules are critics for obstacle and challenge in the administration due to their poor solubility in aqueous solution. Solubilizing these drugs and delivering to a target cancer site have been extensively explored with nanoscale carriers, including micelles, hollow capsules, crosslinked nanogels, cylindrical micelles, and inorganic nanoparticles. However, the versatile drug delivery platform with noncovalent gatekeepers in many kinds of hydrophobic drug molecules without premature drug release, large loading capacity and colloidal stability is still challenging. Hence we developed a simple technique by utilizing the advantage of hardcore mesoporous silica, using the biocompatible non-covalent polymergatekeepers technique. This is a versatile drug delivery platform, where different kind of hydrophobic drugs such as doxorubicin, camptothecin, paclitaxel, curcumin and tomaxifen can be loaded into the core at high capacity, without any chemical modification of the carrier. The polymer shell surface can be easily decorated with different targeting ligands with simple and mild thiol-disulfide chemistry. The drug molecules loaded in the nanocontainers can be released by the degradation of the polymer shell in controlled manner in the intracellular reducing microenvironment, which consequentially induces cell death.

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Characteristics of the antifreeze protein extracted from fish that inhabit the Korea Ocean

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The antifreeze proteins (AFPs) are mainly found in polar and northern-temperate fishs and grouped into five distinct classes (types I~IV and antifreeze glycoproteins). AFP binds to ice crystal and inhibit the growth of ice crystal, thus creating the gap between melting and freezing points of aqueous solution. This property is called thermal hysteresis (TH). Interestingly we found recently that temperate fishes inhabiting near the East sea of Korea also had antifreeze activity in its blood and muscle. In this study, firstly we screened antifreeze activity of fishes near Ulleung island, and secondly attempted to purify and characterize AFPs. We screened the TH activity from muscle tissues of *Priacanthus macracanthus Cuvier*, *Halichoeres tremebundus*, *Hypodytes rubripinnis*, *Hexagrammos otakii*, *Clidoderma asperrimum*, *Pleuronectes herzensteini*, *Eopsetta grigorjewi*, and *Stephanolepis cirrhifer* (8 samples) and found that *Halichoeres tremebundus*, *Stephanolepis cirrhifer* and *Pleuronectes herzensteini* displayed TH accompanied with changes in ice crystal morphology. Muscles of Korean ocean fishes were homogenized in NH_4HCO_3, and supernatant were obtained by centrifugation. Using fast protein liquid chromatography (FPLC), fractions containing antifreeze activity was selected. Further fractionation was carried out using HPLC. The TH activity and characteristics of AFP isolated will be presented.

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Cell-penetrating dimeric α-helical peptides can inhibit transcription of HIV-1 at nanomolar unit

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We designed a-helical peptide dimer using leucine and lysine residue to penetrate cell efficiently and inhibit Tat-TAR interaction. Most LK dimers can penetrate eukaryotic cells easily and inhibit transcription of TAR at low nanomolar concentrations. LK dimers that can inhibit reproduction of HIV-1 effectively are considered as potential anti-HIV-1 drugs.

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Human acyl carrier protein does not sequester its bound acyl chain inside the hydrophobic pocket

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Acyl carrier protein (ACP) is an acidic protein which is essential for fatty acid synthesis(FAS). The synthases of Type I FAS are arranged as large multidomain polypeptides. The growing fatty acid chain is bound covalently during chain elongation and reduction to the ACP domain that is then able to access each catalytic site. In this work, Human ACP was cloned, expressed, and purified. We prepared 15N and 13C labeled ACP and performed the NMR experiments for structural determination. Backbone assignment of ACP was completed and 80 residues are assigned in HSQC spectra. We performed the CD experiments and observed a well defined α-helical structure in the presence of Ca^{2+} ion while it does not adopts any folded conformation without metal ion, implying that divalent cation helps stabilizing the electrostatic repulsion of ACP. On conversion from apo to holo form, chemical shift changes are observed on the ACP residues surrounding the phosphopantetheine attachment site in HSQC spectra. However, there are almost no chemical shift changes when the holo form is modified to octanoyl form. These results imply that Human ACP does not sequester its acyl chain, while Type II bacterial ACPs sequester its acyl chain. This is a significant difference between the Human FAS and bacterial FAS. These difference makes bacterial FAS as an excellent target to design potent antibiotics. In order to understand the fundamentals of Human FAS, tertiary structure of Human ACP will be studied and the dynamic properties will be investigated further.

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Reduction of capsular constructure of silicone implant by biocompatible polymer coating

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Silicone implants are widely used in breast augmentation and reconstruction surgeries because of their transparency, high oxygen permeability and low cost. But limited biocompatibility induces severe side effects such as capsular contracture, an excessive foreign body reaction forming a tight and hard fibrous capsule around the implant. The effects of biomembrane-mimic surface coating of silicone implants to the capsular formation was examined. Biomembrane-mimic polymer, poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC) has biocompatibility, so they prevent nonspecific protein adsorption and fibroblast adhesion on the silicone surface. More importantly, PMPC coated silicone implant show decrease of capsule formation in rats, represented significantly thinner capsules, lower collagen density, and more regular collagen alignment than bare silicone implant. Also reduction of inflammation-related cells, myeloperoxidase, and transforming growth factor-β showed PMPC coating is effective in reducing inflammation in the capsular tissue. The biomembrane-mimic coating of silicone implants are expected to have a high possibility to prevent capsular contracture and to develop biocompatible materials for various biomedical applications.

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Selective manipulation of the droplet including the cell in microfluidic chip

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서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Droplet based microfluidics is a rapidly growing field of research combining physics, biochemistry and microsystems engineering. Precise control of droplet volumes and reliable manipulation of individual droplets allow us to perform chemical reactions inside the droplets under defined conditions.In microfluidic devices, we were fabricated the uniform droplets regulating the flow rates of aqueous solution and oil. For the active manipulation of multiple emulsion droplets, double-layer microfluidic systems with pneumatic valves have been adopted for handling emulsion droplets in microfluidic channels. So, fabricated emulsion droplets were transported along guided channels, which were the protrusion on top of microfluidic channels. By using pneumatic valves, we can control to release the droplets in the trapping region.Consequently, droplets can be selectively released and transported into the other positions in a microfluidic device by the active control of the pneumatic valves.Due to storage and release, we could be realized selective screening on specific region inside a microfluidic device. Therefore, this method could be further ` explored for small scale reaction of analysis in a precisely controlled manner.

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Alteration of Cell Morphology on Hexagonally Close Packed Silica Nanobeads

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숙명여자대학교 화학과

The nanotopological cues are emerging field of in vivo study, because it stimulates changed cell morphology and behavior such as adhesion, proliferation, differentiation, apoptosis and migration. However, it has not studies nanosurface affected cancer cell behavior, therefore, in this study, we determined that effects of the silica nanobeads on cancer cells. For synthesis of silica beads, we made it stober method using basic amino acid (L-arginine) or NH4OH and mixed TEOS by controlling injection rate. We carried out rubbing process to obtain the monolayer silica beads and it used as nanotopological cues for fabrication. It was induced changing cell morphology at 1DIV in group-II (SB-450 and SB-570). However, it was maintained in group-I (SB-120, SB-230) and group-III (SB-1450) like control. Therefore, we separated type-I and type-II surface along with area of cell adhesion and morphology. The characteristic of type-II surface was long distance between contact points, resulting in increase of tension to cells. We found that the morphology rounded up by type-II surface at 1DIV. We described that the nanosurface-induced mechanical tension is associated with alteration of morphology, thus the silica nanobeads used as nanotopological tools for cancer research.

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Isolation, structural elucidation and bioevaluation of ethanolic extract from *Zanthoxylum schinifolium*

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Recently, the hazard may appear due to the use of synthetic preservatives that have been used widely in the existing industry revealed by several studies. Therefore, the development and discovery of natural preservatives is a necessary condition. The natural substance derived from an organic material including lower fatty acid, lysozyme, lactoferrin, bacteriocins, and a polylysine can be frequently employed as a preservative in various foodstuffs. In particular, the utility of preservatives in the cosmetics products is of immense interest. In the present investigation, we have reported the isolation of effective ingredients, structural analysis and bioevaluation of the ethanolic extract of natural materials Sancho (chines pepper, Fruit of *Zanthoxylum schinifolium*). Sancho has been commonly used in the variety of foods because it is highly effective for human health. For example, relieve indigestion, vomiting, diarrhea, relieve dysentery, neurasthenia improvement, sterilization, atopic dermatitis, seborrheic treatment, diuretic, burn treatment, antiviral, hangover, skin care, pain relief etc. The present study demonstrates the anti-oxidation as well as anti-tyrosinase effect of separated product from Sancho assessed by the spectrophotometric analysis.

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Patterning the coiled-coil proteins on gold nanostructures in single-molecule level

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Patterning biomolecules at nanoscale on solid substrates has highlighted increasinglyfor various applications, including platforms for studying biological phenomena at single-molecule level, sensors detecting biomolecules with single-molecule level sensitivity, and means of patterning sub-5-nm inorganic materials at single-particle level. In molecular biology studies, single-protein on substrates enables the study of the kinetics of biological events at single-molecule level, rather than ensemble averages of multiple molecules. In addition, the functionalities of biomolecules can be used to pattern inorganic materials at single-molecule level, by patterning single proteins on substrates, and attaching inorganic nanoparticles, such as quantum dots to the patterned biomolecules. Here, we study the orientations of three coiled-coil protein variants of two lengths attached to patterned nanostructures at the single-protein level. The three coiled-coil proteins are attached to gold nanostructures fabricated precisely by e-beam lithography and lift-off process through cysteine-gold interaction, and their orientations are studied at the single-molecule level using confocal imaging and molecular dynamics simulation. We show that the orientations of the 33-nm-long coiled-coil protein can be controlled by using a gold trench.

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Isolation, structural elucidation and bioevaluation of ethanolic extract from *Paeonia suffruticosa Andrews*

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Recently, because of the wide use of the synthetic preservatives in the existing industry, the significant complication on the human health can be found in the recent research. Alternatively, the natural preservative should be studied substitute to the synthetic preservatives. The preservative extensively used in the foodstuff for their longer life time and especially used frequently in the cosmetics products. The present study was conducted to explore the natural material in order to figure out their preserving ability toward the cosmetics product. *Moutan Cortex Radicis* (MCR), the root cortex of *Paeonia suffruticosa Andrews* (*Ranunculaceae*), is a medicinal plant widely used to control the menstrual irregularity, menstrual pain, bruising, hematemesis, epistaxis, elevated blood pressure, extravasated blood removed, bruises, anti-inflammatory, antispasmodic, analgesic, boils treatment, beginning appendicitis and so on. So we have selected the ethanolic extract of peony (*Paeonia suffruticosa Andrews*) and isolate the different components by using column chromatography as well as high performance liquid chromatography. The isolated components from the ethanolic extract of Paeonia suffruticosa Andrews exhibited appreciable potential against the tyrosinase inhibition and anti-oxidant assays assessed by the spectrophotometric analysis.

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Sensing endoplasmic reticulum membrane fluidity of live cells

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Endoplasmic reticulum (ER) stress is strongly implicated in saturated fatty acid (FA)-induced cytotoxicity, which may involve alteration in ER membrane structure. This study is intended to investigate whether or not the ER stress by saturated FA associated with change of ER membrane fluidity. Hence, using a fluorescent sensor (ER-MFS) designed to target to ER membrane and report its fluidity, spectroscopic characterization of its response to environmental changes and a series of confocal fluorescence microscopic experiments were performed for HeLa cells treated with brefeldin A, tunicamycin or palmitic acid. Consequentially, I found that the ratio of fluorescence intensity of ER-MFS at 518 nm to that at 439 nm (I518/I439) was increased mostly by solvent viscosity change, but not by solvent polarity change, and that ER-MFS is localized mainly in ER membrane, judged by its colocalization with ER-Tracker and its poor solubility in an aqueous solution. And it was found that the I518/I439 in HeLa cells with palmitic acid-treatment was higher than that with the oleic acid-, tunicamycin- or brefeldin A-treatments. This results show that the ER membrane fluidity is significantly reduced by palmitic acid treatment, suggesting that the reduced membrane fluidity by palmitic acid is responsible for ER stress and its cytotoxicity thereby. Elucidation of its mechanism requires further investigation yet.

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Structural and Dynamic features of the Psychrophilic Cold Shock Protein (Csp) from *Cowellia psychrerythraea*

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Csps are proteins expressed when growth temperature drops below physiological temperature. They bind to single-stranded nucleic acids and play a central role in the regulation of gene expression under cold shock conditions as RNA chaperones. *Cowellia psychrerythraea* is considered an obligate psychrophile bacteria and can be found in continually cold marine environments including arctic and actarctic sea ice. Here, in order to understand the structural feature of Csp from a psychrophilic bacterium, *Cowellia psychrerythraea* (Cp-Csp), we investigate the thermal stability of Cp-Csp by circular dichroism (CD) experiment. Cp-Csp is less thermostable with a lower melting temperature (38˚C) compared with psychrophilic *Listeria monocytogenes* Csp (40˚C) and thermophilic *Thermus aquaticus* Csp (76˚C). NMR solution structure of Cp-Csp contains five β strands combined in two antiparallel β sheets making up a β barrel structure : β 1, 2-10; β 2, 15-19; β 3, 27-30; β 4, 48-55; β 5, 60-66. The structural study of Cp-Csp showed that the structural flexibility with shorter β strand length and less hydrophobic core packing may be key factors in determining the thermostability of Cp-Csp. In backbone dynamics study, large R_2 values ($>10\ s^{-1}$) were observed for backbone N-H sites of K7 and W8 and it provide evidence for motions on the μs to ms time scale within the proposed nucleotide binding epitope. Using the molecular beacon system, we confirmed that Cp-Csp functions as a nucleic acid chaperone to prevent the formation of secondary structures in nucleic acids at low temperature. Such a function may be crucial for efficient translation of mRNAs at low temperatures and may also have an effect on transcription.

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DNA Nanoparticles for Immunology: CpG Loading and Dendritic Cell Activation *in vivo*

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We introduce a versatile carrier system based on DNA nanoparticles (NPs). Incorporation of lipid-modified nucleobases to DNA strands enables formation of micelles in uniform size. In a single self-assembly step the micelles can be equipped with immune adjuvant (CpG) and fluorescent probe through Watson-Crick base-pairing. With the NPs we have investigated effect of the CpG concentration in immunostimulation. We observed dose dependent activation of TLR-9 resulting in DC maturation *in vivo*. Such pathogen-associated molecular patterns (PAMP) are presented by flow cytometry, ELISA and confocal microscopy.

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DNA Nunchaku: Dimerization on a Single Scaffold of DNA Origami

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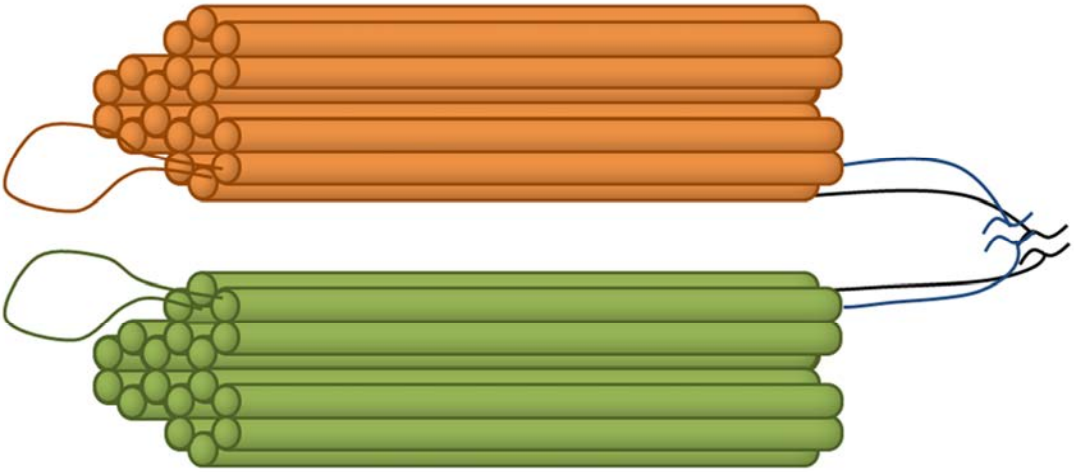
We designed a DNA origami where two triangular prisms are interconnected via M13mp18 scaffold segments. In this experiment, the idea is to build two blocks of identical shapes in different folding strategies. Then addition of locking strands leads to positioning two prisms in close proximity. We investigated effects of Mg^{2+} concentration in folding efficiency and characterized the structures by TEM and AFM. For the first time, we present the use of scaffold as the linkage segments in a single DNA origami using both hexagonal and square lattice motifs as the nanostructure and locker, respectively.



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Structure and motional properties of bovine angiogenin studied by NMRspectroscopy

김민준 김양미*

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Angiogenin is a fundamental molecule inducing angiogenesis. In many tumor and cancer cells, angiogenin is overexpressed and is critical for its capacity to induce neovascularization. Angiogenin is a member of the pancreatic ribonuclease superfamily and has 33% sequence identity with that of RNase A. Although the structure of angiogenin is very similar to that of RNase A, angiogenin contains unique functional features that account for its angiogensis while RNase A does not have angiogenic activity. Also, angiogenin has a weak ribonucleolytic activity than that of RNase A. Therefore, we studied the structure of bovine angiogenin (bAng) and dynamic property to understand the importance of structural flexibility in its function. Circular Dichroism data showed that bANG has a distinct β-sheet structure with melting temperature of 56℃. Backbone resonance assignment was completed by triple resonance NMR experiments for 13C and 15N labeled protein. Chemical shift index showed that bANG has three α-helices and seven β-sheets connected by nine loops. The dynamic properties of bAng were investigated through the use of R1, R2 and heteronuclea NOE experiments. K41, D69 have a significantly large R2 value. K41 is at the ribonucleolytic active site and D69 is at the cell binding site. The reduced heteronuclear NOEs are appeared at K20, G87, R90 near the loop region, implying that active sites and loop regions have great flexibilities. It may suggest these flexibilities are required for structural rearrangements when ligand binds to angiogenin for its enzymatic activities.

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Crystal structure of Z-ring associated protein D (ZapD) from Escherichia coli

손상현 이형호[1,*]

국민대학교 화학과 [1]서울대학교 화학부

Cytokinesis in bacterial organisms is a crucial event, which is followed and performed tubulin-homologue FtsZ. The polymerization of FtsZ into ring-like structure composed of FtsZ is controlled by various components from 'divisome' consisting of positive and negative regulators. The cytoskeleton protein FtsZ is composed of two main domains, of which N-terminal domain is associated with binding of GTP to G-rich motif. The binding of GTP to its N-terminal domain can initiate the polymerization of FtsZ into 'Z-ring', ring-like structures, by GTP hydrolysis. FtsZ polymerization is regularized by GTPase activity. ZapD (Z-ring associated protein D) is known as the positive regulator of FtsZ polymerization and binds to the C-terminal tail of FtsZ directly. To characterize how ZapD contributes to the assembly of FtsZ polymerization, we performed the preliminary structural studies of ZapD from Escherichia coli and carried out GST pull-down assay. It showed ZapD binds to the C-terminal tail of FtsZ in vitro and its surface was highly positively charged. We hypothesize the positive surface of ZapD would contribute its recruitment to the cell membrane.

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Crystal structure of Ni-containing metallo-β-lactamase

최화정 이형호*

서울대학교 화학부

TmMBL (a metallo-β-lactamase from *Thermotoga maritima*) was predicted to have a metallo-β-lactamase (MBL)-like fold (αββα) based on sequence similarity. MBL superfamily consists of various hydrolases which require metals, commonly Zn^{2+}, and have αββα domain but they have low sequence identity each other. MBL contains diverse activities such as phosphodiesterase and β-lactamase. Here, we report the crystal structure of TmMBL diffracted to 1.92 ? resolution and assays for phosphodiesterase and β-lactamase activities. Assay for phosphodiesterase activity was performed using bis-pNPP by monitoring the increase of absorbance at 410 nm and assay for β-lactamase activity was performed with nitrocefin by measuring the increase of absorbance at 485 nm. We tried various metal ions to find its right metal ions because hydrolases in MBL superfamily normally need divalent cations for their activity. TmMBL showed remarkable increase of phosphodiesterase activity with Ni^{2+} and did not seem to have the activity with Ca^{2+}, Zn^{2+}, and Mg^{2+}. Oligomeric state of TmMBL was estimated as a trimer by analytical gel filtration.

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Structural and biochemical insights into the role of TEX14 to inhibit cytokinesis

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Differentiating germ cells do not complete cytokinesis and instead intercellular bridges are formed by the consequence of inhibiting the final cutting of plasma membrane. The interaction of testis-expressed gene 14 (TEX14) to CEP55 is an essential step to prevent the recruitment of ESCRT machinery. In this study, we solved the three crystal structures of CEP55 bound to TEX14 peptide (or its chimera peptides) and performed multi-experiment analysis to characterize the CEP55/TEX14 interaction. Oligomeric state of the CEP55 protein was estimated as a dimer by analytical gel filtration. The central CEP55-EABR (ESCRT and ALIX binding region) domain bound to a 13-residue peptide of TEX14 with a dissociation constant Kd = 300 nM and a stoichiometry of 2:1. We also demonstrated that TEX14 showed a high affinity and a low dissociation rate, and an increase of local concentration to the midbody compared to those of ALIX. We proposed that these binding properties of TEX14 to CEP55 cooperatively contribute to the prevention of ALIX recruitment to the midbody.

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Traceless and site-specific fluorescent labeling of transmembrane proteins in live cells

이의연 권영은*

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Understanding of protein interaction and cellular dynamics is an important step to get insight of biotechnological applications. Therefore, a recent life science research has increasing demands on studying physiological events on the molecular level in real-time. For this purpose, live cell imaging using fluorescent proteins (FPs) has been widely utilized to visualize target proteins under a microscopy by constructing fusion proteins. However, methods of FP-based imaging have a few limitations, such as slow maturation kinetics or issues with photo-stability under laser illumination. In this study, we have utilized Npu DnaE split-intein mediated protein trans-splicing (PTS) reaction for site-specific fluorescent labeling of cell membrane proteins. Trans-splicing reaction is a self-processing reaction and can be used to introduce various synthetic probes to target proteins. We prepared a model cell membrane protein fused to N-terminal fragment of Npu DnaE intein and a C-terminal fragment of Npu DnaE intein fused to a fluorescent probe. Here, we also adopted an engineered Npu intein in order to make this system more practical. As the engineered C-intein is considerably shorter compared to wild-type C-inteins, the preparation of C-intein becomes easier. We demonstrated that engineered Npu intein mediated labeling reaction is comparable to wild-type Npu intein. No external energy was required for the labeling reaction. This approach will lead to new methodologies for investigating protein localization, transportation, and cell signaling.

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Development of inhibitory aptamer against *Mycobacterium tuberculosis* based on inhibition of acetohydroxyacid synthase

문지영 윤문영*

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Acetohydroxyacid synthase (AHAS) in Mycobacterium tuberculosis (MTB) is a promising and potential target for the development of new anti-tuberculosis agents. AHAS from MTB is one of the biosynthetic enzymes, which catalyzes the first common step in the biosynthesis of the essential branched chain amino acids (BCAA's: valine, leucine, and isoleucine). We identified short (30mer) single stranded DNA aptamers as novel inhibitor against MTB AHAS through systematic evolution of ligands by exponential enrichment (SELEX). Total 9 aptamers were identified with strong and specific binding to MTB AHAS. Among identified 9 aptamers, 2 aptamers (Apt 1, Apt 6) are the most potent inhibitors against MTB AHAS with IC50 in the low nanomolar range (28.94 and 22.35, respectively). These two aptamers were modified and changed as minimal inhibitory aptamers. Apt1-17mer and Apt6-20mer were evaluated for In-vitro test and exhibited strong inhibition against multi drug-resistant and extensive drug-resistant MTB strain with low MIC 5.27 μg/ml and 6.16 μg/ml. Taken together, results of this study provide impetus for the development of strong anti-tuberculosis agents and may overcome the issue of drug resistance.

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Peptide functionalized gold nanoparticles for novel targeting agent towardsBrain Glioma stem cell marker CD133

조준행 윤문영[1,*]

한양대학교 자연과학대학 [1]한양대학교 화학과

In the cancer stem cells (CSCs) model, only a small proportion of tumor cells are able to self-renew extensively, while the bulk of cells proceed to differentiate into committed heterogeneous clones. On the basis of the involvement of CSCs in tumourigenesis and treatment resistance, it is conceivable that only eradication of CSCs can lead to a cancer cure.CD133, also known as prominin-1 (PROM-1), is a 5-transmembrane glycoprotein with several isoforms of unknown physiological or pathological function. CD133+ cells was firstly identified as a cancer initiating cell in brain tumor and contributor to the CSC population. Therefore, CD133 are an important target candidate for prevention of relapse and disease progression in brain tumor. In the previous study, we screened the peptide which have higher binding potency to target protein in vitro. To further characterization of found peptides, we investigate the binding properties on cellular level. In addition with this, the peptide conjugated to Gold nanoparticle for novel diagnostic approach.

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Screening of high-affinity ssDNA aptamers against dihydrostreptomycin

하나름 윤문영*

한양대학교 화학과

Dihydrostreptomycin is an aminoglycoside antibiotic consisting of a hydrogenated form of streptomycin, which is usually used in vetinary medicine in cattle, pigs, chicken and sheep. The use of antibiotics to treat food animals has the potential to affect human health. 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 screened the ssDNA aptamers against dihydrostreptomycin. We used the DNA binding plate for fixation of target and screening. We determined the saturation conditions of target binding on the well surface and was found to be 5mM of dihydrostreptomycin. Total 11 rounds of SELEX was progressed including negative selection for kanamycin, streptomycin and we obtained aptamers. These aptamers were synthesized and characterized with respect to their Kd value and specificity using aptamer-based ELISA method. Furthermore, aptamer conjugation with polydiacetylene (PDA) will be discussed in order to development of aptasensor based on colorimetric system for detection of antibiotics.

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Identification of natural product inhibitors for slingshot homologs

이영근 이선영 강효진 정상전*

동국대학교 화학과

The level of protein tyrosine phosphorylation is maintained by coordinated catalysis of protein tyrosine phosphatases (PTPs) and protein tyrosine kinases (PTKs). Protein phosphatase slingshot homologs (SSH), members of dual specific phosphatases (DUSPs), consist of SSH-1, -2 and -3. Each member plays an essential role in controlling actin dynamics by regulating cofilin/ADF activity. Cofilin is important in actin dynamics relevant to states of various diseases such as neurodegenerative diseases, vascular diseases, phagocytic ingestion event for infective microorganism, as well as cancers. We have screened natural product library for inhibitors of SSHs, which may offer a clue to develop therapeutics for aforementioned actin dynamics-related diseases. As a result, we identified seven natural products with SSHs inhibitory activity Interestingly, one of the inhibitors showed selective inhibition to SSH?2 over SSH-1 and -3. Further, we determined type of inhibition by each inhibitor and Ki values. Additionally, binding site prediction of the inhibitors were performed with a crystal structure of SSH-2.

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Natural Product Inhibitors for Cdc25 Phosphatases

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동국대학교 화학과

Cell division cycle 25 phosphatases (Cdc25s) are dual-specificity protein phosphatases that play a key role in the cell cycle transition by dephosphorylating CDK/cyclin complexes. Overexpression of Cdc25s has been observed in a variety of cancers with tumor aggressiveness and poor prognosis. Therefore, Cdc25s have been regarded as attractive drug targets for anticancer therapy, meaning that discovery of selective Cdc25s' inhibitors may be a potential cancer therapeutic approach. We have screened 658 natural compounds for Cdc25 inhibitors through HTS. For several hit compounds showing slow binding and noncompetitive inhibition, we determined IC_{50} and K_i values, confirming mode of inhibition, and defined a potential binding site through molecular docking study. Furthermore, we treated the breast cancer cells with the selected Cdc25s' inhibitors to test if they show anticancer effect *in vitro*.

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Characterization of a novel unclassified hydrolase (LmH) from *Listeria monocytogens*

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A novel type of hydrolase (LmH) from Listeria monocytogenes was identified, characterized, and immobilized for biotechnological applications. Primary sequence analysis indicated that LmH had a catalytic triad (Ser91-Asp192-His222) with a molecular weight of 27.8kDa. Homologs of this enzyme are produced by many Gram-positive bacteria including Bacillus, Staphylococcus, and Enterococcus. Biochemical properties of LmH were investigated by performing mass spectrometry, dynamic light scattering (DLS), enzyme assays, enantioselective analysis, circular dichroism (CD) spectroscopy, fluorescence analysis, and macroscopic hydrogel formations. Interestingly, crosslinked enzyme aggregates (CLEAs) of LmH exhibited enhanced stability and good recycling abilities compared to free LmH. These molecular characteristics of LmH highlight its great potential for the pharmaceutical, biotechnological, and chemical industries.

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Mobile esterases on microbe-templated nanoparticles

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Due to low diffusion rates and large surface areas, nanomaterials have received great interest as supporting materials for enzyme immobilization. Here, the preparation of a cobalt oxide nanoparticle using Bacillus subtilis as a biological template and use of the nanostructure for microbial esterase immobilization is described. Morphological features and size distributions were investigated using electron microscopy (EM) and dynamic light scattering (DLS). Catalytic properties of enzyme-coated nanostructures were investigated using 4-methylumbelliferyl acetate and p-nitrophenyl (PNP) acetate as model substrates. Enzyme-coated nanostructures were observed to retain ～85% of the initial activity after 15 successive reaction cycles, and enzyme immobilization processes could be repeated four times without a loss of immobilization potential. The present work demonstrates that B. subtilis-templated cobalt oxide nanoparticles have the potential to be used as biocompatible immobilization materials, and are promising candidates for the preparation of effective nanobiocatalysts.

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Identification of a Potent Inhibitor of Human Vaccinia-H1 Related (VHR) Phosphatase and its Anti-proliferative Activity against Cervix Cancer Cells

노경민 강효진* 정상전*

동국대학교 화학과

Human vaccinia-H1 related (VHR) phosphatase, encoded by dual specificity phosphatase 3 (DUSP3) gene, is one of the smallest known phosphatase with only 185 amino acids and regulates phosphorylation states of protein. Maintaining the proper protein tyrosine phosphorylation state has been implicated in various human diseases including cancer, type 2 diabetes and obesity. Especially, VHR has been reported that loss of VHR activity cause cell cycle arrest in HeLa cells, suggesting that identification of its selective inhibitors expected potential anticancer drugs. Natural products have been regarded as good source for development of new drugs. Here, we screened natural product library for VHR inhibition to identify hit compounds. Furthermore, kinetic evaluation of the hit compounds identified a potent inhibitor with nM Ki and the hit compounds decreased the proliferation of cervix cancer cells. These compounds may be a promising targeted therapeutic drugs for cervix cancer.

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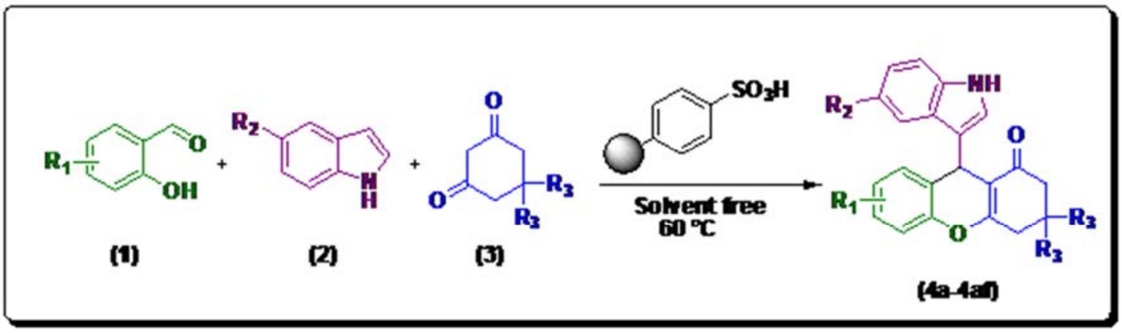
A Metal-Free Tandem C?C/C?O Bond Formation Approach to Densely Functionalized Indolyl 4H-Chromenes Catalyzed by Polystyrene supported p-Toluenesulfonic acid under Solvent-Free Conditions

ShindeVijayVilas 정연태* 이상동

부경대학교 이미지시스템공학과

Abstract: A new environmentally benign and highly convergent protocol for the synthesis of indolyl 4H-chromene derivatives have been developed. This one-pot three-component condensation reaction of salicylalehyde, cyclic 1,3-diketones and indole is promoted by PS-PTSA as a reusable heterogeneous acid catalyst under solvent-free conditions. This protocol demonstrates several notable advantages such as that the catalyst is readily available, can be recovered and reused for at least five runs without any significant impact on product yields, high atom-economy, excellent yields, and efficiency of producing three new bonds (two C?C and one C?O) and one stereo center in a single operation.



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Synthesis of high energy density material

권국태 조은소리 이소정 김승희[1] 김진석[2,*]

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

Sensitivity is one of the important character for the energetic materials. There were many attempts to develop high-performance and insensitive explosives. 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo [5.5.5.0.0]-dodecane is a promissing compound in the field of insensitive explosives. It has similar structural framework with HNIW(CL-20), and like CL-20, it has very high density. However unlike CL-20, it is friction insensitive, possesses low impact sensitivity, anf it can be easily synthesized from cheap starting materials. Synthetic pathway is well known by many other scientists, but yield of last step is not enough. In this presentation, we will show some synthetic schemes and results of syntheses.

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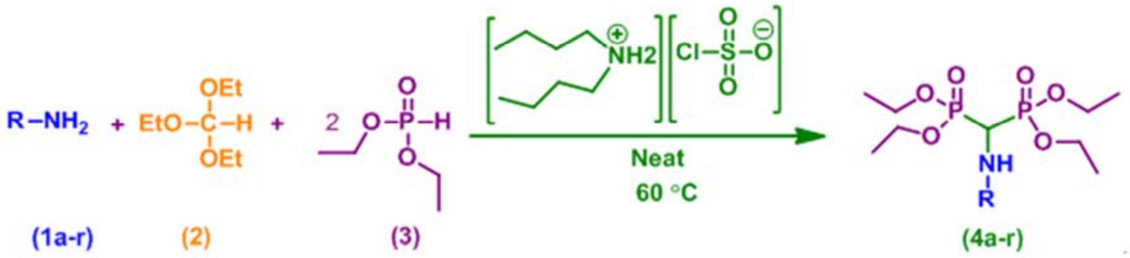
Synthesis of N-containing bisphosphonates under ionic liquid condition

Mudumala Veeranarayana Reddy 정연태*

부경대학교 이미지시스템공학과

The preparation and description of a novel secondary amine ionic liquid, di-n-butyl ammonium chlorosulfonate, is described. The di-n-butyl ammonium ionic liquid (DBA IL) was characterized by FT-IR, elemental analysis, NMR spectroscopies, and wide-angle X-ray scattering techniques, as well as thermogravimetric analysis. The DBA IL functions as an efficient, environmentally benign, and recyclable catalyst with short reaction times and high catalytic activity for the synthesis of a variety of N-containing bisphosphonates in high yields. Another merit of this ionic liquid shown that the purification of products by non-chromatographic method with good to excellent yields of the desired products.



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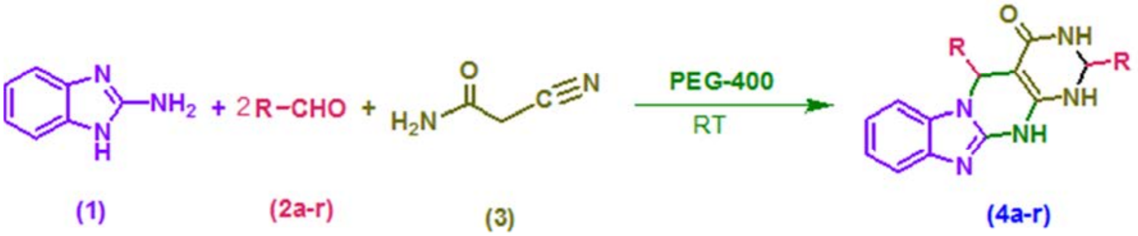
Synthesis of benzo[4,5]imidazo[1,2-a]-pyrimido[4,5-d]pyrimidin-4(1H)-ones under catalyst-free conditions

Mudumala Veeranarayana Reddy 정연태* 이상동

부경대학교 이미지시스템공학과

A simple and an efficient eco-friendly methodology has been developed for the synthesis of benzo[4,5]imidazo[1,2-a]-pyrimido[4,5-d]pyrimidin-4(1H)-ones in excellent yields under catalyst-free-conditions using inexpensive and non-toxic polyethylene glycol (PEG-400) medium. This new protocol offers an environmental acceptability, shorter reaction time, room temperature, low cost, high yields and recyclability of the PEG-400 medium are the important features. This method provides a green and much improved protocol over the existing methods.



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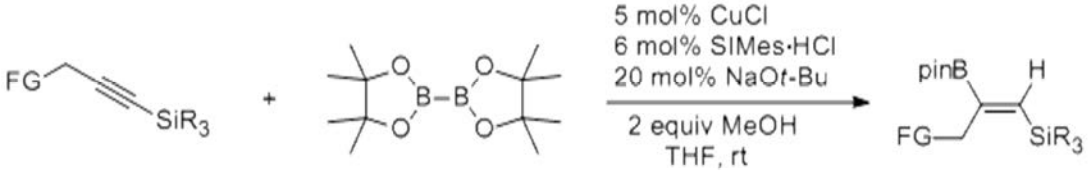
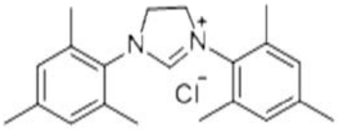
Copper-Catalyzed Regio- and Stereoselective Synthesis of Multifunctionalized Alkenylboronates

김영은 장원준 윤재숙*

성균관대학교 화학과

The borylation of alkynes provided an efficient synthetic approach to alkenylboron compounds, which are useful intermediates in organic synthesis. Recently, our group reported stereocontrolled synthesis of (β-borylalkenyl)silanes using copper catalysts. In this work, we focused on the directing effects of both the silyl and propargylic group in a single compound. It was found that β-monoborylation relative to Si of propargylic silylalkynes occurred with high regioselectivity using an *N*-heterocyclic carbene(NHC)-Cu(I) catalyst.





SIMes·HCl

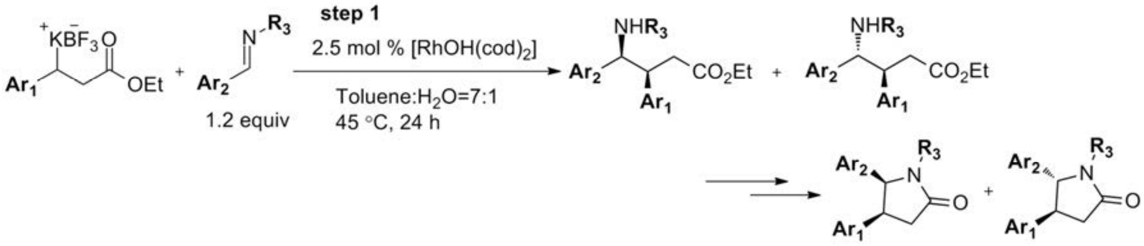
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-658**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Addition of Secondary Alkyl Potassium Trifluoroborate Salts to *N*-Sulfonyl Imines with Rh(OH)(cod)$_2$

이우림 윤재숙*

성균관대학교 화학과

The rhodium-catalyzed 1,2-addition and 1,4-addition of organoboron compounds to electrophiles has become a major area of research. In comparison, alkyl boron derivatives (sp^3 C-B) have been rarely studied as substrates. We investigated an efficient Rh-catalyzed addition of secondary alkyl borate salts to *N*-sulfonyl imines in good yield. This method could be used for the synthesis of *β*,*γ*-diaryl-substituted *γ*-butyrolactames. We also will present our results of the addition of enantiomerically enriched substrates to imines.



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N-heterocyclic carbene-based well-defined ruthenium hydride complexes for direct amide synthesis from alcohols and amines under base-free conditions

김건순 홍순혁*

서울대학교 화학부

Readily synthesized, well-defined N-heterocyclic carbene based ruthenium (II) hydridecomplexes were developed for amide synthesis from alcohols and amines under base-freeconditions. Diverse amides were synthesized in fair-to-excellent yields. In the case of secondaryamines, where direct dehydrogenative amidation is not feasible, a catalytic amount of a base wasrequired to promote the transamidation of esters, which are byproducts of alcohol dimerization

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Ruthenium(Ⅱ)-catalyzed imine synthesis from nitriles and secondary alcohols

김다은 홍순혁*

서울대학교 화학부

Imines are versatile functional molecules used for nitrogen sources in the synthesis of a wide range of products. We developed a redox- and step-economical synthetic method for imines from nitriles and alcohols using ruthenium (II) hydride complexes as catalysts. Diverse imines were synthesized in good yields. To the best of our knowledge, this is the first example of imine synthesis from nitriles and alcohols.

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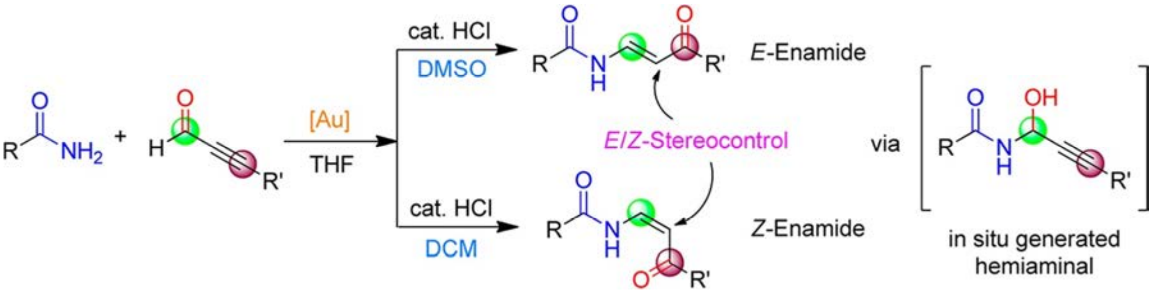
Gold(I)-Catalyzed, Stereocontrolled Enamide Synthesis from Primary Amides and Propargyl Aldehydes Using a Tandem Strategy

김상민 이다본 홍순혁*

서울대학교 화학부

Enamides are very common organic compounds and encompass numerous natural products and drug candidates. In addition, enamides are highly valuable synthetic intermediates for the synthesis of chiral amines, heterocycles, and cross-coupling reagents. Recently, diverse transition metal-catalyzed reactions have been developed utilizing Ru, Rh, Fe, Pd, Au, and Cu, which provide significant advantages over traditional methods. Nevertheless, these reactions are also limited due to difficulty to prepare the necessary starting materials, requirement of particular reaction conditions, and confined scope of the enamide products. We reported a novel strategy for enamide synthesis from primary amides and propargyl aldehydes via Au(I)-catalyzed tandem amide addition and Meyer-Schuster rearrangement. This method provides an atom-economical way to produce enamides from simple and versatile starting materials. This is the first example of transition metal-catalyzed Meyer-Schuster rearrangement of inherently unstable substrates with a carbon-heteroatom bond at the propargyl position. In situ generated hemiaminals were successfully converted to the desired products under the optimized conditions. Enamide stereochemistry was controlled simply by changing solvents and adding a catalytic amount of acid. The developed synthetic strategy provides a new method to synthesize various β-substituted-α,β-unsaturated carbonyl compounds.



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Gold(I)-Catalyzed, Stereo-, Regioselective N-Sulfonyl Enaminone Synthesis via Meyer-Schuster Rearrangement

이다본 김상민 홍순혁*

서울대학교 화학부

Enaminone is a valuable moiety presented in numerous natural products and drug candidates. Also, it is a versatile intermediate for heterocycles, chiral amines and cross-coupling reagents. Especially, N-sulfonyl enaminone is of the greater importance than other simple enaminones because sulfonamides are common in pharmaceuticals and biologically active compounds such as Rosuvastatin, Meloxicam and Sulfamethoxazole.Several synthetic strategies for enaminones have been developed. However, they have limitation on selectivity and accessibility of starting materials. Moreover, N-sulfonyl enaminone is more difficult to synthesize via general addition strategies due to lower nucleophilicity of sulfonamide. Only few synthetic methods with complex substrates or ynoate esters as carbonyl sources have been reported. Therefore, a novel selective synthetic strategy from accessible starting materials is highly required.Recently, our group reported a novel regio- and stereo-controlled enamide synthesis via gold(I)-catalyzed Meyer-Schuster rearrangement. Applying the same strategy, we have developed a gold(I)-catalyzed N-sulfonyl enaminone synthesis from primary sulfonamides and ynones via Meyer-Schuster rearrangement.

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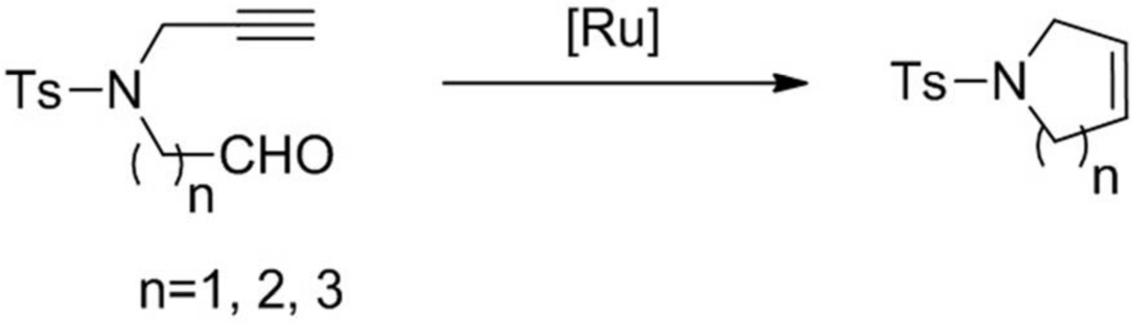
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of N-Heterocyclic Alkenes using N-containing Alkynals

서현옥 한소엽[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학과, 촉매반응?합성연구센터

We report our study on the synthesis of N-heterocyclic alkenes through ruthenium-catalyzed decarbonylative cyclization. The detailed reaction conditions will be discussed at the presentation.



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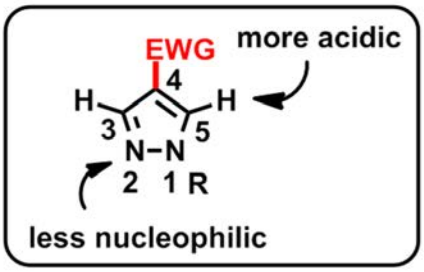
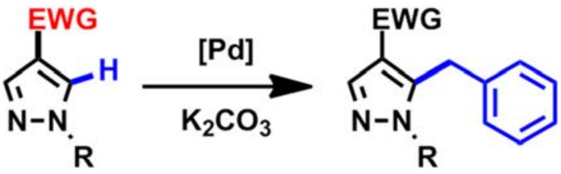
Catalytic C-H Benzylation of Pyrazoles and Imidazoles

배세리 주정민*

부산대학교 화학과

We describe a general approach for the synthesis of benzylated pyrazoles. An electron-withdrawing substituent, such as nitro, chloro, and ester groups, at C4 renders the Lewis basic nitrogen atom to be less basic and the C-H bond more acidic than the ones of the parent ring, enabling Pd-catalyzed C-H benzylation reactions of pyrazoles. The new method expanding the scope of the C-H functionalization of pyrazoles beyond arylation reactions provides a rapid access to complex pyrazole compounds.





EWG = NO_2, Cl, CO_2Et

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An Efficient Preparation of Non-Symmetrical Ureas using MeOTf

김희권

전북대학교 의학전문대학원/핵의학교실

Unit of urea is a common structural feature in a variety of biologically active compounds such as plant and insect growth regulators, antagonists of natural receptors and antitumor agents. We developed an efficient method for the urea structure to produce asymmetric urea. According to the classical method, carbamolylimidazole compounds were prepared by treatment of amine compouns with N,N-carbonyldiimidazole. After MeOTf was used to activate carbonyldiimidazole, reactions with the corresponding amine compounds generated the desired asymmetry urea structures. Our result showed that a variety of compounds containing ureas were easily prepared in higher yield.

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A Practical Preparation of N-Succinimidyl-4-[18F]fluorobenzoate for [18F]-Labeling of Biomolecules

김희권

전북대학교 의학전문대학원/핵의학교실

Positron emission tomography (PET) has been increasingly used in the clinic and preclinical research. N-Succinimidyl-4-[18F]Fluorobenzoate (SFB) is an important compound that is widely used to label biomolecules such as proteins and peptides because of its in vivo stability. Despite the recent studies done on the radiosyntheses PET probes, there have yet to be studies conducted on [18F] SFB on miniaturized devices. Here, we have studied miscroscale-level radiosynthetic conditions by examining several microscale reactions that produced a high radiochemical yield of [18F]SFB. Synthesis of [18F]SFB started with 4-(ethoxycarbonyl)-N,N,N-trimethylbenzenaminium triflate on a microchip. [18F]SFB was successfully prepared with a radiofluorination yield of 71% via three-steps. The [18F]SFB was used for the conjugation with an antibody for immuno PET.

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Unique prototropy of meso-alkylidenyl-thia-(m-benzi)porphyrin bearing single meso-exocyclic C-C double bond

이창희[*] 유재덕[1] Indrajit Saha[2]

강원대학교 화학과 [1]한라대학교 신소재 화학 공학과 [2]Department of Chemistry, Ramkrishna Mahavidyalaya, Tripura-799277

The porphyrinoids bearing exocyclic double bonds at meso-positions have not been studied extensively. The unusual features of these modified porphyrinoids inspired us to synthesize new meso-alkylidenyl-porphyrinoids bearing one exocyclic C-C double bond. Such systems would be excellent model system to probe the relationships between global aromaticity and stabilizing/destabilizing effect of substituents. Herein we report, for the first time, a generic synthesis and spectroscopic properties of meso-alkylidenyl-thia(m-benzi)porphyrin containing one exocyclic carbon-carbon double bond. Acid catalysed [3+1] Mac-Donald type condensation of tripyrane 3 and diol 4 followed by oxidation with DDQ leads to the to the formation of the desired meso-alkylidenyl-thia(m-benzi)porphyrin 1 bearing on exocyclic C-C double bond. This process also resulted in the formation of a core-modified phlorin type compound 2 that contains one sp3 hybridized meso-carbon atom. Phorins are hybrid class of molecules (porphyrinoids) that have intermediate structural features of porphyrins and calixpyrroles, and could be regarded as Calixphyrin. In contrast to the other conventional porphyrinoids, phlorins exhibit multi-electron redox chemistry. The presence of sp3 carbon atom disrupts extended macrocyclic π-conjugation as a result of which electronic properties of phlorin also differ from porphyrin. The detailed structural characterization and spectroscopic properties of 1and 2 will be discussed.

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Syntheses and Characterization of Pyrimidine-Based Conjugated Polymer for Polymer Solar Cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Because of environmental pollution, polymer-based solar cells have been attracting considerable attention for their feature, such as low cost, light weight, and possibility use in flexible devices. PBDTCN, PBDTTCN, PBDTF and PBDTTF with substituted-BDT/BDTT units as the electron rich units and pyrimidines, with cyano or fluoro groups, as the electron deficient units, were synthesized by Stille coupling reaction with Pd(0)-catalyst to provide good solubility in common organic solvents. We synthesized the new conjugated polymers, PBDTCN, PBDTTCN, PBDTF and PBDTTF, which were synthesized by Stille polymerization. The UV-vis absorption onset of PBDTCN, PBDTTCN, PBDTF and PBDTTF were around 700 nm and their optical band gaps were about 1.9 eV. The HOMO energy levels of four polymers (PBDTCN, PBDTTCN, PBDTF and PBDTTF) were at -5.14 ~ -5.5 eV, their LUMO energy levels were at -3.46 ~ -3.85 eV, corresponding to the electrochemical band gap of around 1.7 eV. The HOMO energy levels of PBDTTCN and PBDTTF are lower than those of PBDTCN and PBDTF. The device comprising PBDTTCN and PC71BM (1:1.5) with DIO showed a VOC of 0.86 V, a JSC of 3.14 mA/cm2, and a fill factor (FF) of 0.40, giving a power conversion efficiency of 1.09%. The device comprising PBDTTF and PC71BM (1:1.5) with DIO showed a VOC of 0.82 V, a JSC of 3.28 mA/cm2, and a fill factor (FF) of 0.39, giving a power conversion efficiency of 1.05%.

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Syntheses and Application Indenoindene-Based Conjugated Polymer for Polymer Solar Cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

In order to overcome the growing global energy demand, extensive researches on environment friendly and renewable sources of energies have been attracting considerable attention during the past decade.The polymer, indenoindene contains stilbenechromophore, but the vinylene group is located in the bicyclic [2.2.0] system. In case of indenoindene, it is possible to introduce four alkyl groups in the sp3 carbons in the bicycle, which will increase the solubility of the polymer, without distorting the conjugation. New conjugated polymers, HS-5528 and HS-5529, were synthesized by the palladium-catalyzed Suzuki polymerization and characterized. The UV edge of HS-5528 was670 nm and band gap was narrow in 1.75eV. The UV edge of HS-5529 was 676 nm and band gap was narrow in 1.31eV. HS-5528 and HS-5529 base on bithiophene imide units show HOMO energy levels at -5.72 and -5.39eV, LUMO energy levels at -3.98 and -4.08 eV. The solubility of polymers is important for OPVs device applications. However, the polymers have poor solubility. It’s difficult to fabrication for solar cells.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Conjugated polymers consisting of BTI Unit as Acceptor materials for Photovoltaics

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Organic solar cells have been a greater attention in the past decades, due to the growing global energy demand. BTI units have the advantage of decreased steric henderance achieved by placing the imide group at the center of BTI unit, and this should enable a planar architecture to realize extended conjugation. We report the synthesis and properties of new N-alkyl-2,2′-bithiophene-3,3′-dicarboximide derivatives containing as the acceptor. The polymers have good solubility in common types of organic solvents. HS-5505, HS-5506 and HS-5507 were synthesized by palladium-catalyzed Stille polymerization. The polymers have good thermal stability and good solubility in common types of organic solvents. HS-5505, HS-5506 and HS-5507 containing bithiophene imide units show λmax at 649, 652 and 675 nm. HOMO energy levels at -5.6, -5.5 and -5.7 eV, LUMO energy levels at -3.9, -3.4 and -3.9 eV. The best performance of device with HS-5506:PC61BM layer showed VOC of 0.76 V, JSC of 3.28 mA/cm2, and FF of 0.51, giving the PCE of 1.26%.

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D-A copolymers based on 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI) for narrow band gap and high performance polymer solar cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Organic solar cells (OSC) devices provide a promising way to utilize the solar energy efficiently. 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI) was modified from partial benzene ring in carbazole moiety. Therefore TTI unit have strong electron donating ability likewise cabazole. By replacing six-membered ring of benzene with five-membered ring of thiophene, enhanced ICT effect. TTI unit was expected to have planar structure because it is beneficial to facilitating π-electron delocalization and high charge transport. The PTTIDTBT-h and PTTIDTMBI and PTTIDPP were synthesized through Stille coupling reaction and estimated in OPVs. The band gaps of PTTIDTBT-h and PTTIDTMBI and PTTIDPP using the UV onset rate of the λmax are shown 594 nm, 682 nm and 759 nm, respectively. The HOMO and LUMO energy levels of PTTIDTBT-h and PTTIDTMBI and PTTIDPP were presented at -5.31 and -3.7 eV, -5.20 and -3.7 eV, -5.09 eV and -3.7 eV, respectively. The small molecules have great thermal stability. The device including PTTIDTMBI with PCBM (1:3) showed a power conversion efficiency value of 1.44%.

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Enhanced Photovoltaic performance of OPV based on 6-(2-thienyl)-4H-thieno [3,2-b]indole(TTI) for organic solar cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Polymers have been widely used to BHJ OSCs because of potential for generating renewable energy and PCE depends of the polymers. The advantages of polymers are definite structure, simple purification, good purity and high photovoltaic performance reappearance. 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI) was transformed from carbazole moiety. therefore, ICT effect was improved charge transport because of planar structrure of TTI. The TTIBT(HS-5534) and TTIMBI(HS-5535) were synthesized by stille reaction and estimated in OPVs. The absorption of film state of TTIBT and TTIMBI show maximum peaks at about 553-762 nm and 604-821 nm. The HOMO and LUMO levels of TTIBT and TTIMBI were presented at -5.32 eV and -3.50 eV, -5.29 eV and -3.61 eV, respectively. The small molecule has good thermal stability. The HOMO?LUMO energy bandgaps of this material shows 1.69 eV and 1.57 eV for TTIBT and,TTIMBI.

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Chemistry of of meso-alkylidenyl benzipentaphyrins

이창희* 황선아

강원대학교 화학과

The novel meso-alkylidenyl porphyrins are non-aromatic and conformationally flexible macrocycles that display unusual protonation selectivity and tautomeric equilibrium. Most of the reported compounds show attractive site-selective protonation depending on the number of core N-H hydrogens. As a part of our continuing efforts for the construction of the new expanded version of the congeneric macrocycles, we report the synthesis, characterization, chemistry and conformational characteristics of novel meso-alkylidenyl benzipentaphyrins. The synthesis is accomplished by a typical '3+1' of the mixed-condensation. The structural characterization indicates that the compounds contain two exocyclic carbon-carbon double bonds at meso-positions and different number of inverted pyrroles. The p-benzipentaphyrin for example, adopts asymmetric conformation that one of the pyrrole unit is inverted, which is stabilized through intramolecular hydrogen bonding. On the other hand, the m-benzipentaphyrin adopt symmetric conformation which two pyrrole rings are inverted. The structural characteristics and protonation selectivity upon addition of acid and chemical reactivity will be extensively presented.

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Calix[4]pyrrole-based, Probe-Host integrated, fluorescence ‘turn-on’ receptor for fluoride anion

이창희* <u>김보람</u>

강원대학교 화학과

A calix[4]pyrrole-based, novel anion receptor carrying fluorescence probe has been designed and synthesized. The designed receptor can detect anionic analytes such as fluoride anion selectively by ‘turn-on’ type fluorescence changes. The synthesis has been accomplished by attaching a coumarin unit to one of the meso-position of calix[4]pyrrole. The dimension between fluorophore and binding site were decided by theoretical calculation. When the host molecule was treated with base (tetrabutyl ammonium hydroxide), the coumarin probe unit simultaneously bind to the calix[4]pyrrole cavity accompanying with complete fluorescence quenching. Upon treatment of this receptor-fluorophore complex with fluoride anion, complete displacement of bound coumarin by fluoride anion was observe. Large fluoride anion-dependent fluorescence enhancement was also observed. The synthesized receptor showed good anion selectivity toward fluoride anion. This ‘turn-on’ type fluorescence chemosensor system showed excellent fluoride selectivity. The ‘turn-on’ process can be reversed upon addition of alkaline metal ion such as Li+ or Na+.

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Anion Binding Properties of Calix[4]pyrrole Carrying Benzimidazole at the Diametrical meso-Positions

이창희* **bezaendalemulugeta**

강원대학교 화학과

Calix[4]pyrroles bearing benzimidazole at diametrically crossing meso-positions have been synthesized and fully characterized. The synthesized receptors are expected to recognize anionic guests through hydrogen bonding and anion-pi interaction. The guest binding pocket created by the two meso-benzimidazole and four pyrrole N-Hs interact cooperatively with anionic guests. The size discrimination is also expected due to the limited dimension of the binding pocket. The anion binding studies carried out in organic solvent displayed enhanced binding affinity toward anions. The cone conformation resulting from the complexation with anion creat pi-rich cavity. The opposite side, electron rich cavity can interact with counter cations to form stable ion-pair complexes. Different cation selectivity is also expected. The results indicate that the synthesized receptor show cooperative interactions of hydrogen bonding and anion-pi interaction. The binding affinities and spectroscopic changes upon ion binding will be presented.

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Non-linear Allosteric Regulation of Anion Binding by Tetracationic Receptor

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강원대학교 화학과 [1]Department of Chemistry, Ramkrishna Mahavidyalaya

A covalently coupled, capsular tetra-cationic calix[4]pyrrole homodimer bearing fluorescent anthracene linkers has been synthesized and characterized. The designed receptor displayed exclusive binding with fluoride anion accompanied with large enhancement of fluorescence. Moreover, the first fluoride anion binding to one of the binding pockets result in increase in affinity for the second fluoride anion binding by a factor of ~311. Such distinctive cooperativity and F- selectivity in positive allosteric fashion are quite rare and unique. Anion induced preorganization of one binding site makes the second binding thermodynamically more favorable. This unique fluoride selective allosterism is associated with the cooperative effects of conformational flexibility of the calix[4]pyrrole and charge interaction. The homoditopic capsular receptor acts as a selective fluorescent chemosensor by exhibiting a nonlinear turn-on fluorescence response. The two identical binding sites, which are suitable to accommodate fluoride anion only, exhibited highly cooperative binding. The clean sigmoidal binding isotherms clearly indicate the positive allosteric binding behavior of the designed host. Moreover, each binding event was distinctly characterized thermodynamically. The development of such non-linear fluoride binding architectures would be very useful for the construction of highly sensitive and selective sensory systems as well as fluoride transport agents

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Metal complexes and properties of meso-alkylidenyl porphyrinoids

이창희* **SILTEABEJEABEBAYEHU**

강원대학교 화학과

meso-Alkylidenyl porphyrinoids are non-aromatic, conformationally flexible macrocycles which are most recently joined macrocycle in porphyrin community. These compounds display unusual protonation selectivity, unique tautomerism and conformtional irregularity. Most of the reported compounds showed unusual regioselective protonation depending on the number of core N-Hs. As a part of our continuing efforts for the construction of the new meso-alkylidenyl porphyrin families, we here report the synthesis, characterization, chemistry and conformational characteristics of novel metal complexes of meso-alkylidenyl porphyrins. The synthesis of metal complexes were straight forward and most of the metallation were possible by reaction of ligand with metals salts. Most of the synthesized metal complexes are stable but some metal complexes such as Ag(I) need axial ligands for stabilization. The structural characteristics and spectroscopic properties will be discussed extensively.

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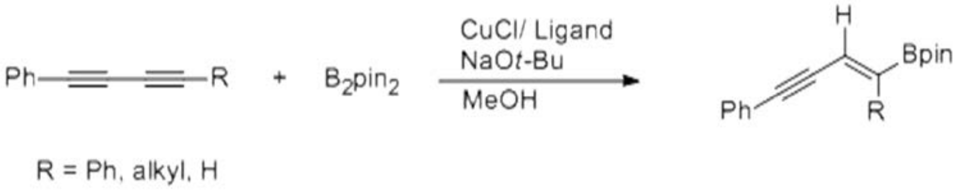
Regioselective Cu-B Addition to Unsymmetrical Conjugate Diynes

LI DINGXI 장수연 윤재숙*

성균관대학교 화학과

We have developed a copper-catalyzed regio- and stereoselective monoborylation method of conjugate diynes with bis(pinacolato)diboron, which produced enynylboronates in a good yield. The reaction is especially suitable for unsymmetrical conjugate diynes. In particular, the internal unsymmetrical diynes with allyl, TMS afford highly-functionalized enynes which can be used for coupling reaction.



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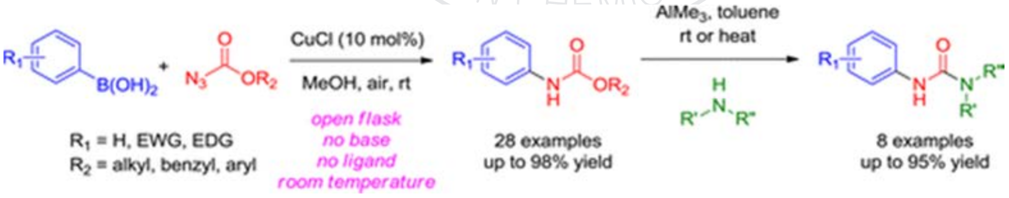
A Synthetic Approach to *N*-Aryl Carbamates via Copper-Catalyzed Chan?Lam Coupling at Room Temperature

KIMUBIN 성단비 김원석*

이화여자대학교 화학 나노과학과

A mild and efficient synthesis of *N*-arylcarbamates was achieved by reacting azidoformates with boronic acids in the presence of 10 mol % of copper chloride catalyst. The reaction proceeds readily in an open flask at room temperature without additional base, ligand, or additive. Rapid access to urea analogues via a two-step one-pot procedure is enabled by reacting *N*-arylcarbamates with aluminum?amine complexes. In addition, among several boronic acid derivatives prepared, dimethylphenyl boronate was found to react rapidly in its reaction with benzyl azidoformate, invoking *in situ* generation of this species in the catalytic cycle.



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Synthesis of novel 2-nitroimidazole Derivatives for Hypoxia Imaging Agents

권영도 김희권[1,*]

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Hypoxia, a condition of low oxygen level, results in preventing chemo and radio therapy because of malignant progression. 2-nitroimidazole undergoes a reduction which is reversible in normal cells, but not hypoxic cells. We developed 2-nitroimidazole derivatives with ^{18}F, which can detect hypoxia in Positron Emission Tomography (PET). Two types of intermediates were prepared separately: 2-(2-Nitro-1H-imidazol-1-yl)ethanamine was synthesized from 2-bromoethylamine and 2-(tert-butyldimethylsilyoxy)ethyl 4-nitrophenyl carbonate was synthesized from ethyleneglycol. Subsequently, the amide bond formation, deprotection of TBDMS group and mesylation produced new precursors for hypoxia imaging. The precursors were used for the radiosynthesis for hypoxia imaging.

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Synthesis of Various 2,7-diphenyl oct-4-enedials as Key Subunits for Unnatural Carotenoids

박명남 구상호[1,*]

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Carotenoids are an important class of organic molecules which exhibit various functions.It is newly found that carotenoids containing conjugated polyene chains would offer an extra stability and excellent electrical conductivity compared with those of natural carotenoids.Thus it is of importance to study the syntheses of such unnatural carotenoids.First, we synthesized the titled dials by coupling of substituted phenyl acetic acid ethyl ester to 1,4-dibromo-2-butene, followed by $LiAlH_4$ reduction and swern oxidation.Next, we tried the coupling and double elimination reaction of above-mentioned dials with allylicsulfone to provide unnatural carotenoids.The conductance of synthesized carotenoids is measured andinteraction of phenyl groups and beta-carotene is analyzed.

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Tandem Catalytic Oxidative Deacetylation of Acetoacetic Esters and Heteroaromatic Cyclizations

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1,5-dicarbonyl compounds from conjugate addition of ethyl acetoacetate to α,β-unsaturated carbonyl compounds underwent Mn(III)/Co(II)-catalyzed oxidative deacetylation to produce 1,4-dicarbonyl compounds, which are converted into furan, thiophene, and pyrrole using the Paal?Knorr reaction.The mechanisms of oxidative deacetylation were studied and one-pot syntheses from 1,5-dicarbonyl compounds were found possible.The oxidative deacetylation and reductive cyclization of β-ketoesters derived from ethyl acetoacetate and o-nitrophenzyl bromides efficiently produced diversely substituted indoles. The yields were optimized and substituent effects were studied.

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Synthesis and Biological activity of Carotenoids Stabilized by Various Substituents

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Carotenoids can exert important physiological functions in wide range of organism including plants and humans. Here, two types of unnatural carotenoids were synthesized. One type carotenoids with phenyl group substituents at C-13 and C-13' position that was synthesized by the coupling of allylic sulfone subunit and dialdehydes containing phenyl groups subunit. Another carotenoids containing pyrenylene group at middle position that can be synthesized by the coupling of allylic sulfone and substituted pyrene. The synthesized unnatural carotenoids were selected for biological study of antioxidation based on the stabilizing of substituent groups.

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Regioselective Preparation of 1,3- and 1,2-Tocopheryl Glyceride Ethers of Carboxylic Acids

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Phosphorylcholine derivatives of 1,2-diglycerides are basic structure of cell membranes. We studied the perparation of diverse glycerides for self-assembly installation into cell membranes or liposomes. It would be an interesting topic for intracellular metal ion transporters or drug delivery vehicles to synthesize new functional membranes or liposomes from unnatural glycerides of biologically active alcohols or acids. Phophatidylcholine is composed of a hydrophilic head group and two hydrophobic fatty acids parts. We replaced one of the fatty acid part with α-tocopherol. We were able to synthesize regioisomeric diglycerides by the regioselective epoxide ring opening with acid nucleophiles, which were efficiently utilized for the formation of diversely substituted phosphatidylcholine derivatives. Self-assembly patterns of phosphatidylchoine compounds in aqueous solution were studied by optical microscopy.

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Synthetic method for Unnatural carotene wire

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Unnatural carotenoids containing various phenyl substituents show excellent characteristics in terms of stability as well as electronic conductance. 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.

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Chain extension method for appocarotenoid

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Carotenoids are used as element of cosmetics, health foods and also plays mecinal role, example, preventing cancer. Carorenoids are characterized by the long conjugated polyene chain that shows distinctive red color. Chain extension of isoprenoid using Kocienski reaction efficiently provided fully conjugated crotenoid compound. The novel C5 benzothiazolyl(BT) sulfone containing an acetal group was prepared as an element for the chain-extension of apocarotenoids. The Julia-Kocienski olefination of the C5 BT-sulfone with C10 2,7-dimethyl-2,4,6-octatrienedial and deprotection of the acetal groups efficiently produced C20 crocetin dial. The compound of C30 and C40 apocarotenoids were prepared from C20 crocetin dial by the repeated application of the Julia-Kocienski olefination of the C5 BT-sulfone and hydrolysis.

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A chain extension method for apocarotenoids

강세인 구상호[1,*]

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Carotenoids are medically and biologically important natural products. We synthesized the natural carotenes using sulfone-mediated coupling reaction, protection of alcohol and double elimination. Lycopene and lycophyll were efficiently produced using Julia-Kocienski olefination by the coupling of C10 geranyl benzothiazolyl(BT) sulfone with C20 crocetin dialdehyde. Julia-Kocienski olefination of C5 BT-sulfone and C10 2,7-dimethyl-2,4,6-octatrienedial was utilized as a chain-extension method for the synthesis natural carotenoid products. The procedure of olefination could be used to synthesize the extended polyene of apocarotenoid.

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Design and Synthesis of Medium Ring Heterocyclic Glycosides for Bio-mimicking Studies

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Based on "amide-triazole bioequivalence" principle1, 1,2,3-triazole-fused medium ring heterocycles capable of mimicking lactams were designed and coupled with different sugar to obtain the corresponding glycosides. Their syntheses were accomplished by intramolecular [3 + 2] cycloaddition of different azidoalkynes3 followed by reaction with sugar in refluxing ethanol2. The bio-equivalent lactam-containing glycosides were obtained by similar reaction sequence where the previously constructed lactams were glycosylated in aforementioned condition. The process is capable of obtaining the triazolo-fused heterocyclic and lactam containing glycosides to study their comparable biological activities.

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Unusual Alkylation between p-Cresol and Benzyl Alcohol

한인숙* <u>정은정</u>

강원대학교 과학교육학부

Heating a mixture of p-cresol and benzyl alcohol in the presence of the catalytic amount of p-TsOH at 100℃ gave 2,2-di(1-hydroxy-4-methyl-2-phenyl)propane (1) in addition to 2-benzyl-4-methylphenol (2) and 2,6-dibenzyl-4-methylphenol (3). The yields of the products were varied depending on the molar ratio of p-cresol and benzyl alcohol. The structure of 1 was established by the spectroscopic methods. The 4o carbon atom of the propane moiety in 1 seemed to be derived from the methylene carbon atom of the benzyl alcohol via initial formation of 2. Successive elimination of the methylene protons in 2, the addition of p-cresol to the carbon, and the rearrangement of the methyl groups seemed to involve in the formation of 1.

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Areans endcapped by bulky silane group as Host Materials for Phosphorescent Organic Light Emitting Diodes

김좌진 김세현 윤승수*

성균관대학교 화학과

Here, we demonstrate triphenylsilane-substituted arenes as host materials for phosphorescent organic light-emitting diodes (PhOLEDs). Particularly, a device using 9,9-dimethyl-7-(4-(triphenylsilyl)phenyl)-9H-fluoren-2-yl)triphenylsilane as host material for green phosphorescent dopant showed the efficient green emission. Therefore, these results suggest that triphenylsilane-substituted arenes have the good potentials as the phosphorescent hosts for OLEDs .

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Synthesis and electroluminescent properties of 9,10-diphenylanthracene derivatives with electron-donating N-containing group

김영석 김동영 윤승수*

성균관대학교 화학과

This paper reports synthesis and electroluminescent (EL) properties of a new series of blue and green emitting materials based on 9,10-diphenylanthracene derivatives with electron-donating groups such as carbazole or diphenylamine. They have been prepared by Suzuki coupling and Buchwald-Hartwig cross-coupling reactions. The OLEDs were fabricated in the following sequence: ITO / NPB (50 nm) / emiting materials (30 nm) / Bphen (30 nm) / Liq (2 nm) / Al (100 nm). All devices using these materials as emitters exhibited good EL properties. Therefore, these results suggest that the introduction of electron-donating group at the anthracene would be applied to develop device performances.

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Blue fluorescence materials of arylanthracenyl-bispiro[anthracene-fluorene]-type for organic light emitting diode

이현우 정수진 윤승수*

성균관대학교 화학과

In this study, we have synthesized three blue materials based on bispiro-type by Suzuki coupling. To explore electroluminescence properties of materials, following device was fabricated: ITO / NPB (50nm) / blue emitting materials (30nm) / Bphen (30nm) / Liq /Al. All devices showed deep blue emission and good electroluminescent properties. Therefore, these results suggest that bispiro-type materials have the good potentials as the efficient blue emitters for OLEDs .

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Molecular Engineering of Dye-Sensitized Solar Cells for Retarding Back Electron Transfer

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울산과학기술대학교(UNIST) 에너지공학과 [1]울산과학기술대학교(UNIST) 친환경에너지 공학부

One of acceptor unit, benzothiadiazole (BT) has a great attention in DSC due to its high electron negativity, resulting in strong intermolecular charge transfer and thereby a broad absorption, but the poor device performances are generally obtained because of strong back electron transfer from TiO_2 electrode to oxidized dye. By using BT unit, however, DSC have achieved the highest power conversion efficiency (PCE) of 13% when the back electron transfer is reduced by the spacer unit. Thus, the understanding and insight of spacer unit can be critical issue to increase the device performance of DSC. In this presentation, we develop four different dyes that consist of D (triphenyl amine)-BT-Spacer (benzene, thiophene, toluene, and hexylthiophene)-A (cyanoacetic acid) to investigate the back electron transfer according to the change of dihedral angle between BT and acceptor. This is because the change of dihedral angle is one of key parameter to control the back electron transfer. Density function theory (DFT) calculations of these dyes provide further insight into molecular geometry, especially dihedral angle and the impact of spacer unit on the back electron transfer and photovoltaic performance. In addition, we find that the back electron transfer can be dramatically reduced under thin TiO_2 film (1.6 ㎛) compared with thick TiO_2 film (6 ㎛). As a result, organic dye with thiophene space unit reaches 7.3% of PCE with open-circuit voltage (Voc)of 660 mV, current density (Jsc) of 14.9 mA/cm² and fill factor (ff) of 0.74 under 1.6 ㎛ TiO_2 film while 5.4% of PCE with Voc of 630 mV, Jsc of 11.9 mA/cm² and fill factor (ff) of 0.72 under 6 ㎛ TiO_2 film.

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발표코드: **ORGN.P-694**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Silver(I)-Mediated C-H Amination of 2-Alkenylanilines

고태윤 김윤아 윤소원*

한양대학교 화학과

For many years, a variety of synthetic methods of indoles have been developed because of their excellent biological properties. Sustainable and more efficient methods for the preparation of indoles are of constant interest. Recently we have developed a silver(I)-mediated intramolecular C-H aminaton reaction for the synthesis of indole derivatives. There are many benefits in our optimized conditions, such as broad substrate scope, high functional group tolerance, simple/fast/high-yielding reaction, and recovery/reuse of the inexpensive silver(I). Furthermore, we could also observe an uncommon migratory process of β-monosubstituted 2-alkenylanilines with solvent-dependence.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-695**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Iron(III)-Catalyzed C-H Amination

장수산 윤소원*

한양대학교 화학과

Intramolecular oxidative C-H amination is one of the straightforward and powerful routes to highly valuable, bioactive nitrogen heterocycles. Recently, we reported a DDQ-mediated intramolecular oxidative cyclization reaction of *N*-Ts-2-styrylanilines to afford a variety of 2-substituted indoles in high yields. Very interestingly, it was found that the addition of catalytic amount of Fe(III) salt in this reaction system could alter the regioselectivity, leading to 3-substituted indoles. Herein we report our preliminary investigations into this unprecedented and unique migratory process.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigations into Pd-Catalyzed Regioselective C-H Amination Using Two Directing Groups

조윤형 이은미 윤소원*

한양대학교 화학과

Carbazoles play various roles in biological and material science as a pharmaceutical agent and organic photovoltaic device. Therefore, a lot of synthetic methods involving transition-metal-catalyzed intramolecular C-C or C-N bond formation have been reported. Previously, we reported a Pd-catalyzed intramolecular oxidative C-H amination of *N*-Ts-2-arylaniline derivatives. In view of our continued interest in Pd-catalyzed regioselective oxidative C-H amination, we were interested in developing a regioselective C-H activation at a sterically more demanding *ortho*-position of C3'-substituted substrates by two directing groups. Herein we report our preliminary investigations into a regiodivergent process.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Multicatalytic One-Pot Reaction for the Synthesis of Phthalides

유현지 윤소원*

한양대학교 화학과

Phthalides are versatile building blocks and pervasive motifs in many bioactive natural products. Therefore, a number of synthetic strategies have been developed for their construction. Recently, we reported an efficient N-heterocyclic carbene (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. As part of our continued interest in multicatalytic processes, we investigated a multicatalytic one-pot reaction for the preparation of phthalides using commercially readily available reagents, obviating the need for starting material forming processes.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Indoles

장영호 김이현 윤소원*

한양대학교 화학과

Recently, we reported a variety of intramolecular oxidative cyclization reaction of *N*-Ts-2-styrylanilines to afford 2-substituted indoles. In parallel with our efforts to develop a highly efficient catalytic system for heterocyclic synthesis, we were interested in developing an intermolecular oxidative one-pot reaction between readily available anilines and olefins for the synthesis of indoles, whereby a single catalytic system would invoke sequential C-C and C-N bond formations in an efficient manner. Herein we report our preliminary investigations into this straightforward one-pot process.

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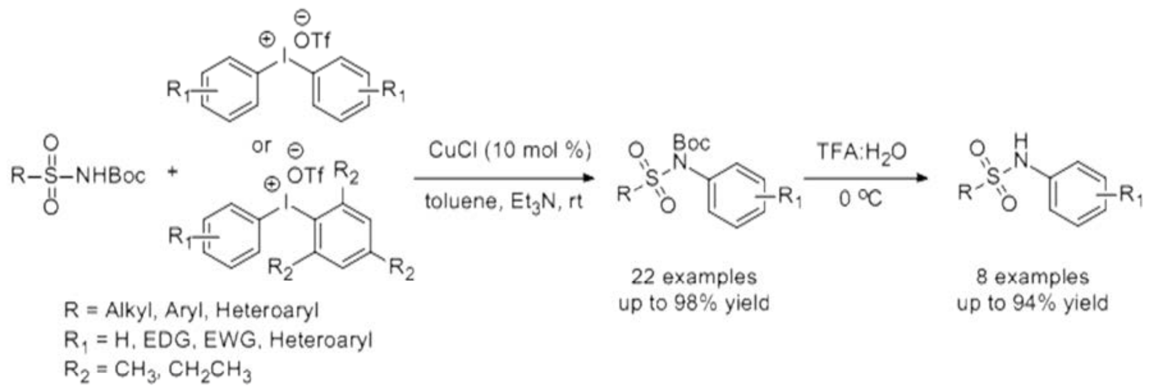
발표코드: **ORGN.P-699**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

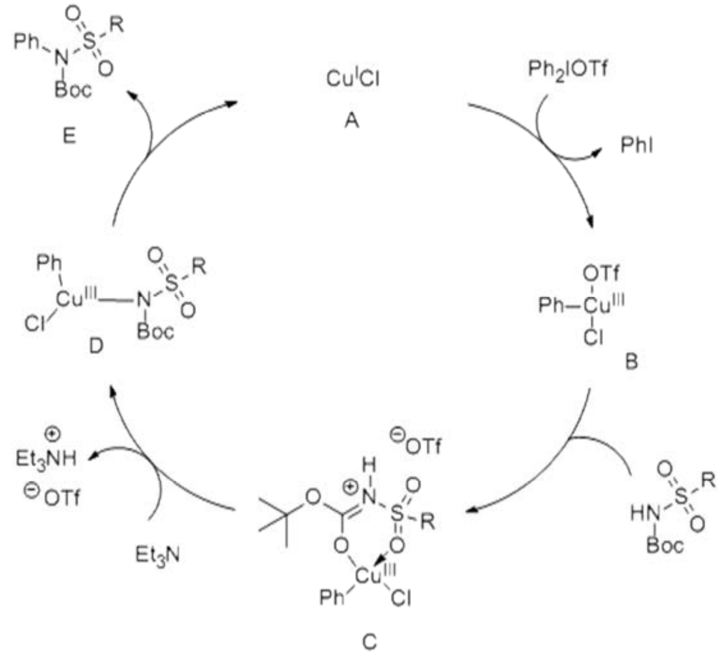
Copper-Catalyzed N-Arylation of tert-Butyl N-Sulfonylcarbamates with Diaryliodonium Salts at Room Temperature

정서희 김원석*

이화여자대학교 화학 나노과학과

N-Arylsulfonamides are a common moiety present in a large number of pharmaceutically interesting compounds. These arylsulfonamide derivatives have become popular in SAR studies in medicinal chemistry research since the early discovery of their anticancer, antibacterial, anticonvulsant and HIV protease inhibitory activities. Thus, various methods have been developed to synthesize N-arylsulfonamides. Herein, a new and mild synthetic approach for the synthesis of N-arylsulfonamides under copper-catalyzed conditions at room temperature has been developed. The reaction requires 10 mol % of CuCl catalyst and Et3N as a base at room temperature. The scope of this method has been explored employing different tert-butyl N-sulfonylcarbamates and diaryliodonium salts. Furthermore, a one-pot coupling/Boc-deprotection sequence utilizing aqueous trifluoroacetic acid was investigated to successfully furnish mono N-arylsulfonamides in good to excellent yields.


R–S(O)(O)–NHBoc
+
OTf
or
OTf
R1
R2
CuCl (10 mol %)
toluene, Et3N, rt
Boc
TFA:H2O
0 °C
22 examples
up to 98% yield
8 examples
up to 94% yield
R = Alkyl, Aryl, Heteroaryl
R1 = H, EDG, EWG, Heteroaryl
R2 = CH3, CH2CH3


Cu^ICl
A
Ph2IOTf
PhI
OTf
Ph–Cu^III
Cl
B
HN
Boc
OTf
Cu^III
Ph
Cl
C
Et3N
Et3NH
OTf
Ph
Cu^III
Cl
D
Boc
Ph
N
Boc
E

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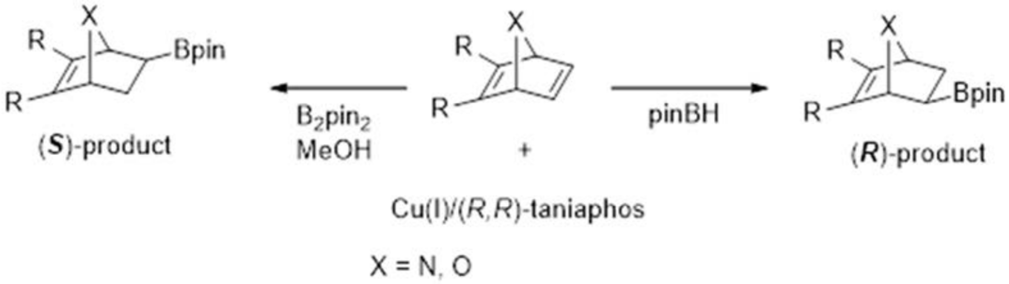
발표코드: **ORGN.P-700**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

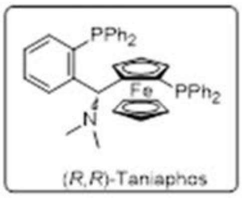
The Reversal of Enantioselectivity in the Copper(I)-Catalyzed Asymmetric Hydroboration

이혜수 한정태 윤재숙*

성균관대학교 화학과

Highly enantioselective results were achieved in the copper(I)-catalyzed asymmetric hydroboration of bicyclic alkenes. Using a copper(I)-(*R*,*R*)-taniaphos catalyst and pinacolborane (pinBH) as the hydroborating reagent, we obtained (*R*)-products with high enantioselectivity up to >99% ee for various bicyclic alkenes including oxa- and azabicyclic alkenes. On the other hand, with the same chiral copper?ligand combination, (*S*)-products were obtained using bis(pinacolato)diboron (B_2pin_2) and MeOH as the borylating reagent. Thus, the reversal of enantioselectivity in the copper-catalyzed asymmetric hydroboration of bicyclic alkenes was observed using different boron source for the first time based on altenative mechanism pathways.





일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-701**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A simple fabrication routes for colorimetric paper strips for the detection of Hg^{2+} and methylmercury ions

전창훈 하태환[1,*]

과학기술연합대학원대학교(UST) 나노바이오공학과 [1]한국생명공학연구원 바이오모니터링연구센터

In the development of selective and disposable mercury chemosensor, four different mercury chelators were synthesized and attempted to graft on cellulose filter paper. Three of them are azobenzene derivatives bearing dithiaazadioxa crown ether moiety as core chelator for Hg^{2+} in common, which vanish their colors in the presence of Hg^{2+} ions (*colorimetric*). In order to modulate spectral features of azobenzene-based chelators, two fluoronitroaniline compounds (2,4-dinitro-5-fluoroaniline, DNFA, and 4,5-difluoro-2-nitroaniline, DFNA) were linked to *N*-phenyl dithiaazadioxo ring through diazotization reaction, in addition to original 4-carboxylaninline that had been previously reported. On the other hand, the fourth chelator is rhodamine-based and turn-on type mercury binder, which also responded with methylmercury ions as well as Hg^{2+} ions, revamping the typical pink color of rhodamine dye (*colorimetric*) along with strong fluorescence (*fluorometric*); thiosemicarbazide moiety was assumed to selectively bind with Hg^{2+} ions for the rhodamine dye. For the paper immobilization, the cellulose filter paper was first primed with 3-aminopropyltrimethoxy silane (APTMS). Two azobenzene-based and the rhodamine chelator could be immobilized on the paper by simply soaking them in Petri dishes at room temperature, without further activation steps. Once tethered azobenzene-based chelators demonstrated enough color changes to discern Hg^{2+} ions of ~1.0 ppm, while fluorescent signals detecting 0.1 ppm level of methylmercury ions by rhodamine-based chelator.

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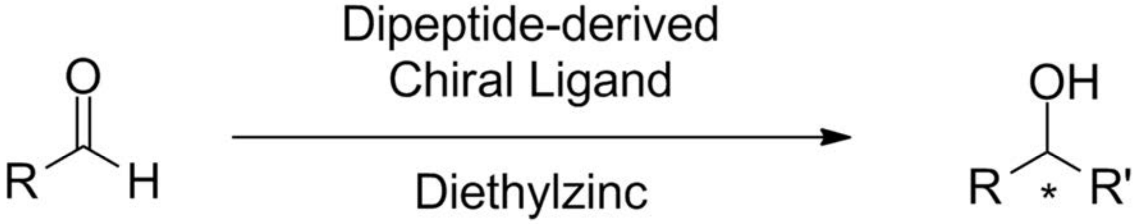
발표코드: **ORGN.P-702**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

D-Phenylglycine-*L*-Proline-derived Catalysts for the Enantioselective Addition of Diethylzinc to Aldehydes

강석용 박용선*

건국대학교 화학과

A new class of modular chiral catalysts derived from various amino acid-*L*-Pro dipeptides was prepared, and the catalysts were tested for their ability to catalyze the enantioselective addition of diethylzinc to aldehydes. *D*-Phg-*L*-Pro derivatives were identified as effective catalysts for the addition with up to 96:4 *er*.



일시: 2015년 4월 15~17일(수~금) 3일간
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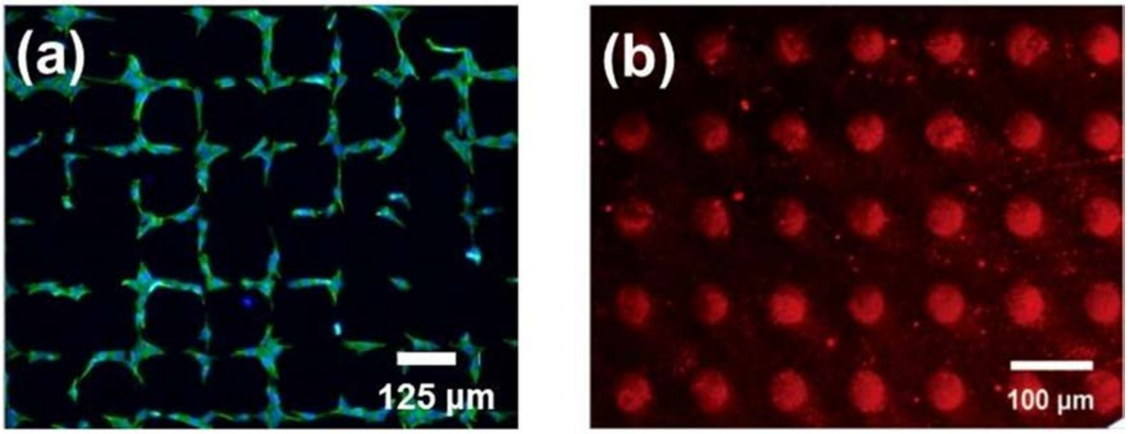
발표코드: **ORGN.P-703**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct Patterning and Biofunctionalization of a Large-AreaPristine Graphene Sheet

한경엽 이정규[1,*] 홍대화[2] 최인성[2,*]

경북대학교 화학과 [1]경북대학교 자연대/화학과 [2]한국과학기술원(KAIST) 화학과

Chemical functionalization and patterning of a large-area graphene sheet on a solid substrate promises many technological applications in optoelectrical and bioanalytical devices, neuroelectronics, energy conversion and storage, and environmental pollution management, as well as providing a research platform for understanding the fundamental phenomena involved in interfacial reactions.[1] Although a pristine graphene sheet has been functionalized by simple chemical reactions, such as halogenation, hydrogenation, phenylation, radical additions, Diels?Alder reactions, and trimethylsilylation,[2] these functionalized graphene sheets lack post-functionalizability for immobilizing biologically relevant molecules. However, these approaches involved the disruption of sp2-hybridized connections over the entire graphene surface, precluding the applications to graphene-based bioelectronics, such as biosensors and neuroelectronics. Therefore, We demonstrate direct pattern of streptavidin and NIH 3T3 fibroblast cells over a large-area pristine graphene sheet on Si/SiO2 by aryl azide-based photografting with the conventional UV lithographic technique and surface-initiated, atom transfer radical polymerization of oligo(ethylene glycol) methacrylate.


(a)
125 µm
(b)
100 µm

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct preparation of new organozinc reagents, aminophenylzinc iodides, and their applications

주성류 김승회*

단국대학교 화학과

New organozinc reagents, 4-aminophenyl zinc iodide (A) and 3-aminophenyl zinc iodide (B), have beengenerated easily and effectively by the direct insertion of active zinc to iodoanilines which possess acidicprotons. The subsequent coupling reactions of the organozincs with various acid chlorides turned out tobe an efficient tool for the preparation of aminophenyl ketones.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective fluorescence sensing of salicylic acid derivatives using Imidazole appended receptors

Anup Pandith 안미란 김홍석*

경북대학교 응용화학과

Developing of highly selective chemosensors for the detection of aromatic carboxylic acids attracts great interest in supramolecular chemistry due to the wide applications and its biological importance. In that sense various attempts has been made to develop fluorescent chemosensors for the detection of salicylic acid (SA) derivatives. Recently pyrene appended receptor has been developed for the detection of SA's derivatives based on "*turn on*" mode response. Particularly, potential secondary amine proton as well as imidazole plays vital role to hold the carboxylic acid moiety in great strength furthermore non-conjugated system gets destroyed after it binds to carboxylic acids. Same way anthracene and pyrene appended receptors were developed for "*on-off*" mode of response, by keeping weakly electron withdrawing CONH group by direct attachment for extending conjugation of pyrene and anthracene fluorophore. Based on this concept designing and synthesis of series of potential chemosensors will be presented.

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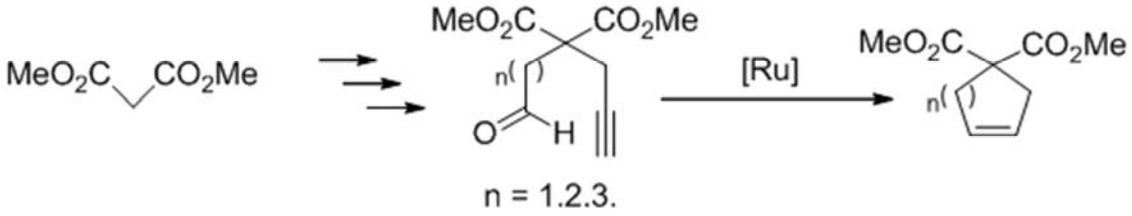
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Successful intramolecular olefination of aldehyde with alkyne using Ru catalyst, starting from dimethyl malonate

문지현* 한소엽[1]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학과, 촉매반응?합성연구센터

We have studied eagerly on intramolecular decarbonylative olefination of aldehydes with alkynes using ruthenium catalysts. Our study on successful intramolecular olefination will be described in details at the presentation.



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발표코드: **ORGN.P-707**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pyrene appended probes for selective fluorescence sensing of salicylic acids

Ashwani Kumar **Anup Pandith** 김홍석*

경북대학교 응용화학과

Pyrenesulfonamide and pyreneamide probes (2-5) were synthesized, and they were used in the sensing of salicylic acid derivatives. The ability of imidazole appended pyrenesulfonamide probe 3 to sense various salicylic acid derivatives was examined by UV-visible, fluorescence, and ^{1}H NMR spectroscopy; it was further supported by DFT calculations. The sensing of salicylic acid derivatives resulted in a significant quenching of the pyrene monomer emission. Among the tested salicylic acid derivatives, probe 3 exhibited the highest binding constant with 3,5-dinitrosalicylic acid ($K_a = 2.65 \times 10^5$ M^{-1}, measured at a 1:1 molar ratio in EtOH).

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-substituted Benzimidazoles or Imidazopyridines with Heteroaromatic diamines from Thioamides

<u>김건우</u> 이언진 정대일[*] 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Benzimidazole moiety plays an important role in chemistry and is also present in a variety of biologically active and therapeutically useful compounds. A simple and efficient transformation using readily available reagents under solvent-free and metal-free conditions is considered as a key solution for pollution problems generated by large-scale reaction. In contract to oxygen, which in a biradical in the ground state, sulfur in less reactive. We tried synthesis of novel thioamides, Benzimidazole and Imidazopyridine with Heteroaromatic diamines.And also we report a chemoselective method for an oxidative coupling reaction of alkylamine with Heteroaromatic diamines for the formation of substituted 2-carbodiimides Benzimidazoles.

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발표코드: **ORGN.P-709**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the Synthesis of novel 2-Amino-N,4-disubstituted-thiazoles

신하윤 송주현 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

A vast array of thiazole derivatives having excellent broad spectrum activity forms an invaluable part of the present armory of the clinicians. Especially thiazole devatives are important compounds in medicinal chemistry due to their broad range of biological activities. Thiazoles are found in a variety of specialized products, often fused with benzene derivatives, the so-called benzothiazoles. This type of heterocycles have shown wide variety of pharmaco active protection as anti-inflammatory, anti-tubercular, antibacterial, fungicidal, local anesthetic, tranquilizers, insecticidal, anti-microbial, anti-tumor and diuretic. Considerable efforts have been devoted to the synthesis of this type of compounds. Taking in consideration the advantages of microwave heating on solvent-free reactions, we report the rapidly solventless synthesis of a series of 2-amino-4-aryl-1,3-thiazoles under microwave irradiation, prepared from the cyclocondensation of heteroaromatic ketones with thiourea and iodine. We report synthesis of 2-amino-4-substituted thiazoles with ketones and thiourea under microwave irradiation and synthesis of 2-amino-N,4-disubstituted-thiazoles with 2-amino-4-substituted thiazoles and various active reagents

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 3-Amino-N-substituted-Quinazolinone-4(3H)-ones from Anthraniloyl hydrazine

강성영 이도훈 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

The Quinoline and Isoquinoline nucleus is found to be very important in pharmacy field. Especially quinazolinone compounds are class of fused heterocycles compounds well known for a long time and still continue the object of considerable interest. Quinazolinones have been reported to be biologically versatile compounds posses variety of activity including anticancer, antifungal, antibacterial activities. The quinazolinones have immense interest because of their broad spectrum of in-vitro activity and their in-vivo chemotherapeutic activity. Recently, the synthesis of 2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids has been described and their catalyst free synthesis in ionic liquids or 2,2,2-trifluoroethanol has also been reported. We now report reactions of anthraniloyl hydrazine(or salicylamide) and aldehydes with diphenyl phosphate (cyanuric chloride , tungstosilicic acid or phosphotungstic acid)as a catalysts.In order to obtain novel bioactive compounds, We also tried synthesis of 3-Amino-N-substituted-quinazolinone-4(3H)-ones from Anthraniloyl hydrazine

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

아릴나프탈렌락톤 리그난 천연물의 전합성 및 유도체화 연구

김태정 이윤서[1] 함정엽*

한국과학기술연구원(KIST) 천연물연구소 [1]강릉원주대학교 해양자원육성학과

아릴나프탈렌락톤은 다양한 식물군에서 발견되는 리그난류 천연물로 암을 비롯하여 염증, HIV, 뇌질환, 골다공증 등에서 다양한 유효 활성을 나타내는 것이 보고되고 있다. 이 중 대표적으로 손꼽히는 천연물로 다이필린, 저스티시딘류, 실리나프탈렌류 및 타이와닌류 등이 있으며, 이들은 나프탈렌락톤(naphtho[2,3-c]furan-1(3*H*)-one)을 중심골격으로 유사한 구조를 가지고 있다. 그러나 이러한 유사 구조를 가지고 있음에도 불구하고 치환기의 위치나 종류에 따라 전혀 다른 생리활성이 발현되어 현재까지 여러 화합물에 대한 연구 내용이 논문이나 문헌을 통해 보고되고 있다. 한편, 아릴나프탈렌락톤 리그난류 천연물은 많은 유기합성 그룹의 연구를 통해 전합성이 달성되어 있으나 현재까지 보고된 모든 방법이 아릴기(-Ar)를 합성 초기단계에 도입하는 방법으로 다양한 유도체화를 통한 SAR 연구를 수행하기에는 비효율적이다. 이에 본 연구진은 아릴나프탈렌락톤 리그난류 천연물의 중심골격인 나프탈렌락톤을 합성 초기단계에 구축한 후, 마지막에 여러 가지 아릴기를 도입하는 새로운 방법을 통해 13 종의 천연물을 비롯한 다양한 유도체를 효율적으로 합성하는데 성공하였다. 본 포스터발표에서는 상기의 연구내용에 대해 상세히 보고하고자 한다.

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장소: 일산 KINTEX
발표코드: **ORGN.P-712**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of (-)-Bassianolide and Study on Its Biological Activity

문보현 이윤미*

광운대학교 화학과

Bassianolide is an insecticidal cyclodepsipeptide isolated from Beauveria bassiana, which is an entomopathogenic fungi. Bassianolide is known to cause atonic symptom to the larvae of Helocoverpa and is toxic to silkworm larvae. It also inhibits acetylcholine-induced smooth muscle contraction. To investigate biological activity of bassianolide as potential anti-cancer agents, we synthesized it and tested for its activity. One total synthesis of bassianolide was reported by Suzuki and co-worker in 1977. However, the overall yield was low with 7.2%. Herein, we describe more facile and efficient synthesis of bassianolide involving coupling reactions between methylamines and carboxylic acids with Ghosez`s reagent (1-chloro-N,N,2-trimethyl-1-propenylamine). D-α-hydroxyisovaleic acid was used as a starting material and synthesis of (-)-bassianolide was achieved in 10 steps with 36.5% overall yield.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Cu-catalyzed Electrophilic Amination of Heteroarenes with O-benzoyl hydroxyamines

윤홍주 이윤미*

광운대학교 화학과

Heteroarylamines are highly valuable components in biologically active natural substances and pharmaceuticals. Therefore, the versatile and practical synthetic strategies for the formation of C(sp2)-N bond have been intensively studied. Among them, copper-catalyzed C-N bond formation with organometallic reagents and electrophilic amines has been widely developed in recent years as one of the most important approaches. Various organometal reagents including zincs, zirconiums, borons, and silicons were used for the Cu-catalyzed electrophilic aminations. In this study, we developed a practical and efficient method for the synthesis of heteroarylamines through the reaction of easily synthesized heteroarylaluminum reagents with readily prepared O-benzoyl hydroxyamines in the presence of a low-cost copper catalyst. Heteroarylaluminum reagents are prepared from the lithiation of heteroarenes with n-BuLi, followed by transmetallation with readily available Et2AlCl and used without further purification. It can be stored under N2 gas for several days. Catalytic aminations with only small amount of Cu salt (1~3 mol %) can be proceeded to complete conversion within a few hours, providing desired heteroarylamines with high yields (up to 98%).

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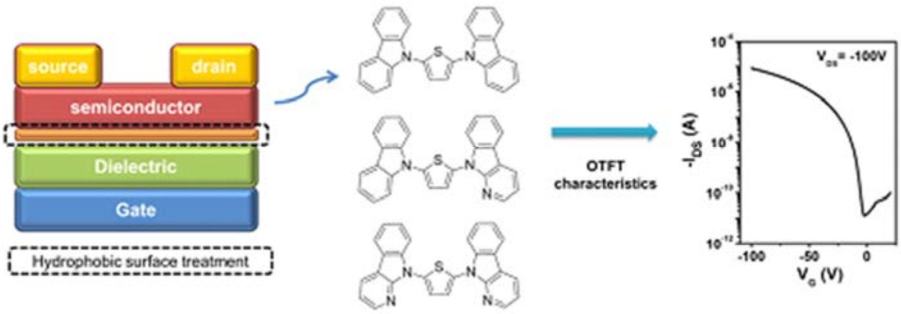
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbazole- and α-Carboline-based Thiophene Derivatives as Organic Semiconductors for Organic Thin-film Transistors

서초현 서성용*

부경대학교 화학과

New thiophene derivatives, end-functionalized with carbazoles (9-(5-(9H-carbazol-9-yl)thiophen-2-yl)-9H-carbazole), carbazole and α-carboline (9-(5-(9H-carbazol-9-yl)thiophen-2-yl)-9H-pyrido[2,3-b]indole), and α-carbolines (9-(5-(9H-pyrido[2,3-b]indol-9-yl)thiophen-2-yl)-9H-pyrido[2,3-b]indole) were synthesized and characterized as organic semiconductors for organic thin-film transistors (OTFTs). The best device performance was achieved via a hexamethyldisilazane dielectric surface treatment of thermally grown Si-SiO2 substrates prior to vapor-phase semiconductor deposition. Within this family, the semiconductor having an electron-donating (carbazole) and an electron-withdrawing (α-carboline) substituent exhibited the highest p-channel characteristic with a carrier mobility as high as 0.014 cm2/Vs and a current on/off ratio of 7 ? 105 for top-contact/bottom-gate OTFT devices. The device characteristics have been correlated with the film morphologies and microstructures of the corresponding compounds.



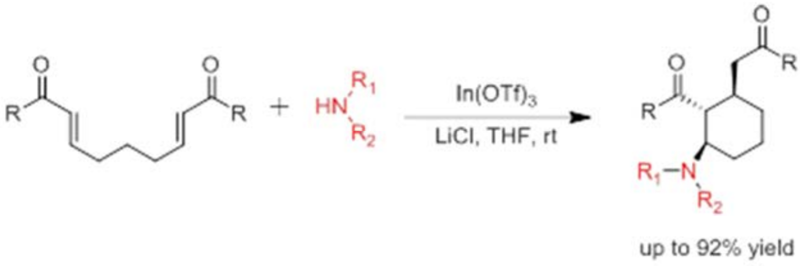
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-715**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereoselective Tandem Intramolecular Conjugate Addition of Secondary Amines to α,β-Bisenones Catalyzed by Indium Triflate

NGUYENPHAMTHANHVAN 서성용*

부경대학교 화학과

We report an indium triflate-catalyzed stereoselective intramolecular tandem conjugate addition of secondary amines to α,β-bisenones to afford a 1,2,3-trisubstituted six-membered ring bearing diketone substituents in good to excellent yields at room temperature. Various kinds of α,β-bisenones and amines were employed to expand the scope of this chemistry. Intramolecular trapping of indium-enolate by the tethered electrophiles resulted in the stereoselective formation of three contiguous stereogenic centers.



일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-716**

발표분야: 유기화학

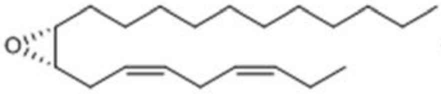
발표종류: 포스터, 발표일시: 수 16:00~19:00

Practical synthesis of (9S,10R)-9,10-epoxy-(3Z,6Z)-henicosadiene: The major pheromone of the saltmarsh caterpillar moth Estigmene acrea

고요한 chirumarrysridhar 신동수*

창원대학교 화학과

An efficient synthesis of (3Z,6Z)-cis-9,10-epoxy-3,6-henicosadiene (1), the major component of sex pheromone of saltmarsh caterpillar moth, Estigmene acrea (Drury), was accomplished from commercially available pentadec-3-yn-1-ol and bromoundecane. Chirality was introduced by employing Sharpless asymmetric dihydroxylation on cis-olefin intermediate in the synthesis of 1 as first time. The other key reactions include metal dissolving coupling, Lindlar's catalyst assisted partial hydrogenation, one-pot three step epoxidation from vicinal diol and Wittig olefination. The overall yield of 1 was noted to be 24.7% in 8 steps. The efficiency and simplicity of this synthesis allow the potential use of pheromone 1 in pest management programs.



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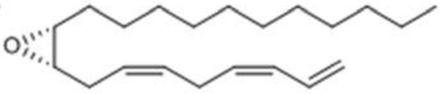

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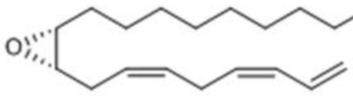

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일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
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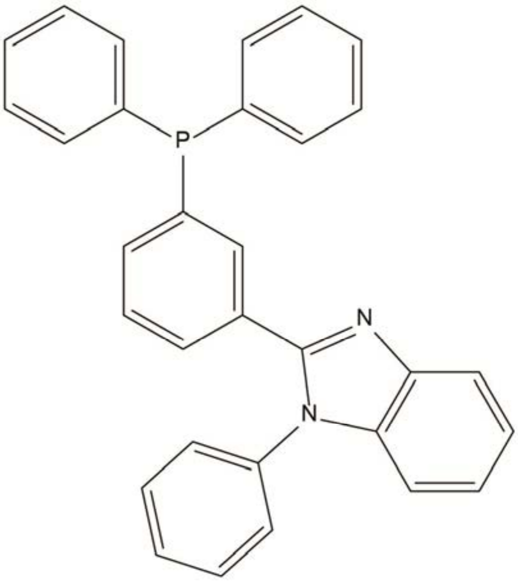
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Electroluminescent Properties of 2-(3-(diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (3-DPPI) and 2-(2-(diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (2-DPPI)

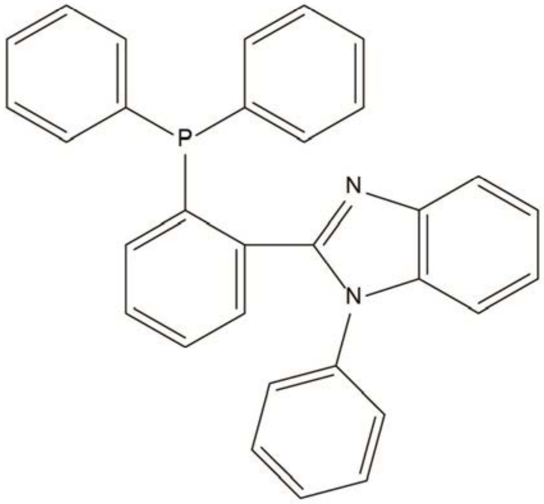
김경현 이범종[1,*] 조현희

인제대학교 화학과 [1]인제대학교 의생명화학과

Novel light-emissive materials, 2-(3-(diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (3-DPPI) and 2-(2-(diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (2-DPPI), have been synthesized. An intermediate (BPBI) for 3-DPPI synthesis was synthesized from 3-bromobenzoyl chloride, 2-aminodiphenylamine and triethylamine in THF. And then, 3-DPPI was synthesized from this BPBI and chlorodiphenylphosphine, and 2-DPPI from 2-diphenylbenzoic acid and 2-aminodiphenylamine. The chemical structures of 3-DPPI and 2-DPPI were determined by FT-IR, 1H-NMR, 13C-NMR, and UV-vis. These compounds show strong blue emission under excitation by UV lamp of 365nm. The photoluminescence (PL) and electroluminescence (EL) properties will be discussed.



3-DPPI



2-DPPI

일시: 2015년 4월 15~17일(수~금) 3일간

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발표코드: **ORGN.P-718**

발표분야: 유기화학

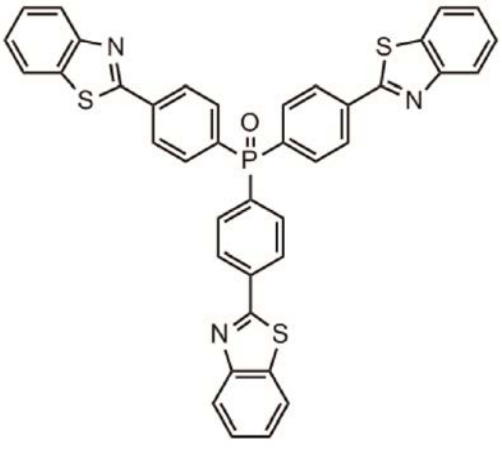
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Tris(4-(benzo[d]thiazol-2-yl)phenyl)phosphine oxide (4-TBTPO) and Tris(4-(benzo[d]oxazol-2-yl)phenyl)phosphine oxide (4-TBOPO) as Materials for OLED

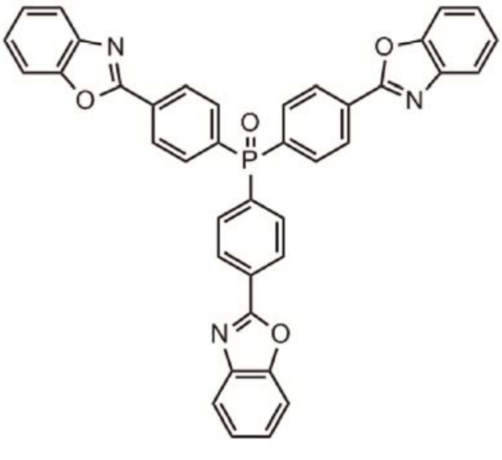
조현희 김경현 이범종[1,*]

인제대학교 화학과 [1]인제대학교 의생명화학과

New organic light emitting devices (OLED) which is configured on the basis of tris(benzothiazolyl or benzooxazolyl)phosphine oxide structure were designed. The in situ synthesis of tris(4-(benzo[d]thiazol-2-yl)phenyl)phosphine oxide (4-TBTPO) and tris(4-(benzo[d]oxazol-2-yl)phenyl)phosphine oxide (4-TBOPO) have been carried out with tetrabutylammonium bromide (TBAB). The chemical structures were characterized by 1H-NMR, 13C-NMR, FT-IR. 4-TBTPO and 4-TBOPO show respectively yellow and blue emission under excitation by UV lamp of 365nm. We will discuss the physical and OLED characters by DSC, UV-Vis, PL and EL measurements.



4-TBTPO



4-TBOPO

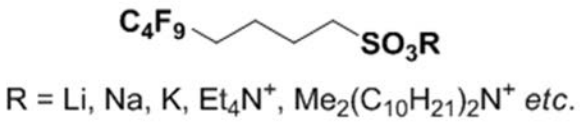
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-719**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

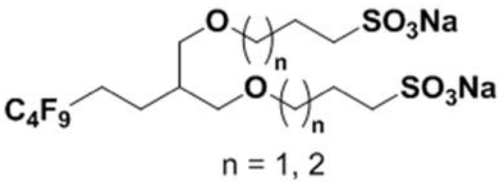
Mono and di-branched hemifluorinated PFOS alternatives synthesis and their property studies

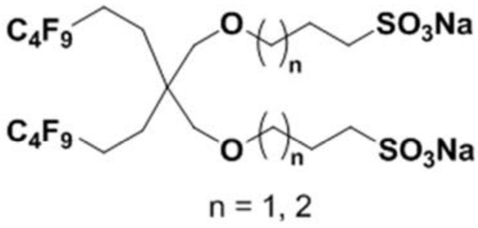
VAIDYARAGHAVENDERRAO chirumarrysridhar 신동수*

창원대학교 화학과

Perfluorobutyl substituted alkanesulfonates derivatives were synthesized and characterized as alternative substances to perfluorooctanesulfonic acid (PFOS, 1), a well-known surfactant. On the other hand PFOS related substances are toxic towards health and environment due to its non-biodegradability. The perfluoroalkyl chain can be substituted with hemifluoro alkyl chain to gain biodegradable substances. In this purpose, we used fluorous alkyliodides coupled to ethyl vinylsulfonate in presence of Zn/CuI in ionic liquids as well as in formamide to obtain ethylperfluoroalkylsulfonate. Simultaneously, we have synthesized di-sulfonates starting from hemifluorinated alkylhalide to avail monoalkyl and dialkyl derivatives. The biodegradability and surface tension reduction properties were also measured.







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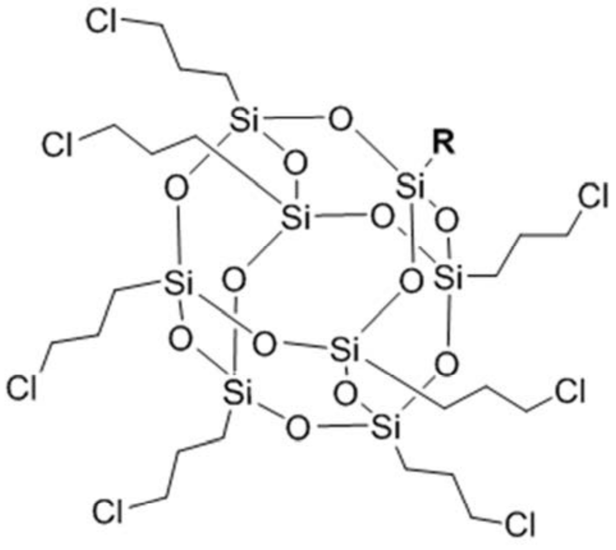
발표코드: **ORGN.P-720**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and synthesis and of hepta(3-chloropropyl)-tricycloheptasiloxane trisodium silanolate and its derivatives

<u>PATILKALPESHTUMADU</u> 이주용 **chirumarrysridhar** 신동수*

창원대학교 화학과

Polyhedral oligomeric silsesquioxanes (POSS) are biodegradable nanostructures with the empirical formula RSiO1.5, consists of a rigid and cubic silica core with a 0.53 nm side length surrounded by eight organic corner groups. Incompletely condensed silsesquioxanes (trisilanols or trisilanolate-T7) having one silicon atom short of T8 cube are of great importance due to the presence of a reactive trisilanolate or trisilanol site and are used as excellent platforms for synthesizing new hybrid materials. Thus, synthesis of trisilanols with seven reactive organic groups is a promising task in the design of hybrid materials with high-performance in several applications. Here, we report the first synthesis of incompletely condensed (with seven reactive groups) POSS, hepta(3-chloropropyl)-tricycloheptasiloxane trisodium silanolate (7Cl-T7-(ONa)3 in gram scale. The reactivity of the chloride functional groups in 7Cl-T8-R makes it an attractive synthetic platform on which to build new compounds for inorganic and organic derivatives of POSS molecules.



R = H, Alkyl or Aryl

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of fluorescence sensors for the reversible detection of mitochondrial thiols

유지혜 최기항*

고려대학교 화학과

Glutathione (GSH), a tripeptide composed of the amino acids L-glutamate, L-cysteine and glycine, is the most abundant thiol in biological system. It acts as a major antioxidant inside cells and, therefore the detection of cellular thiol concentration changes has emerged as an important issue. Mitochondria are the main intracellular location of oxygen consumption and reactive oxygen species (ROS) generation. Because GSH plays an important role in ROS regulation, the monitoring of mitochondrial thiol concentration changes is especially important to understand cellular mechanisms of redox dependent signallings.Herein, we have designed reversible fluorescence sensors capable of monitoring the thiol concentration in the mitochondria. These sensors with a cyanoacrylamide electrophile react with GSH in a rapid and reversible manner. The sensors are also equipped with a tripenylphosphonium, and successfully localized inside mitochondria. As a result, we could monitor, for the first time, the mitochondrial thiol concentration changes in real time.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Introducing Various Amino Groups into Metal-Organic Frameworks

함형우 하현빈 김민*

충북대학교 화학과

금속-유기 골격체(Metal-Organic Framework, MOF)란 금속 이온 또는 단위체에 유기 리간드가 결합하여 다공성을 갖는 구조를 말하며, 기체 저장, 분리, 촉매 등으로 다양한 분야에서 적용이 가능하다. MOF 의 합성에 사용되는 리간드는 금속과 배위할 수 있는 그룹 외에 특정 작용기를 포함할 수 있는데, 아민이나 할로젠 같은 작용기를 포함하는 리간드를 사용할 경우, MOF 의 다공성 구조 내에 해당 작용기를 효과적으로 도입할 수 있다. 본 연구에서는 상대적으로 MOF 의 합성에서 널리 활용되는 작용기인 아민 리간드에 변형을 주어, 여러 종류의 아민 작용기 유도체를 합성한 후, 이를 MOF 합성에 응용한 결과를 논의하고자 한다. 특히, 아연과 지르코늄을 중심 금속으로 하는 MOF 의 합성에서 나타나는 독특한 특성에 대하여 발표하고자 한다.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Selective C-C Bond and C-N Bond Formations of Benzoxazoles

유광호 김영조* 김민*

충북대학교 화학과

질소, 산소 등의 헤테로원소를 포함한 고리형화합물은 자연에 존재하는 유기 물질에서 자주 관찰되고, 전합성, 약학, 농화학등 다양한 분야에서 중요한 기본 골격물질로 최근에 많은 연구가 이루어 지고 있다. 최근, 전이금속 촉매를 이용하여 헤테로 고리를 가지는 화합물을 시작물질로 목표 분자를 합성하거나 다양한 작용기를 도입하는 연구가 다양하게 진행되고 있다. 특히,헤테로 원자 옆의 탄소-수소 결합은 상대적으로 산성도가 높기 때문에,새로운 결합을 이 위치에 도입하는 연구가 활발하게 진행되고 있다. 주로 팔라듐, 로듐 등의 후전이금속이 사용되고 있으며, 최근 니켈이나 구리 등의 상대적으로 값이 저렴한 촉매를 이용한 헤테로고리 화합물의 작용기화 연구가 널리 진행되고 있다. 본 발표는 대표적인 헤테로고리 화합물 중에 하나인 벤조옥사졸을 시작 물질로 하여 아릴화 반응을 진행시킨 결과를 보고하고자 한다. 특히, 탄소-수소 결합 위치에 대한 아릴화 반응과 고리 열림 탄소-질소 결합 형성 반응 사이의 선택성에 대한 논의를 중점적으로 발표할 것이다.Acknowledgement 본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행 된 연구 결과임. (과제번호 2014H1C1A1066874).

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Synthesis of Group 13 Element-Containing Bezene Dicarboxylic Acids

하현빈 김수연 김민*

충북대학교 화학과

벤젠다이카복실산 유도체는 최근 다양한 분야에서 연구 되고 있는 유기/무기 혼성 구조체인 금속-유기 골격체(Metal-Organic Frameworks, MOFs)를 합성하기 위하여 가장 널리 사용되는 리간드다. 특히, 벤젠의 6 개 수소 중에서 두 개의 카복실산 외에 남은 4 개의 위치에 여러 종류의 작용기를 도입할 경우, MOF 구조 내에 특정 작용기를 도입할 수 있다. 이 전략을 이용하여 기존에 아민이나 할로젠 등의 작용기를 포함하는 벤젠다이카복실산을 이용한 MOF 의 합성이 다양하게 보고 되고 있다. 본 연구에서는 MOF 연구에서 상대적으로 연구된 바가 적은, 13 족 원소를 포함하는 작용기를 벤젠다이카복실산 유도체에 도입하여 성공적으로 리간드를 합성하고, 이를 이용하여 MOF 의 합성과 성질 연구를 진행하고자 한다.Acknowledgement 본 연구는 교육부와 한국연구재단의 지역혁신인력양성산업으로 수행된 연구 결과임. (과제번호 2014H1C1A1066874).

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Cobalt-Catalyzed Selective Transformations of Oximes

김세은 김영조* 김민*

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본 발표에서는 전이금속 중 코발트 촉매를 이용한 옥심의 전환 반응에 대하여 발표하고자 한다. 옥심은 탄소와 질소 사이에 이중 결합을 가지고, 질소에 수산화기를 가진 작용기로, 산업적으로 아마이드를 형성하는 반응에 사용되는 중요한 합성 중간체이다. 알데히드 혹은 케톤을 시작 물질로 하여 쉽게 합성할 수 있는 옥심은 나이트릴을 형성하는 탈수화 반응과 아마이드를 형성하는 재배열 반응이 가능하고, 또한 가수분해를 통한 카복실산의 형성, 그리고 탄소 위치에 친핵체의 공격 등이 가능한 반응성이 매우 높은 화합물이다. 본 연구에서는 신규 코발트 촉매를 이용하여 옥심을 여러 종류의 화합물로 전환하는 반응을 연구하였다. 특히, 기존에 유기 반응에 사용되지 않았던 오쏘-나이트로 페놀산 형태의 리간드를 사용하여 코발트의 반응성을 관찰하였다. 흥미롭게도 코발트를 중심 금속으로 사용하는 비슷한 반응 조건에서 다이나이트로페놀산 리간드가 반응에 참여한 경우에는 탈수화 반응이 우세하여 나이트릴이 주 생성물로 얻어졌으며, 나이트로 나프톨을 리간드로 사용한 경우에는 재배열 반응이 우세하여 아마이드가 주 생성물로 얻어졌다. 이러한 형태의 리간드 조절에 의한 반응성의 조절은 매우 드문 예로, 같은 시작 물질인 옥심과 중심 금속인 코발트를 사용하여 나이트릴과 아마이드를 선택적으로 높은 수율로 합성할 수 있었다. 본 발표에서는 신규 리간드가 배위 된 촉매의 구조 및 다양한 옥심에 대한 반응성에 대하여 논의하고자 한다.Acknowledgement 본 연구는 교육부와 한국연구재단의 지역혁신인력양성 사업으로 수행된 연구 결과임.(과제번호 2014H1C1A1066874).

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Spiropyran-Fluorescein Chemosensor

신은주* 김빛나

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Artificial sensors for sensing and recognition of various metal ions have received considerable attention. Especially, the design and synthesis of sensors for colorimetric and fluorimetric detection of metal ions is a challenge to many chemists. Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, undergoing reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.Fluorescein(Fl) is highly fluorescent and widely used as a fluorescent tracer for many applications and a useful fluorescence probe for important biomolecules, and also known as a color additive. Incorporating Fl into SP is expected to lead to excellent light-controlled fluorometric ion sensing system. In this study, SP-Fl dyad with spiropyran and fluorescein units, was prepared. Their spectroscopic properties and photochromic reaction were investigated using absorption and fluorescence spectroscopy.

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Facile efficient synthesis of styrenated phenol

신은주* 김빛나

순천대학교 화학과

The functionalization of arenes is of great importance in the synthesis of pharmaceuticals, agrochemicals, and fine chemicals. These synthetic routes were conventionally performed by Friedel-Crafts alkylation and acylation reactions. Normally, these reactions are catalyzed by different Lewis acid catalysts, however, drastic reaction conditions were employed resulting in lower product selectivity and over-alkylation. Intermolecular hydroarylation reaction of vinyl arenes with various electron rich arenes has attracted considerable importance in both chemistry laboratory and chemical industry in view of the demand for efficient, economic, and environmentally friendly processes. Hydroarylation of alkenes derivatives was successfully catalyzed by various homogeneous Lewis acid catalysts. However, all these catalysts have limitations, such as high amount of catalyst, low recyclability and require tedious workup procedure for the catalyst separation. Thus, identification of an efficient reusable heterogeneous catalytic system for hydroarylation of alkenes remains an intriguing challenge. In the recent years, heteropoly acid catalysts are represented as green solid acid catalysts for various acid-catalyzed reactions. Polyoxometallates (POMs) among heteropoly acid catalysts possess high acidic strength, safe to handle, and non-corrosive solid acid catalysts. In this work, efficient reusable heterogeneous catalysts have been explored for the addition of phenol to the styrene derivatives under solvent-free conditions.

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Synthesis and spectroscopic properties of rhodamine derivative containing indole moiety

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Design and synthesis of artificial sensors for sensing and recognition of various metal ions have received considerable attention. Especially, the design and synthesis of sensors for colorimetric and fluorimetric detection of metal ions is a challenge to many chemists. Rhodamine dyes are widely used as colorimetric and fluorescent chemosensors for the detection of various metal cations, owing to their strong absorption and fluorescence in the visible region accompanying by the structural change from the spirolactam ring-closed (c-Rh) form to ring-opened form (o-Rh). In general, rhodamine with spirolactam ring (c-Rh) is red-orange color and is non-fluorescent. However, its ring-opened form(o-Rh) is formed by the addition of metal cations and it display a pink color and strong fluorescence. Therefore, rhodamine-based chemosensors detectable with the naked eye has attracted a great interest in recent years.Introducing indole into rhodamine is expected to lead to excellent light-controlled colorimetric and fluorometric ion sensing system. In this study, rhodamine derivative containing indole moiety was synthesized. Their spectroscopic properties and photochromic reaction were investigated using absorption and fluorescence spectroscopy.

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Synthesis and spectroscopic properties for quinoline-substituted spiropyran derivative

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Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, undergoing reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.Incorporating quinoline ring into SP is expected to lead to excellent light-controlled fluorometric ion sensing system. In this study, quinoline-substituted spiropyran derivative was synthesized and its spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

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Spectroscopic Properties of Spiropyran derivative with naphthalene ring

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Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, whose molecular structure can be altered after exposure to light, temperature, pH or electrochemistry. They would undergo reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.On the other hand, the naphthalene moiety is one of the most useful polycyclic aromatic compounds in the construction of fluorogenic chemosensors for a variety of important chemical species. Incorporating naphthalene into spiropyran is expected to lead to interesting photoresponsive system with the properties of which can be manipulated by light. In this study, spiropyran derivative with naphthalene ring was prepared and its spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

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Synthesis of Natural benzofuran derivatives

서영화 전종갑[1,*]

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Chalcones are widespread in plant kingdom and they were reported to have various biological activities such as antitumor, anti-parasitic, anti-leishmanial, anti-oxidative, antibacterial, superoxide scavenging, PTP1B inhibitory activity. Previously, we synthesized licochalcones A-E and their derivatives. benzofuran derivatives under current study were isolated from *R. rugosa* belongs to the genus of rose that grows in Yu Nan Province of China. Their anti-tobacco mosaic virus activities were already known. Synthesis of these natural products was not yet reported. Herein we wish to describe the synthesis of natural benzofuran derivatives using α-bromination of acetophenones and the Rap-stoermer reaction of the resulting phenacyl bromides with substituted salicyladehydes as key steps.

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Synthesis of Natural Prenylated Chalcones

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Chalcones are widespread in plant kingdom and they were reported to have various biological activities such as antitumor, anti-parasitic, anti-leishmanial, anti-oxidative, antibacterial, superoxide scavenging, PTP1B inhibitory activity. Previously, we synthesized licochalcone A-E and their derivatives. The first chalcone which we attempted synthesis was isolated from the hairy roots of *G. glabra*. and the second one was isolated from the stem bark of the plant *Erythrina abyssinica*. The key steps of the present approach are Al_2O_3-mediated prenylation and Claisen-Schmidt condensation

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Synthesis of Natural Cinnamylphenols

정종운 전종갑[1,*]

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cinnamylphenol compounds isolated from Dalbergia nigrescens Kurz (Leguminosae). cinnamylphenol compounds were showed inhibitory activities against Epstein Barr virus early antigen activation induced by 12-*O*-tetradecanoylphorbol-13-acetate in Raji cells (anti-tumor promoters). We attempted synthesis of cinnamylphenol compounds through Cu(OTf)$_2$-catalyzed Friedel-Crafts-like alkylation reaction as the key step.

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Novel Xylene-linked Maltoside Amphiphiles (XMAs) for Membrane Protein Study

조경호 채필석*

한양대학교 생명나노공학과

Integral membrane proteins carry out a number of vital functions such as signal transduction, material transfer and cell-cell recognition across lipid barriers. Amphipathic agents, called detergents, are inevitably used for membrane protein study and play fundamental roles in determining the success of protein structure analysis. Here we introduce a novel class of amphiphiles with a benzene scaffold, which two alkyl chains and four hydrophilic groups project from. These novel agents were evaluated for a set of membrane proteins including a G-protein coupled receptor (GPCR) and some of them (XMA-4 and XMA-5) displayed favorable behaviors in terms of membrane protein stabilization. These results indicate that novel BMAs have a significant potential in membrane protein structural study.

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Synthetic Amphiphiles Bearing a New Hydrophilic Group for Membrane Protein Study

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Membrane proteins perform a variety of essential cellular functions and account for about one-third of proteins encoded in the human genome. Successful membrane protein solubilization and stabilization are prerequisites for their structural and functional characterizations. Thus, conventional detergents with an alkyl chain and a polar head group are used as essential tools for membrane protein study, but are often limited in stabilizing the native structures of membrane proteins. Here we designed and prepared a new class of amphiphiles bearing a glucose-derived hydrophilic group to overcome the limitations of conventional detergents. The efficacies of these novel agents will be evaluated for a number of membrane protein systems.

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A Novel Class of Glucose-containing Amphiphiles for Membrane Proteins Study

sadafaiman 채필석[1,*]

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More than 50% of pharmaceutical drugs target integral membrane proteins reflecting their pivotal roles in biological function and drug discovery. Despite their immense significance, the detailed structural and functional information of membrane proteins is very limited, indicating difficulties associated with handling of these membrane-inserted proteins. Conventional detergents are commonly used for membrane protein manipulation, but membrane proteins encapsulated by these agents tend to lose their structural integrity. Hence we prepared several novel glyco-amphiphiles with an ether or amide linkage that will be evaluated for their abilities to extract and stabilize a few membrane proteins. Because of synthetic convenience and expected promising efficacy, these agents will serve as essential tools in membrane protein research

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Fluorescein-labeled deoxyuridine as a pH probe

이정연 황길태*

경북대학교 화학과

세포 내 pH 를 모니터링 하는 것은 살아있는 세포에서의 생리학적 및 병리학적인 과정을 이해하는데 매우 중요하다. 지금까지 세포 내 pH 를 모니터링 하는 여러 방법이 개발되고 있다. 그 중에서도 형광 센서들은 간단하고 민감하여 많은 관심을 끌고 있다. 바이오 시스템에서 pH 변화를 모니터링 하기 위해 pH 를 센싱하는 형광 분자가 많이 알려진 반면, pH 에 민감한 형광 뉴클레오사이드는 거의 알려져 있지 않다. 따라서 본 연구에서는 4-bromophthalic anhydride 와 2-nitrotesorcinol 의 친핵성 방향족 치환반응으로 fluorescein 유도체를 합성하고 Sonogashira 반응을 통해 2’-deoxyuridine 에 도입하여 fluorescein 을 기반으로 하는 2’-deoxyuridin 을 합성하였다. Fluorescein 은 산성이나 중성 pH 에서 형광을 띄는 quinone 형태로 존재하며, 염기성 pH 에서 형광을 띄지 않는 spiro 형태로 존재하는 특징을 가지고 있다. 이러한 특징을 토대로 우리는 산성 조건에서부터 염기성 조건까지 다양한 pH 에 따른 형광 변화를 조사하였다. 이를 이용하여 바이오 시스템에서 pH 에 민감한 형광 뉴클레오시드로써 사용할 수 있을 것이라고 기대하고 있다.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Sequential detection of Cu(II) and iodide anion based on *turn-on* and *turn-off* fluorescence probe

안미란 임치섭 **Anup Pandith** 김홍석*

경북대학교 응용화학과

The developments of *turn-on* and *turn-off* fluorescent probes have been attracted. A sensor of sequential detection system for Ga(III)/ HSO_4^-, and Cu(II)/I^- were reported recently. A new highly selective fluorescent probe of simple 2-(2’-aminophenyl)thiazole (1) was synthesized and investigated for the quantification of copper(II) and iodide anion.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photochemical Characteristics for Aggregation-Induced Emission of Photoisomerizable Fumaronitrile

정한빈 고경국 이재관[1,*]

조선대학교 탄소소재학과 [1]조선대학교 화학교육과/탄소소재학과

Aggregation-induced emission (AIE) of π-conjugated organic molecules has received a great deal of attention in the field of organic optoelectronics owing to its fascinate and unprecedented optical phenomena. Despite the intermolecular interaction via π-π stacking between π-conjugated molecules generally leads to photoluminescence (PL) quenching, several specific π-conjugated organic molecules such as tetraphenylenthene (TPE) and cyanostilbene presented the opposing properties that enhance the emission in solid-state but quench in solution. It has been reported that these AIE features were originated from aggregation-induced planarization of π-conjugated molecules. The AIE-active π-conjugated organic molecules often have structurally diarylalkene motifs, which exhibited twisted structures by internal steric repulsion between lager aryl groups in diluted solution but planar structure by tight π-π intermolecular packing in concentrated solution or solid-state. Among various diarylalkene motifs, we have interested in the AIE-active molecules having unsymmetrically aryl-substituted alkene motifs such as cyanostilbene. They can present a typical E/Z isomerization under light-irradiation. Herein, we report the synthesis and photochemical characteristics of fumaronitrile-based π-conjugated molecules

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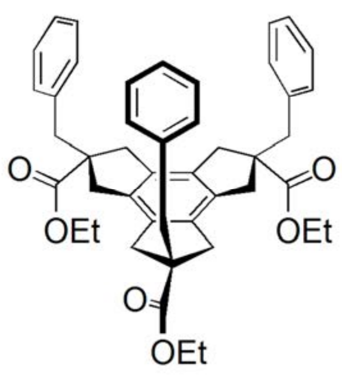
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Tripodal Trindane-based Anion Molecular Receptors with 2-aminobenzimidazole Recognition Motif for HSO_4^- Sensing

김원 최흥진[*]

경북대학교 응용화학과

Novel C_{3v}-symmetric tripodal anion receptors having guanidine recognition motif were synthesized from *cis,cis,cis*-2,5,8-tribenzyltrindane-2,5,8-tricarboxylate (1) condensing with 2-aminobenzimidazole. The C_{3v}-symmetric scaffold 1 has non-polar benzyl moieties on one side and polar ester moieties on the other side. These moieties were selectively functionalized to afford the C_{3v}-symmetric anion molecular sensors to recognize selectively and effectively towards the anions with C_{3v}-symmetric guests such as F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, HSO_4^-, NO_3^-, expecting shape-selectivity.Interestingly the tripodal receptor which has 2-aminobenzimidazole recognition motif showed a superior recognition towards $H_2PO_4^-$ by NMR titration, but selectively recognized with HSO_4^- emitting blue fluorescence under UV irradiation, which can be further developed to HSO_4^- selective fluorescent anion sensors. New compounds 2 with electron-donating or electron-withdrawing groups 5,6-disubstituted on benzimidazole moieties are being currently searched for more red-shifted fluorescence light emission in the visible range than the unsubstituted one.



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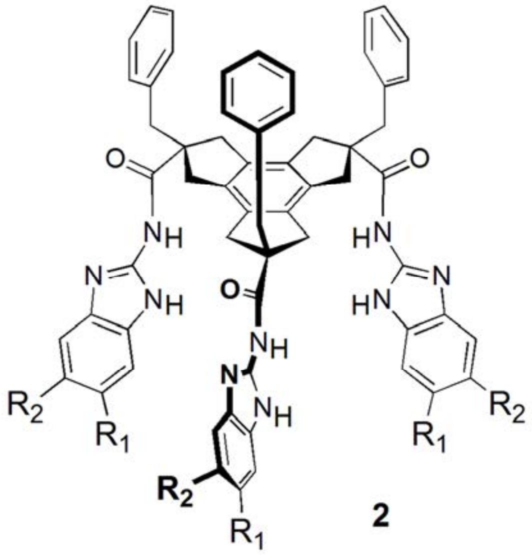

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일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-741**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Biomimetic Oranocatalytic Enantioselective Decarboxylative Aldol Reaction of Malonic Acid Half Thioesters to Trifluoromethyl Ketones

심재훈 송충의*

성균관대학교 화학과

We have discovered that cinchona-based bifunctional organocatalysts efficiently promote biomimetic decarboxylative Michael addition reaction[1] and aldol reaction[2] using malonic acid half thioesters (MAHTs) as enolate precursors (e.g., up to 99% yield and 99% *ee* in the Michael reaction of MAHT with nitroalkenes; up to 94% yield and 96% *ee* in the aldol reaction of MAHT with aldehydes).In this symposium, we present the first metal-free biomimetic enantioselective decarboxylative aldol reaction of MAHTs with various trifluoromethyl ketones using cinchona-based bifunctional organocatalysts to afford chiral β-trifluoromethyl β-hydroxy thioesters. A range of aromatic and nonaromatic trifluoromethyl ketones were smoothly converted into the corresponding aldol products in good to excellent yields and enantioselectivities (up to 91% *ee*). The simple and mild protocol for the synthesis of chiral β-hydroxy thioesters having a trifluoromethyl-substituted quaternary stereogenic center will lead to various applications in the field of medicinal chemistry.References 1. H. Y. Bae, S. Some, J. H. Lee, J.-Y. Kim, M. J. Song, S. Lee, Y. J. Zhang, C. E. Song, *Adv. Synth. Catal.* 2011, *353*, 3196.2. H. Y. Bae, J. H. Sim, J.-W. Lee, B. List, C. E. Song, *Angew. Chem. Int. Ed.* 2013, *52*, 12143.

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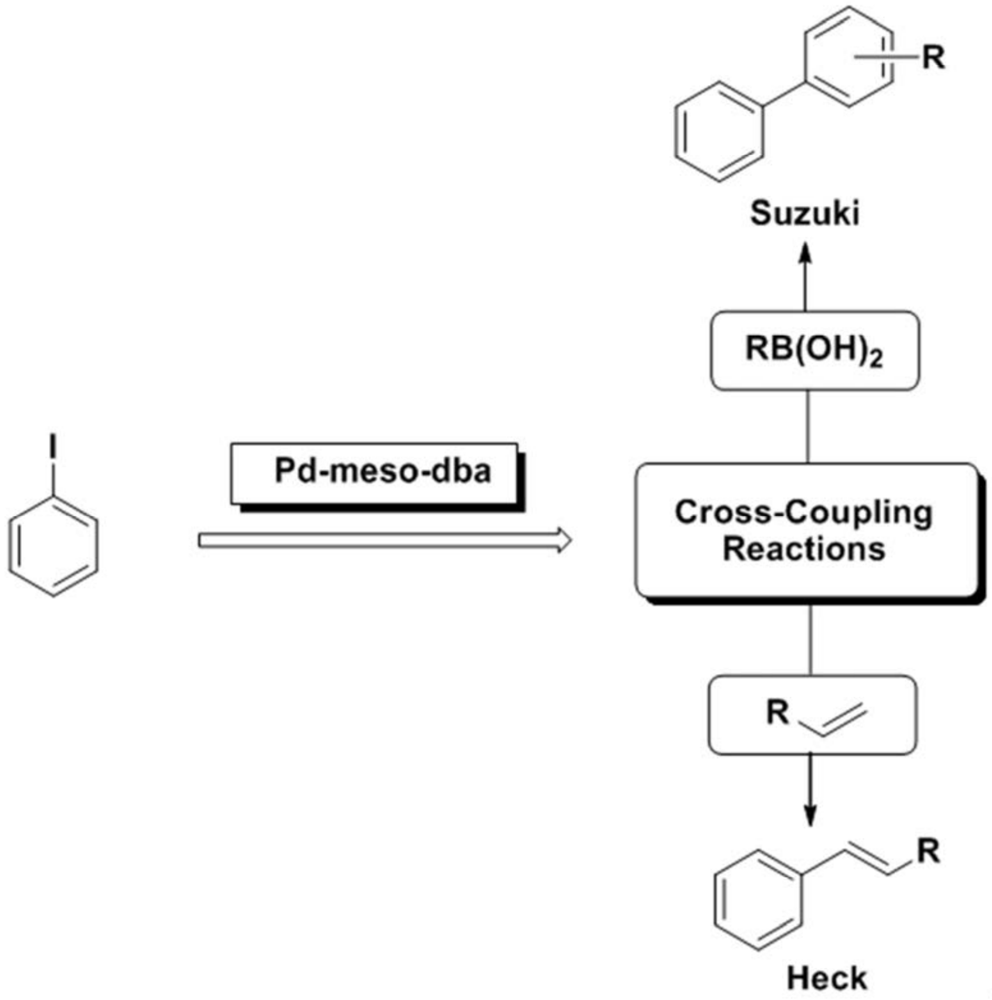
장소: 일산 KINTEX
발표코드: **ORGN.P-742**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Recoverable mesoporous catalyst Pd-Meso-DBA: Synthesis and applications

chirumarrysridhar 신동수*

창원대학교 화학과

SBA-15, mesoporous silica with different textural and structural properties have been synthesized and studied extensively recently. This substance meet the key factors for improved catalytic activity with distinguished properties such as high surface area, narrowly and highly ordered pore system, high hydrothermal stability and surface functionalities that present inside and outside of pores. These heterogeneous mesoporous silica supported catalysts achieve the catalyst-free product with better yield when compared with the conventional catalysts. We herein, present a new mesoporous silica based palladium(0) complex 'Pd-Meso-DBA', along with its applications towards Suzuki and Heck coupling reactions.


R
Suzuki
RB(OH)2
I
Pd-meso-dba
Cross-Coupling Reactions
R
R
Heck

일시: 2015년 4월 15~17일(수~금) 3일간
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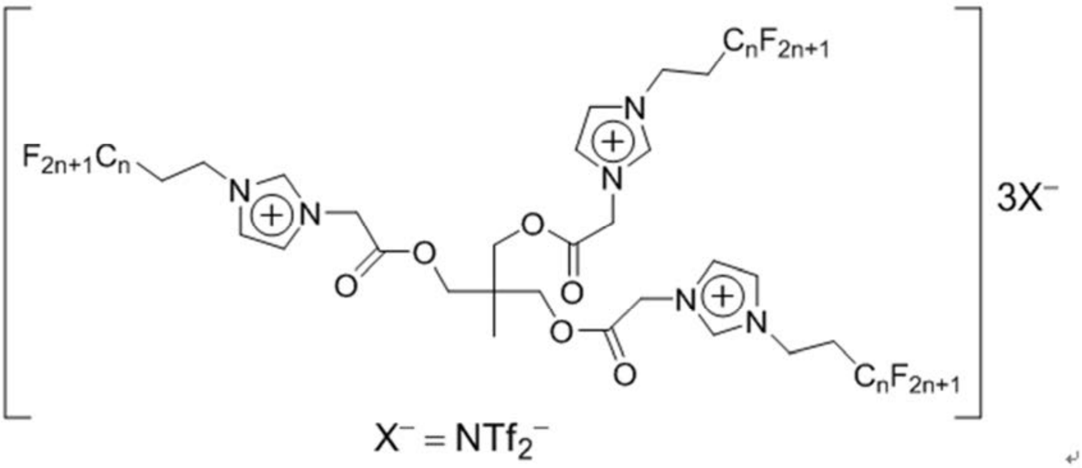
발표코드: **ORGN.P-743**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of novel hydrophobic fluorinated ionic liquids and its application

chirumarrysridhar 이태균 장지수 이동준 김한솔 신동수*

창원대학교 화학과

In this study, we reported the synthesis of series of novel tris-cationic ionic liquid surfactants containing ester groups formulated from imidazole cations with appended hemi fluorous tails form readily available starting materials in high yields and function as surfactants when added to conventional ionic liquids, facilitating the emulsification of fluoroalkanes with IL. Long hemifluornated 'ponytail' is attached to tris imidazolium cation prepared IL by starting from commercially available 1H,1H,2H,2H-nonafluorohexyl iodide, imidazole, chloroacetyl chloride and 1,1,1-tris(hydroxymethyl)ethane. Biodegradability and surfactants properties of the tris imidazaolium hemi fluorinated ionic liquids were investigated



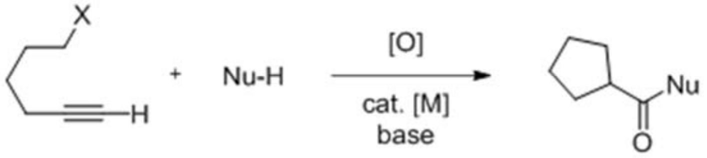
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-744**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Transition Metal-Catalyzed Oxidative α-Addition and β-Alkylation of Terminal Alkynes

윤희경 김인수 이철범*

서울대학교 화학부

We describe the transition-metal catalyzed cyclization and oxygenative nucleophilic addition of terminal alkynes. The reaction can be carried out with a broad range of nucleophiles such as alcohols and amines in the presence of a suitable base and oxidant. The proposed mechanism involves the formation of a disubstituted metal vinylidene intermediate via β-alkylation. This transformation can provide diverse ester and amide products while forming 5-membered cyclic ring moiety followed by transfer oxygenation to form a metalloketene which then undergoes nucleophilic addition.



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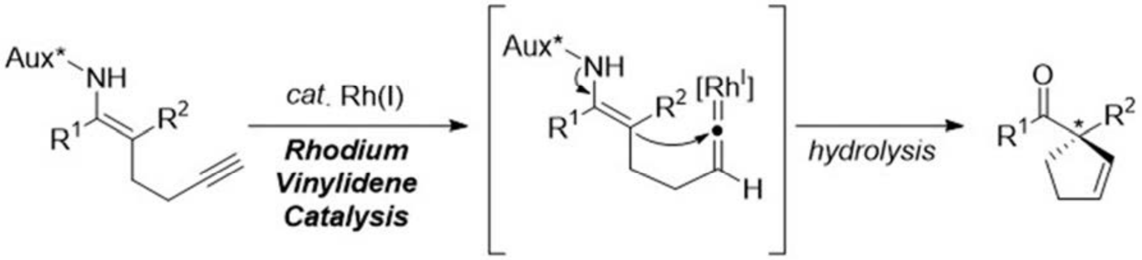
장소: 일산 KINTEX
발표코드: **ORGN.P-745**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium-Catalyzed Carbocyclization of Alkynylenamines for the Stereoselective Construction of Quaternary Carbon Centers

최경민 이철범*

서울대학교 화학부

In this poster, we present the asymmetric 5-endo-dig carbocyclization of alkynylenamines to construct cyclopentene derivatives with a quaternary carbon center. The reaction proceeds via a rhodium-vinylidene intermediate, which reacts with enamine nucleophile to form a C-C bond. The use of an enamine from a chiral primary amine enables asymmetric carbocyclization with high stereoselectivity. It is the first example of asymmetric C-C bond formation by rhodium-vinylidene-mediated catalysis that takes place through asymmetric 5-endo-dig carbocyclization with terminal alkyne.



일시: 2015년 4월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-746**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Regiochemistry-Directed Syntheses of Polyhydroxylated Alkaloids from Chiral Aziridine

최지혜 이원구[1,*] 하현준[*]

한국외국어대학교 화학과 [1]서강대학교 화학과

We have established a new method for the asymmetric synthesis of natural or unnatural polyhydroxylated alkaloids represented by calyculin fragment C_{33}-$C_{37}$and many azasugars and their analogs starting from form commercial chiral aziridine-2-carboxylate. The keys reactions contain stereoselective dihydroxylation, regioselective aziridine ring-opening reaction and double reductive amination of aziridine amine with ketone and aldehyde. Especially, different classes of compounds were elaborated from regioselectivity-directed branches of 2-substituted aziridine as a common synthetic intermediate into different rings such as pyrrole, piperidine pyrridizine and indolizine with specific examples of 1,4-dideoxy-1,4-imino-l-ribitol and analogs of hyacinthacine, swainsonine, catnospermine and deoxynojirimycin. We also established one-pot sequential reactions consisted of aziridine ring-opening, debenzylation and double reductive aminations from 2-[3,6(or 7)dioxo-1,2-dihydroxy]yl-aziridines to prepare 8-deoxyhyacinthacin and (3*R*)-methyl-8-deoxyswainsonine with remarkable stereoselectivity in high yield.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

CO_2 Fixation to Cyclic and Acyclic Carbonates

임유나 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Generally, carbonates were synthesized either by phosgenation using toxicity CO derivatives, oxidative carbonylation using transition metal complexs and CO, or synthetic protocols using CO_2. Specially, the use of carbon dioxide (CO_2) as a C1 building block for chemical synthesis has recently attracted much interest because of its abundance, cost-efficiency, nontoxicity, and high potential as a renewable source. Efficient and high-yielding synthesis of organic carbonates has been investigated due to wide usage of oranic carbonates as alkylation agents, carbonylation agents, fuel additives, electrolytes of lithium ion batteries, and monomers for the polymer synthesis. In this study, the direct coupling of carbon dioxide and alcohols for synthesis of cyclic and acyclic carbonates was achieved by using organic base and CH_2Br_2 in the absence transition-metal complexes and Mitsunobu-type reagents.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synethesis of N-Sulfenylimines by copper-catalyzed oxidative cross-coupling of amines and thiols

이찬 장혜영[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

Although sulfenylimines has been utilized in the preparation of N-sulfinylimines, N-sulfonylimines, β-lactams, vinyl formamides, and H2S-releasing reagents, the efficient and catalytic methods to prepare sulfenylimines have not been actively explored. Herein, an efficient copper-catalyzed aerobic coupling of amines and thiols to form N-sulfenylimines were reported. Using commercially available copper catalyst and oxygen as an oxidant, N-sulfenylimines were synthesized in good yields without over-oxidation to form sulfinylimines and sulfonylimines.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative esterification of allylic alcohol catalyzed by N-Heterocyclic carbene using TEMPO

강예원 장혜영[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

Using of organic oxidants, avoiding transition-metals appears very promising in terms of economic and environmental benefits. In particular, carbene-catalyzed oxidation using N-heterocyclic carbene and 2,2,6,6,-tetramethylpiperidine N-oxyl (TEMPO) is proposed for the synthesis of esters. In this study, we used TEMPO with a combination of catalytic amount of N-heterocyclic carbene and 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) for the one-pot oxidation/esterification of allylic alcohols. The effect of HFIP is to promote the rapid conversion of aldehydes to ester, resulting in high yields of oxidative esterification.

일시: 2015년 4월 15~17일(수~금) 3일간
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

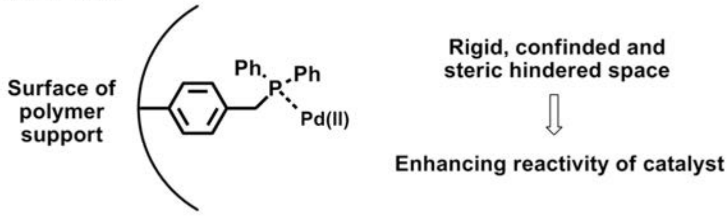
Highly ordered polymer supported phosphines as the ligands for organometallic reaction

김황석 이희윤*

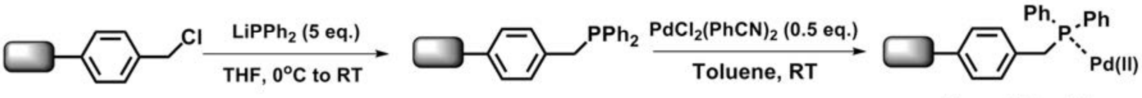
한국과학기술원(KAIST) 화학과

Palladium-catalyzed cross-couplings are widely used tools in organic synthesis. To utilize aryl chlorides with low reactivity, many elegant ligands for activating the palladium metal were reported. While those ligands have electron-rich, sterically bulky properties for elevating the reactivity of catalyst, they are air-unstable and require high cost or synthetic efforts. We envisioned that the phosphine on the highly ordered mesoporous polymer surface as the sterically hindered ligand could serve for activating palladium catalyst. This catalyst system facilitated the Suzuki cross-coupling of various aryl chlorides as well as the unreactive aryl bromides at room-temperature with high yields.

Conceptual view of idea

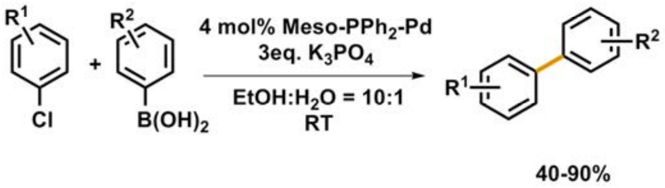


Simple preparation of catalyst



Meso-PPh$_2$-Pd

Catalytic activity of catalyst



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-751**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Cytotoxicity test of Isobenzofuran-1-(3H)-ones and Isoindolo[2,1-a][1,5]benzodiazepin-1,2-ones

김은비 이용균 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

In recent years, Isoindolin-1-one derivatives have been reported to possess diverse pharmacological properties, such as antihypertensive, antiulcer, anesthetic, and antipsychotic, as well as efficacy as vasodilatory agents. The alkaloids containing the isoindolin-1-one core unit have been received wide attention as they are found to be potent MDM2-p53 interaction inhibitors, and U-II receptor antagonists. Moreover, Isoindolin-1-ones are also used as the important synthons for the synthesis of various drugs and natural products. Also, 1,4-and 1,5-benzodiazepine scaffolds structures have already proven their utility in medicinal chemistry. Recent trends in drug discovery show an attempt to move away from flattened aromatic structures to their saturated counterparts. Implementation of this idea to 1,4 and 1,5-benzodiazepine scaffolds, as well as to their fused analogues gives rise to three-dimentional molecular frameworks which potentially might preserve the 'privileged' status of their aromatic preunsorp. Herein, we report two-step reaction sequence for the preparation of isoindolo[2,1-a][1,5]benzodiazepin-1,2-ones. In the first step, phthalaldehydic acid reacted with ketones to give isobenzofuran-1(3H).-ones Cyclization reaction of isobenzofuran-1-(3H)-ones with o-phenylenediamine or heteroaromatic diamines led to the formation of isoidolo-[2,1-a][1,5]benzodiazepin-1,2-ones.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

An activatable fluorescent probe for g-glutamyltranspeptidase in the murine model of colon cancer

박석안 김해조*

한국외국어대학교 자연과학대학 화학과

g-Glutamyltranspeptidase (GGT), as a cell surface-associated enzyme, has been reported to be overexpressed in liver, breast, and colon cancer. [1-3] Herein, we report a new activatable fluorescent probe from hemi-cyanine for selective and sensitive detection of the tumor-enridched GGT. The probe exhibited a dramatic fluorescence enhancement (F/F0 = 10 at 557 nm) upon the addition of GGT with a limit of detection of 0.15 mU/mL and was applied for the successful detection of colon cancer in the mouse model.Keywords: activatable fluorophore, colon cancer, colorimetric probe, cyanine, ?g?glutamyltranspeptidaseReferences[1]. Urano, Y., Sakabe, M., Kosaka, N., Ogawa, M., Mitsunaga, M., Asanuma, D., Kamiya, M., Young, M. R., Nagano, T., Choyke, P. L., Kobayashi, H. Sci. Transl. Med. 2011, 3, 110.[2]. Hou, X., Yu, Q., Zeng, F., Yu, C., Wu, S. Chem. Commun. 2014, 50, 3417. (a) Curr. Neurovasc. Res., 2011, 8, 258 (b) Clin. Toxicol. 2011, 49, 471[3]. Fiala, S., Trout, E., Pragani, B., Filala, E. S. Lancet 1979, 313, 1145

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An activatable fluorescent probe for targeting cellular membrane through the biothiol-mediated hydrazone-to-pyrazole transformation

나상윤 김해조[1,*]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

Biological thiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) play essential roles in maintaining cellular redox homeostasis.[1] Among the biothiols, GSH exists in cells at a high concentration of about 5 mM and plays a critical role as an antioxidant in animals.[2] Abnormal levels of GSH, however, exhibit a severe resistance against cancer therapy.[3] Therefore, it is of growing importance to monitor the level of GSH in living cells. A nonfluorescent coumarin-hydrazone conjugate probe was transformed into a strongly fluorescent pyrazolyl coumarin through a thiol-mediated cyclization reaction with F/F0 50. Interestingly, the probe was initially expressed at the cellular cytoplasm but translocated into the membrane regions of cells upon reaction with cellular enriched glutathione, which allowed us to obtain clear membrane imaging in the living cells. References[1]. (a) Dalton, T. P.; Shertzer, H. G.; Puga, A.; Annual Review of Pharmacology and Toxicology, 1999, 39, 67; (b) Wu,G.; Fang, Y. Z.; Yang, S.; Lupton, J. R.; Turnur, N. D.; Journal of Nutrition, 2004, 134, 489.[2]. Lushchak, V. I.; Journal of Amino Acids, 2012, 2012, 736837.[3]. Seshadri, S.; Beiser, A.; Selhub, J.; Jacques, P. F.; Rosenberg, I. H.; D'Agostino, R. B.; New England Journal of Medicine, 2002, 346, 476.

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Mitochondria Targeting Iron Oxide Nanoparticles in NIR triggered Hyperthermia

정효성 이재홍 엄수진 김형석 정유진[1] 이지하[2] 정종화[2] 강철훈[3] 김종승[*]

고려대학교 화학과 [1]고려대학교 유기화학 [2]경상대학교 화학과 [3]경희대학교 동서의학대학원

Mitochondria are organelles that are readily susceptible to temperature elevation. We prepared a new mitochondria-targeting iron oxide NP fabricated with two functional groups: TPP as the mitochondrial targeting unit and coumarin as a fluorescent signalling unit. Upon irradiation with a 740 nm NIR laser at 2.0 W/cm2, the solution temperature of Mito-CIO was increased by 13 °C, whereas no such changes occurred in an NP-free solution. Laser irradiation of HeLa cells incorporating Mito-CIO increased the cellular temperature by 2.1 °C within 5 min. In HeLa cells, Mito-CIO and CIO were localized to the mitochondria and the ER, respectively. Mito-CIO induced significantly more cell death after 20 min NIR irradiation than did CIO, and the differential cytotoxicity can be attributed to the mitochondrial localization of NPs. Furthermore, in vivo therapy using mitochondria-directed hyperthermia clearly displayed tumour suppression, which is in agreement with the in vitro cytotoxicity results. Together, these results strongly support our hypothesis that mitochondria are more susceptible to hyperthermia than the ER. From this study of both the in vitro and in vivo effects of mitochondria-targeted MPs, we conclude that this heat generating system can enhance the therapeutic efficacy of hyperthermia in cancer treatment and may allow the development of new photothermal therapeutics.

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Synthesis of Unsymmetrical Fr?chet-type Dendrimers using dual click chemistry

김소연 이재욱*

동아대학교 화학과

Click chemistry, which is the Cu(I)-catalyzed Huisgen [2+3] 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 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 groups. Therefore, the click chemistry as a concept of simplifying synthesis is very useful tool to produce functional polymers and dendrimers. In addition, Staudinger/aza-Wittig reactions (new click reaction) are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Recent investigation of the click chemistry, the Staudinger/aza-Wittig reaction between an organic azide and an aldehyde, has attracted attention which has found many applications in organic chemistry, materials science and synthesis of various dendrimers. Taking advantage of these facts, herein we will use the first click reaction (Staudinger/aza-Wittig reaction) leading to the alkyne-functionalized Fr?chet monodendrons containing the benzene at a core, and then will use the second click reaction (1,3-dipolar cycloaddition reaction) with azide-dendrons leading to the formation of unsymmetrical Fr?chet-type dendrimers.

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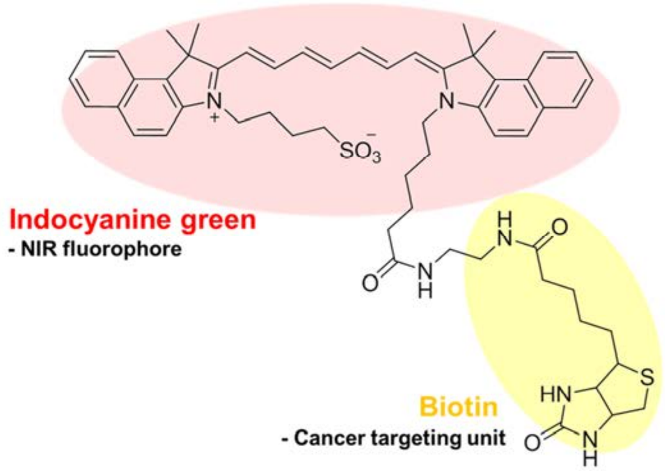
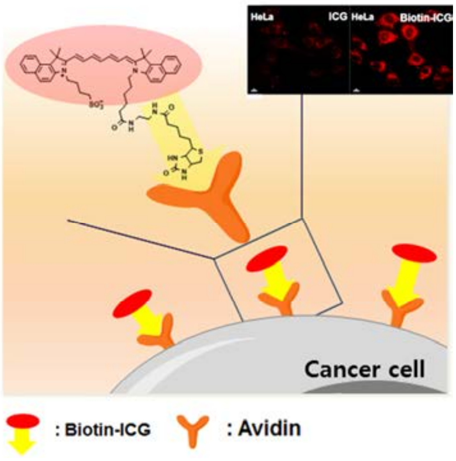
Targeted Imaging of Cervical Cancer Cells Using The Biotin conjugated Indocyanine Green (Biotin-ICG)

엄수진 정효성 김원영 김형석 최주아 김종승*

고려대학교 화학과

In clinical practice, the major method to treat cancer is surgical resection. In that sense, precise spatial discrimination between cancer and healthy tissue is the main issue. To reach this goal, image guided cancer surgery using near-infrared (NIR) fluorescence has emerged as attractive approach. Among NIR fluorophores, which provide advantages of improved contrast and deep tissue penetration, only indocyanine green (ICG) is approved by FDA for clinical use. However, ICG is limited by a lack of target specificity. Herein, we present the design, synthesis and contrast efficacy of a novel tumor targeted NIR contrast agent, Biotin-Indocyanine green (Biotin-ICG), which can specifically target the cancer cell. The intracellular uptake experiments prove that the targeting efficacy of the Biotin-ICG was more effective than that of free ICG in biotin receptor-positive HeLa tumor cells. Furthermore, the results from cell viability tests also confirm that Biotin-ICG did not show any cytotoxicity.





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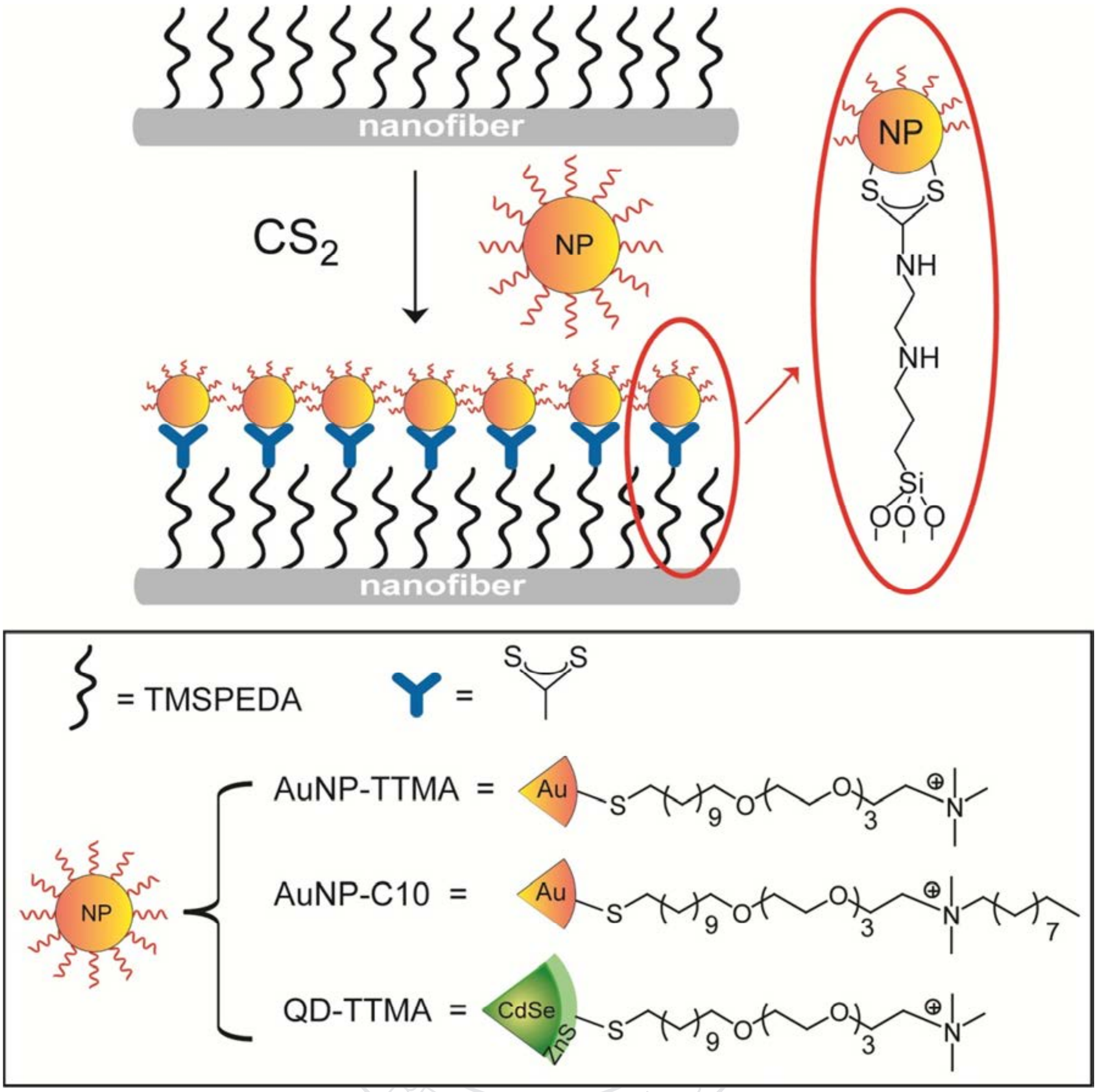
Fabrication of functional nanofibers through post-nanoparticle functionalization

정은희* Yi-Cheun Yeh[1] Vincent M. Rotello[1]

강릉원주대학교 화학신소재학과 [1]University of Massachusetts Amherst, U.S.A.

A facile method has been developed to functionalize nanofiber surfaces with nanoparticles through dithiocaramate chemistry. Gold nanoparticles (AuNPs) and quantum dots (QDs) have been immobilized on nanofiber surface. These surfaces provide scaffolds for further supramolecular functionalization, as demonstrated through FRET pairing of QD-decorated fibers and fluorescent proteins.


nanofiber
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NP
nanofiber
NP
S
S
NH
NH
Si
O O O
= TMSPEDA
=
S
S
AuNP-TTMA =
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AuNP-C10 =
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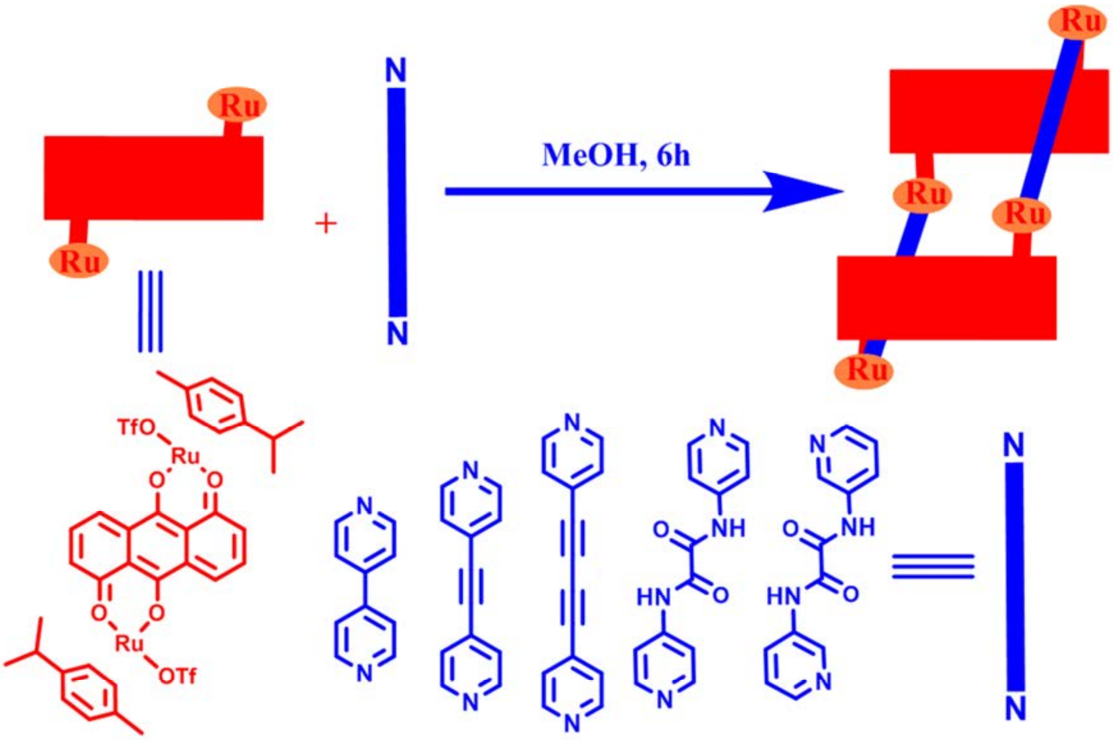
Coordination-driven self-assembly of molecular parallelograms incorporating pyridyl donors and a new Ru(II) *p*-cymene acceptor

SINGH NEM 송영호 지기환*

울산대학교 화학과

In the past two decades, coordination-driven self-assembly has emerged as an effective tool for constructing functionalized metalla-supramolecules with promising applications such as molecular recognition, separation, catalysis and encapsulation of various guests. In the search for new building blocks for the synthesis of supramolecular archetectures with modified properties, there has been an increasing interest in using bimetallic transition metal complexes. The present work demonstrates the use of a newly designed Ru(II) *p*-cymene acceptor for spontaneous formation of molecular parallelograms by its coordination-driven self-assembly with various linear pyridyl donors (scheme 1). The resulting supramolecular parallelograms have well-defined internal cavities to stack large guest molecules. All the new complexes have been characterized by various spectroscopic and single crystal X-ray diffraction. The poster will address a detail comprehensive account of the mentioned work.



Scheme 1: Synthetic route to the self assembled metall-parallelograms

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DOSY and 2D ROESY NMR spectroscopy in the characterization of coordination-driven self-assembled architectures

송영호 **SINGH NEM** 지기환*

울산대학교 화학과

NMR spectroscopy is a unique and powerful methodology for the characterization of self-assembled architectures. The classic 1D NMR spectra provide evidences about complexation-induced chemical shifts and the symmetry of architecture. However, it is unable to provide evidences about whether the assembly is 1+1, 2+2 or 3+3 architecture. Conventional 2D NMR experiments, especially NOESY and ROESY have opened new perspectives by efficiently detecting interactions within or between the molecules. DOSY NMR experiment provide concrete evidence about the size and number of components available in the solution. The poster will address comprehensive applications of the ^{1}H-^{1}H ROESY and DOSY NMR spectroscopy in the detection of mono and catenane structures and in host-guest interactions.

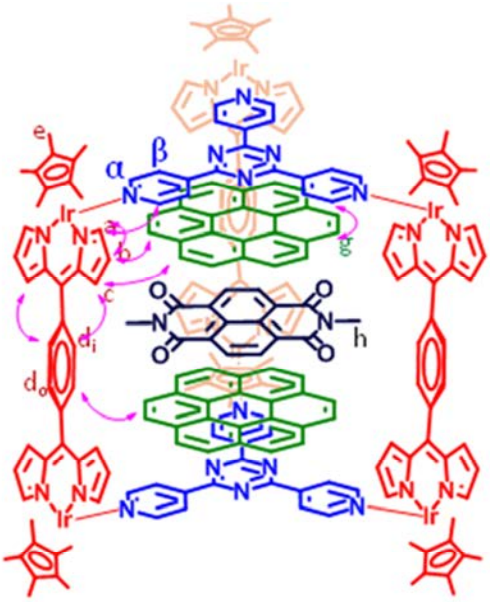

Figure 1: Pink arrow showing observed coupling interactions in ^1H-^1H ROESY NMR spectrum in a host-guest archetecture

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Immobilizing fluorescent material onto silica surface by NHS-functionalized methallylsilane

김수현 심용균 전철호*

연세대학교 화학과

Organic-inorganic hybrid material is interesting material that has both organic and inorganic character. This organic-inorganic hybrid material has the adventage that overcome individual limit. We can use mesoporous silica as an inorganic material which is used for immobilizing fluorescent material (N-dansylethylenediamine) by NHS-functionalized methallylsilane. Immobilization ratio can be easily determined directly by elementary analysis. We developed three immobilization methods: grafting method, chemical modification(CM) method, purified chemical modification(PCM) method. Grafting method is immobilization of NHS-functionalized coupling reagent onto silica surface, followed by reacting the fluorescent material onto silica surface. CM method is to react fluorescent material with coupling reagent first, and then to immobilize this modified coupling reagent onto silica surface. In this protocol, excess coupling reagent, which is redundant, can be readily discarded (purification) by following process. This purification process can be carried out by using scavenger. This purification method is called PCM method. For these new protocols, facile preparation of organic-inorganic hybrid materials can be possible.

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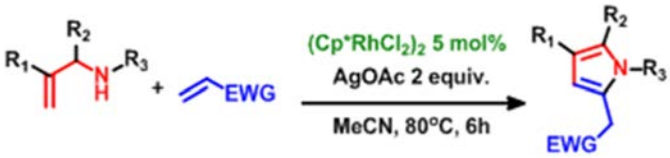
Synthesis of Multi-substituted Pyrroles via Rh(III) catalyzed N-annulation

서용식 김동수 전철호*

연세대학교 화학과

N-heterocyclic compounds are one of interesting compounds due to their biological activities. Particularly, pyrrole is used as building block for the synthesis of valuable drugs. For this reason, it is desirable to develop synthetic methods of multi-substituted pyrrole from simple starting materials. Recently we successfully developed synthetic methods of N-hetrocyclic compounds such as isoquinoline, pyridine via Rh(III)catalyzed N-annulation. Using the same catalytic system, we devise an efficient synthetic method of multi-substituted pyrrole compounds from simple allylamines and olefins having an electron withdrawing group. This new synthetic methods proceed via unreactive C-H bond activation by transition metal catalyst. This mew protocol has many advantages in term of atom-economy, efficiency and selectivity.



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Bis-ureidoquinoline as a Selective Fluoride Anion Sensor through Hydrogen-Bond Interactions

조윤희 조동규*

인하대학교 화학과

Bis-ureidoquinoline shows a characteristic UV-vis absorbance and turn-on fluorescence changes in the presence of the fluoride anion. Such selective changes probably originate from the hydrogen-bond interactions, as shown by the ^{1}H NMR titration and DFT calculations. Bis-ureidoquinoline can be used as a fluoride-selective sensor for the detection of fluoride anions under illumination from a laboratory hand-held UV lamp.

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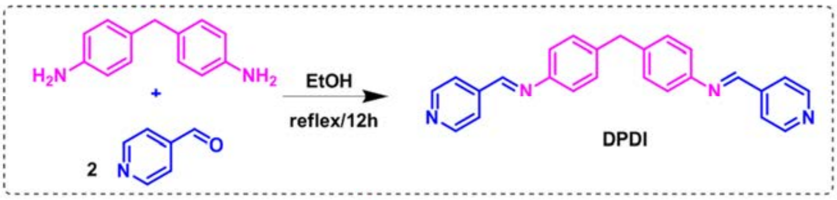
Organometallic Ruthenium(II) Supramolecular Self-assemblies of Dipyridyl-Diimine Based N,N-donor

PALANIELUMALAI <u>김동환</u> 지기환*

울산대학교 화학과

The design of metalla supramolecules is of enduring interest because of their importance in basic supramolecular chemistry and crystal engineering and their potential uses in functional materials, sensing applications, transportation processes and biodicinal chemistry. In particular, the organometallic based metallacycles are promising candidates for the above mentioned applications. However, the biological applications such as cytotoxicity, cellular uptakes, bioimaging studies and anti-tumor properties of the organometallic self-assembled coordination complexes (SCDCs) are scare. The SCDCs constructs by a multible of metal acceptors and suitable organic donors ligands and have extended beyond a simple two-component paradigm to encompass selective self-assembly, in which multiple assemblies form from a mixture of subunits, to multicomponent assemblies.[1-4] Herein, we report the dipyridyl-diimine based ligand with arene ruthenium based supramolecular self-assemblies. The arene-ruthenium supramolecular architectures were achieved from flexible dipyridyl-diimine(DPDI) and organometallic arene ruthenium acceptors(A-D).



Ruthenium (II) aceptors

References:

[1] Cook, T. R.; Vajayee, V.; Lee, M. H.; Stang, P. J.; Chi, K-W. *Acc. Chem. Res.* **2013**, *46*, 2464.

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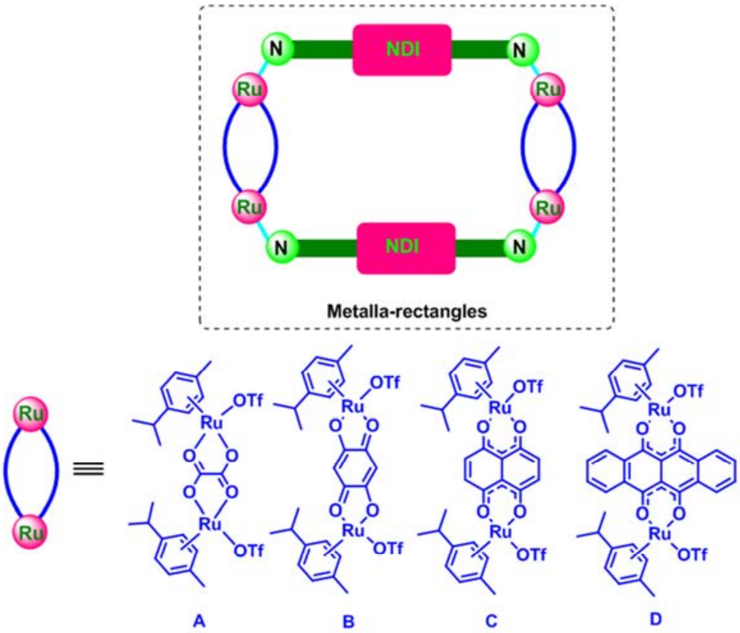
Ruthenium(II) Supramolecular Self-assemblies of Rigid Dipyridyl Based Naphthalene Diimides: Synthesis and Structural Aspects

PALANIELUMALAI 김태근 지기환*

울산대학교 화학과

Fascination with supramolecular coordination self-assemblies (SCDSs) over the last few decades has led to the synthesis of an ever-increasing number of elegant and intricate functional structures with sizes that approach nanoscopic dimensions. The design and synthesis of SCDSs via the rational combination of bridging multidentate ligands with various platinum group metal ions (Pt, Pd, Ru, Rh, Ir and Os) are of intense interest in the current field of supramolecular chemistry, and many complexes have been constructed in this aspect to exhibit either appealing architectures or encouraging the chemical properties such as biomedicines, catalysis, photoluminescence, sensors and nano material devices.[1-4] Herein, we report the series of supramolecular self-assembled metalla-rectangles of arene-ruthenium acceptor with rigid naphthaline diimide ligand. The organometallic arene-ruthenium based metalla cycles architectures were achieved from the arene-ruthenium acceptors (A-D) and meta-pyridyl based ditopic napthaline diimide N,N-donor (NDI)



Ruthenium (II) aceptors

References:

[1] Han, Y-F.; Jin, G-X. *Chem. Soc. Rev.* **2014**, *43*, 2799.
[2] Mukherjee, S.; Mukherjee, P. S. *Chem. Commun.* **2014**, *50*, 2239.
[3] Cook, T. R.; Vajayee, V.; Lee, M. H.; Stang, P. J.; Chi, K-W. *Acc. Chem. Res.* **2013**, *46*, 2464.
[4] Dubey, A.; Min, J. W.; Koo, H. J.; Kim, H.; Cook, T. R.; Kang, S. C.; Stang, P. J.; Chi, K.-W. Chem. Eur. J. **2013**, *19*, 11622.

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Reductive amination of aldehydes by hantzsch ester using S-benzyl isothiouronium iodide

이민희 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

Reductive amination of carbonyl compounds is one of the most powerful methods for a C-N bond formation. Hantzsch ester has proven to be a powerful reductive reagent and solve some of the problems encountered with the traditional reductive reagents. However, in some cases, this reducing agent was found to be ineffective without catalysis. Previously, thiourea catalysts were the best in this mechanism. Recently S-benzyl isothiouronium has been reported as more effective catalyst which makes NH parts more acidic than thioreuas accelerating reaction rate. In this presentation we will discuss the molecular design of isothiouronium compounds and organocatalytic effectiveness.

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Synthesis of Ethoxy Dibenzooxaphosphorin Oxides via Palladium-Catalyzed C-H Bond Activation/C-O Bond Formation

신서현 손정유 이필호*

강원대학교 화학과

Unreactive $C(sp^2)$-H and $C(sp^3)$-H bonds are ubiquitous in organic compounds, so that the development of methods for the transition metal-catalyzed C-H activation is one of the challenging goals in organic synthesis. so that the development of methods for the transition metal-catalyzed C-H activation is one of the challenging goals in organic synthesis. Recently, a variety of C-H activations by using new phosphoryl-related directing groups have been reported by our and other groups. We have developed an efficient synthetic method for a wide range of ethoxy dibenzooxaphosphorin oxides starting from 2-(aryl)arylphosphonic acid monoethyl esters and employing Pd-catalyzed $C(sp^2)$-H activation/C-O formation under aerobic condition.

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The direct reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes using S-benzyl isothiouronium iodide as an organocatalyst with Hantzsch ester

이하늬 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

Hantzsch esters have proven to be a powerful reductive agent, because they overcome some of the problems encountered with traditional reductive reagents such as hydrogen gas/metal and metal hydrides, for instance, their limitations in the case of sensitive, acid-labile, or polyfuntional substrates. However, in some cases, this reducing agent was found to be ineffective without catalysis. Isothiouronium salts have been explored recently as a new class of hydrogen-bonding subunit as thioureas. Isothiouronium group has more advantages because it enhances the NH acidity compared to the corresponding thiourea.S-benzyl isothiouronium iodide has been successfully developed as a novel class of noncovalent organocatalyst for the direct reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes. A wide range of aldehydes amines as well as nitroalkenes were found to give the expected products in moderate to excellent yields and short times. The isothiouronium catalyst has certain valuable charateristics such as high hydrogen-bonding propensity and the ability to be recovered and reused.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Method of Benzooxaphosphorinanone Oxides through Palladium-Catalyzed Carbonylation

신서현 최원석 이필호*

강원대학교 화학과

Because inhibition of β-lactamases remains a practical method to maintaining the efficacy of β-lactam antibiotics, the investigation for inhibitors of these enzymes has continued during the past 80 years. Since the cyclic phosphonates have been known to be reversible covalent inhibitors of the P99 β-lactamase, a new synthetic approach to these compounds was required. So, we have developed an efficient phosphaanuulation by Pd-catalyzed carbonylation of C-H bonds of phosphonic and phosphinic acids, leading to the construction of oxaphosphorinanone oxides, which are novel phosphorus heteocyclic privileged structures. Thus, this transformation opens a new avenue to sequential C-C/C-O bond formation in one pot vecause carbon monoxide represents an economical and atom efficient C1 building block.

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Metal-Free Azaphosphaannulation of Phosphonamides via Oxidative C-N Bond Formation

서보람 신서현 이필호*

강원대학교 화학과

Organophosphorus compounds have been broadly used in agricultural and pharmaceutical chemistry and material science, development of an efficient synthetic method for these compounds has been continuously required. In this regard, we were interested in transition-metal-catalyzed C-H activation/C-N bond formation and developed a Rh-catalyzed C(sp^2)-H activation/annulation and oxidative alkenylation/aza-Michael reaction directed by phosphonamide and phophinamide groups. We report an efficient metal-free azaphosphaannulation of myrid of phosphonamides through intramolecular oxidative C-N bond formation using $PhI(OAc)_2$ and iodine in acetonitrile under air, thus leading to the formation of benzazaphosphol-3-one 1-oxides, which are novel phosphorus heterocyclic privileged structures.

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Diastereoselective Synthesis of Tetrahydrofurano- and Hexahydropyrano-dihydropyrroles Containing *N*,*O*-Acetal Moieties through Rhodium-Catalyzed Transannulation of Alkynes, Sulfonyl Azides, and Oxacycloalkenes

김철의 신서현 이필호*

강원대학교 화학과

Rh-catalyzed [3 + 2] cycloaddition using iminocarbene intermediates derived from *N*-sulfonyl triazoles is well established. In this regard, we have developed a method for synthesis of pyrroles from the transannulation of *N*-sulfonyl triazoles with alkenyl alkyl ethers/elimination reaction. Tetrahydrofuranodihydropyrroles (THF-DPs) and tetrahydropyranodihydropyrroles (THP-DPs), which combine two unique heterocycles of dihydropyrroles and oxacycloalkanes, are valuable privileged structural motifs found in natural products. Herein, we have reported a diastereoselective synthetic method of tetrahydrofuranodihydropyrroles and tetrahydropyranodihydropyrroles containing *N*,*O*-acetal moieties *via* Rh-catalyzed denitrogenative transannulation of *N*-sulfonyl-1,2,3-triazoles with oxacycloalkenes. A myriad of functionalized pyrroles bearing hydroxyalkyl moieties at C3-position could be prepared *via* Rh-catalyzed denitrogenative transannulation/acid-catalyzed ring-opening reaction.

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Hetero Aromatic Oligomers : Synthesis, Characterization and Properties

김영선 김종현 김인태*

광운대학교 화학과

Conjugated polymers have emerged as an important material for numerous applications in the photovoltaic devices, light emitting diodes (LEDs), field effect transistors (FETs), and electrochromic devices, etc. Conjugated oligomers show similar properties to conjugated polymers, with certain advantages including their well-defined structure, the possibility to introduce functionalities, easier purification, and fewer defects. In this work, we synthesized several oligomers and observed their properties. The structure of the compounds was ascertained by 1H NMR,13C NMR, and FT-IR spectroscopy. We also observe UV/Vis absorption, photoluminescence(PL) spectra for the synthesized the compounds. Through this work, we can find the possibilities of hetero aromatic oligomers for organic photovoltaic devices (OPVs).

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Synthetic Method of 2-Aryl-2*H*-benzotrizoles from Azobenzenes and *N*-Sulfonyl Azides Catalyzed by Rhodium

최원석 손정유 이필호*

강원대학교 화학과

Development of synthetic methods of 2-aryl-2*H*-benzotriazole derivatives from easily accessible reactants is highly significant because it is an essential component of pharmaceuticals, UV stabilizers, and organic electronic materials. Because benzotirazoles exist as N^1-, N^2-, and N^3-substituted isomers, the selective preparation of benzotriazole represents an important synthetic challenge. Although a variety of synthetic methods for N^1-arylation of benzotriazole have been reported, a selective N^2-arylation of benzotriazole is still needed. For this reason, the selective synthesis of 2-aryl-2*H*-benzotriazoles has been continuously in demand. In our continuing efforts to develop efficient C-H activations, we report herein an efficient synthetic method for 2-aryl-2*N*-benzotriazoles from azobenzenes and *N*-sulfonyl azides through sequential Rh-catalyzed amidation (C-N bond formation) and oxidation (N-N bond formation) with $PhI(OAc)_2$ in one pot.

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Synthesis of Dihydroazepines and Dihydropyrroles from *N*-Sulfonyl-1,2,3-triazoles with 1, 3-Dienes through Aza-[4+3] and Aza-[3+2] Annulations

김철의 최원석 이필호*

강원대학교 화학과

Azaheterocycles are a highly important class of compounds due to their biological activities and pharmaceutical usabilities. In particular, dihydroazepines, dihydropyrroles, and pyrroles are constituents of a valuable privileged structure in organic chemistry. For this reason, the development of efficient synthetic methods of multi-substituted azaheterocyclic compounds from simple and easily accessible starting materials has been continuously required. Now, we report an efficient aza-[4 + 3] annulation and aza-[3 + 2] annulation starting from terminal alkynes, sulfonyl azides, and 1,3-dienes in a one-pot.Recently, 1-sulfonyl-1,2,3-triazoles easily prepared from copper-catalyzed 1,3-dipolar cycloaddition of terminal alkynes with sulfonyl azides have been extensively investigated as precursors of α-imino metal carbenes. High reactivity of α-imino metal carbenes toward nucleophiles is caused by intrinsically electrophilic properties of the metal carbene species. In addition, it can react with electrophiles because the α-imino group having nitrogen atom is inherently nucleophilic. Accordingly, these amphiphilic α-imino metal carbenes smoothly react with nitriles, alkynes, allenes, isocyanates and isothiocyanates, furans, aldehydes and imines, α,β-unsaturated aldehydes, indoles, arenes, alkenes, amides, and furans to afford a multitude of heterocycles. More recently, we have reported that the reaction of triazoles with alkenyl alkyl ethers give rise to pyrroles through the corresponding dihydropyrroles. Next, we were interested in whether 1,3-diene can act as the dipolarophile to construct a dihydroazepine and dihydropyrrole scaffold.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-TBAF-Catalyzed C-N Formation of Sulfoximines with Aryl Siloxanes

최원석 신서현 이필호[*]

강원대학교 화학과

An efficient copper-TBAF-catalyzed C-N bond formation of sulfoximines with arylsiloxanes in dichloromethane at room temperature, affording the desired *N*-aryl sulfoximines in good to excellent yields under an oxygen atmosphere, is reported. The present method complements the previously reported synthetic approaches due to some advantageous properties of aryl siloxanes such as availability, low toxicity, ease of handling, high stability, and environmentally benignity under mild conditions, thus opening a new approach to practical C-N bond formation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Tumor targeted phototherapeutic topoisomerase inhibitor: programmed activation of cancer cell apoptosis

신원섭 장주희 구세영 최주아 이동엽 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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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of Rhodamine-labelled dieckol as an anti-inflammatory agent

구세영 이재홍 장주희 신원섭 이봉호[1] 김종승[*]

고려대학교 화학과 [1]한밭대학교 응용화학생명공학부

Dieckol, belonging to a special class of natural polyphenols called phlorotannins, is isolated from several brown algae of genus Eisenia and Ecklonia. Dieckol has been reported to show various biological activities, such as anti-inflammatory, antioxidative, hepatoprotective, anti-diabetic, anti-allergic, antiviral and anticancer activities. Since dieckol has shown various biological activities, we introduced a rhodamine fluorophore into dieckol by a click reaction to investigate its local ization within living cells using confocal laser microscopy. We also evaluated the levels of inflammatory mediators such as NO, TNF-a, and IL-6, and intracellular signal pathways like MAPK and NF-kB activation in LPS-stimulated RAW 264.7 macrophages. Rhodamine B-labelled dieckol (Compound 1) was mainly located in the ER and it strongly regulated inflammatory mediators such as NO, TNF-a, and IL-6, and intracellular signal pathways like MAPK and NF-kB activation in LPS-stimulated RAW 264.7 macrophages. The anti-inflammatory activity of 1 was found to be considerably stronger than that of dieckol itself. According to the ER distribution of 1 and its potent anti-inflammatory activity, it is predicted to be an effective treatment of inflammation or inflammation-related disease.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Challenges in Designing Organelle-Selective Water-soluble Fluorescent Sensors for Cu(II)

이윤학 선우경 김창회 김원영 정유진[1] 김종승*

고려대학교 화학과 [1]고려대학교 유기화학

A novel water-soluble fluorescent naphthalimide derivative as a sensor for Cu(II) has been synthesized. The sensor, conjugated with DPA (as the Cu(II)-binding moiety) and TPP (as the mitochondrial-targeting moiety) was further decorated with a galactose unit at the fluorophore’s terminal using the click reaction. Although confocal fluorescence imaging revealed that probe 1 was not localized in mitochondria, and was neither quenched under Cu-overloading conditions, the probe 1 did exhibit a high selectivity for Cu(II) ions over various metal ions in HEPES-buffered solutions. Furthermore the fluorescence was dramatically quenched upon the addition 1 equivalent of Cu(II), and the response was stable in the range of pH 6-10.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly selective two-photon fluorescent probe for cysteine detection and its application in live cell imaging

선우경 이윤학 김창회 이동엽 김종승*

고려대학교 화학과

In the past few decades, intracellular biothiols such as cysteine (Cys), homocysteine (Hcy), glutathione (GSH) have drawn great attention because of the significant roles in biological systems. Among thiols, cysteine is most essential in protein synthesis, cellular detoxification, and post-translational control. The detection of intracellular cysteine level in cancer cells would be a fundamental and significant approach for discovering correlation between its concentration and pathogenesis. It is highly desired to develop a novel fluorescence probe that can distinguish cysteine from other biothiols, moreover can be monitored by the two-photon fluorescence spectroscopy. Herein, we present a novel two-photon fluorescent probe for cysteine which is highly selective over Hcy and GSH consist of a chromene fluorophore and the selective reaction site for cysteine.

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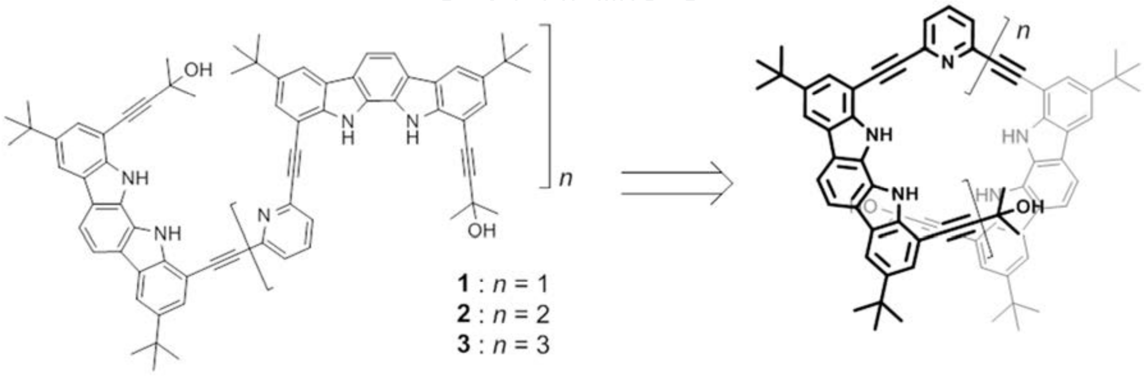
발표종류: 포스터, 발표일시: 수 16:00~19:00

Folding Features of Indolocarbazole-pyridine Foldamers

전해근 정규성*

연세대학교 화학과

Indolocarbazole-pyridine foldamers 1-3 were prepared by connecting indolocarbazoles and pyridines alternatively through ethynyl spacers by Sonogashira reactions. Computer modeling studies suggest that the foldamers fold into a helical conformation with an internal tubular cavity. All the existing indolocarbazole NHs and pyridine nitrogen atoms are convergent in the cavity, which is energetically favorable owing to dipole-dipole interactions. The helical folding of 3 was unambiguously determined by single crystal X-ray diffraction which showed three water molecules entrapped in the cavity forming multiple hydrogen bonds. These folding features were also probed by 1D-, 2D-^{1}H NMR, and UV-visible spectroscopy. Details will be described in the poster presentation.



일시: 2015년 4월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-780**
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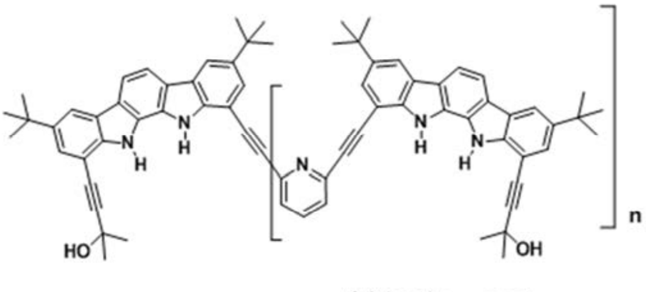
발표종류: 포스터, 발표일시: 수 16:00~19:00

Helical foldamers based on indolocarbazole and pyridine

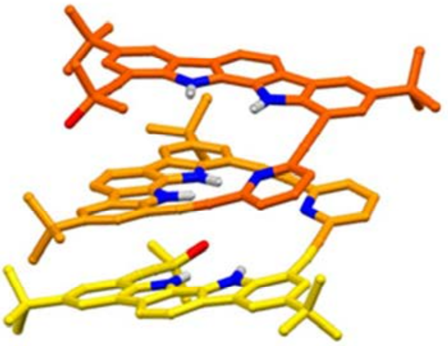
정진영 정규성*

연세대학교 화학과

We have designed and prepared helically foldable synthetic oligoindolocarbazoles, which are linked by pyridine. The single crystal X-ray structure of trimer (1) shows that indolocarbazole NH and pyridyl nitrogen are placed in the same direction owing to dipole-dipole interaction, and it gives rise to preference of helical conformation. According to ^{1}H NMR spectroscopic study, pentamer (2) folds into helical structure in dichloromethane but the unfolded conformation is predominant in the presence of dimethyl sulfoxide. Helical foldamers of this type afford an internal cylindrical cavity surrounded by multiple hydrogen bond donors for anions. Consequently, pentamer (2) transports chloride ion across a POPC membrane by a channel mechanism, while trimer (1) does not due to short length of chain. Details will be described in the presentation.



1 (trimer) : n = 1
2 (pentamer) : n = 2



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발표코드: **ORGN.P-781**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

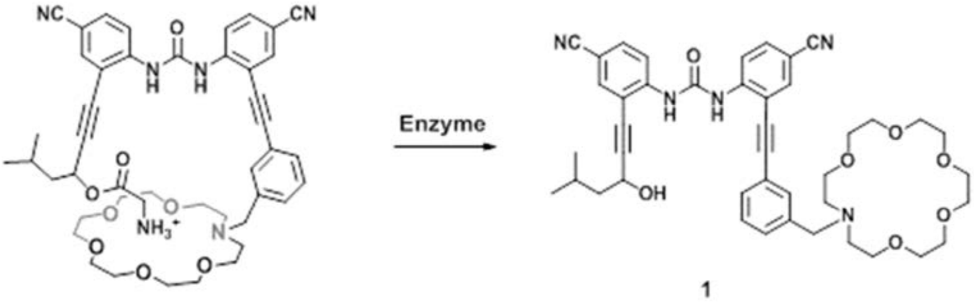
Stimuli-responsive Synthetic K-Cl Cotransporters via Symport

김지선 정규성*

연세대학교 화학과

Potassium chloride co-transporters (KCCs) are a class of important regulators of intracellular chloride concentration, and their action is known to be activated by dephosphorylation.[1]We prepared a ditopic receptor 1[2] that contained 18-azacrown-6-ether as a potassium ion binding site and diphenyl urea as a chloride binding site, thus facilitating KCl transport in a POPC membrane. To develop a synthetic KCC mimic with the controlled activity, the hydroxyl group in 1 has been modified into a α-ammonium ester which interferes with the binding and transport of potassium and chloride ions. The K-Cl transport can be activated upon removal of the protecting group by enzymatic hydrolysis. Details including synthesis and enzyme-dependent transport activity will be described in the presentation.

References
1. Chen, Y. F.; Chou, C.Y.; Ellory, J.C.; Shen, M.R. *Am J Transl Res*. 2010, *2(4)*, 345?355.
2. Lee, J. H.; Lee, J. H.; Choi, Y. R.; Kang, P.; Choi, M. -G.; Jeong, K. -S. *J. Org. Chem*. 2014, *79*, 6403?6409.



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발표코드: **ORGN.P-782**
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Fluorescence study upon extending the structures of conjugated benzotriazole containing oligomers

이미림 이동환*

서울대학교 화학부

Benzotriazole is an essential component of pharmaceuticals, UV stabilizers, and organic electronic materials. Among N^1-, N^2-, and N^3-substituted isomers of benzotriazoles, N^2-substituted moiety shows strong fluorescence. In this study, fully conjugated oligomers were synthesized using highly fluorescent N^2-substituted benzotriazoles. To check the change in the fluorescence property upon extending the structure of the oligomers, series of different length of molecules were synthesized and characterized by UV?Vis and Fluorometer.

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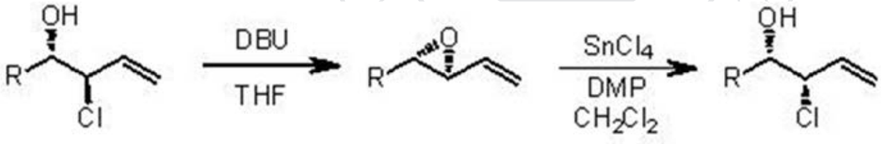
Stereochemical Conversion from anti-Vinyl chlorohydrins to syn-Vinyl chlorohydrin via trans Vinyl oxyranes

이은혜 방지윤 유찬모*

성균관대학교 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of Lewis acid catalysts are some of the most attractive methodologies. A highly diastereoselective synthesis of syn-vinyl chlorohydrin was achieved from the reaction of trans vinyl oxirane prepared from syn-vinyl chlorohydrin. The method described herein is successful with various substrates in good yields and high levels of diastereoselectivity. Scope and mechanistic aspects will be presented.



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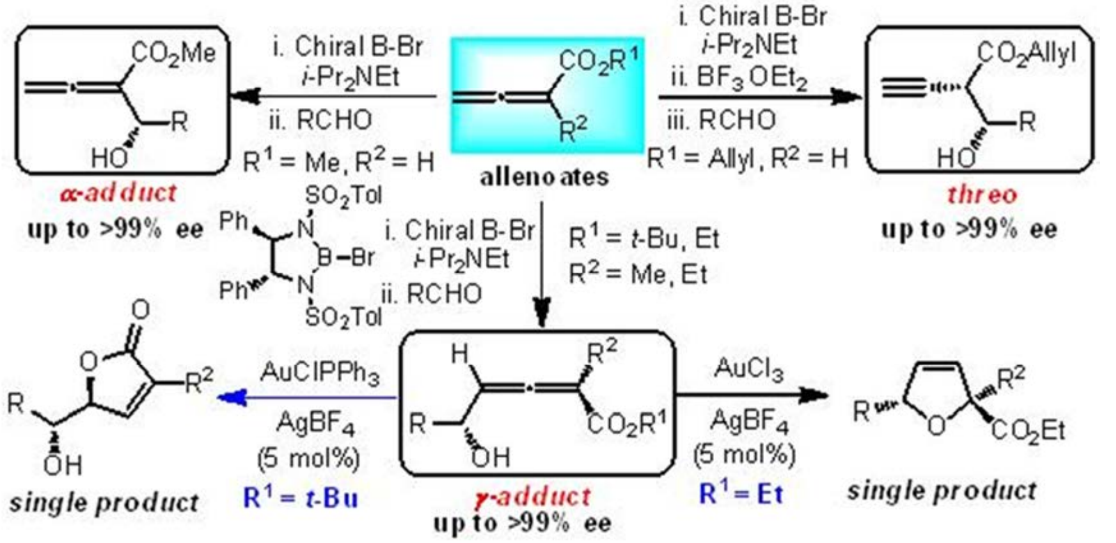
Regulation of Stereochemical Routes for Asymmetric Aldol Reaction of Allenoates: Governing Factors and Synthetic Applications

방지윤 김명훈 이은혜 유찬모*

성균관대학교 화학과

As part of our investigations utilizing allenes as versatile substrates, we present herein our discovery of control elements to regulate selective formation of isomeric alpha-addition, threo addition, or gamma-addition adduct from allenoates with aldehydes, which allows there action in good yields with high levels of stereoselectivity as highlighted below Scheme. We will present regulation factor for reactions and synthetic applications including natural product (+)-sylvone. Appilcation of gamma-adducts using Au(I) or Au(III) catalysts will also be discussed.



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발표코드: **ORGN.P-785**

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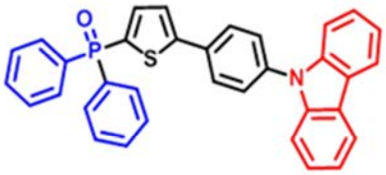
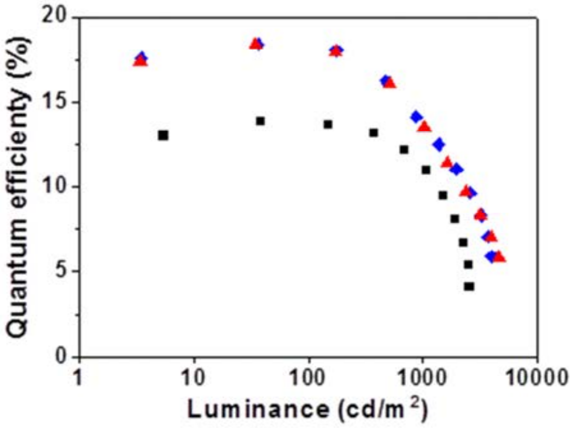
Synthesis of Novel Carbazole Derivative as a Host Material for Blue Phosphorescent Organic Light-Emitting Diodes

machireddy rajeshkumar reddy 서성용*

부경대학교 화학과

A novel bipolar compound with a thiophene modified 9-phenylcarbazole and phosphine oxide moieties, (5-(4-(9H-carbazol-9-yl)phenyl)thiophen-2-yl)diphenylphosphine oxide (CPTPO), was synthesized and characterized as a high triplet energy host material. Bipolar charge transport character and a high triplet energy of 2.72 eV of CPTPO allowed the development of blue phosphorescent organic light-emitting diodes with an external quantum efficiency of 18.4%.





일시: 2015년 4월 15~17일(수~금) 3일간
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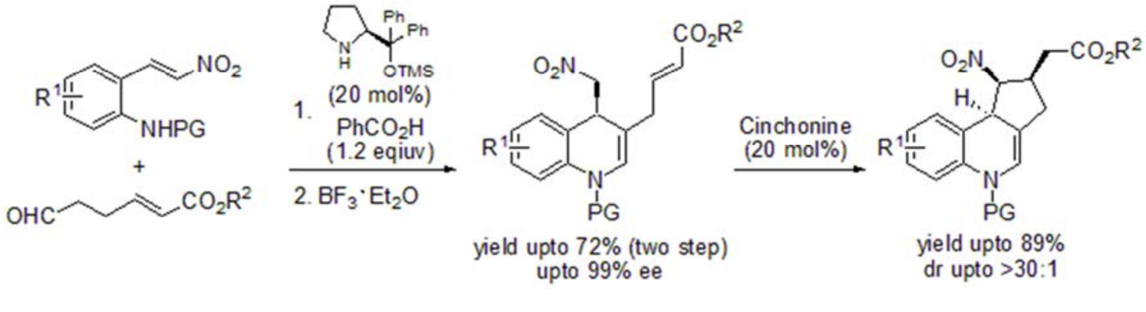
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric synthesis of densely polycyclic-fused dihydroquinolines: Enantioselective organocatalytic Michael addition/aza-cyclization and Michael addition sequential reactions

유미림 김성곤*

경기대학교 화학과

A highly efficient sequential process to the asymmetric synthesis of polycyclic-fused dihydroquinolines utilizing organocatalysis has been developede. In this synthesis, an asymmetric organocatalytic Michael/aza-cyclization domino reaction of 5-formylpent-2-enyl esters with N-protected-2-amino-β-nitrostyrenes followed by dehydration allows the process to proceed to afford corresponding α,β-unsaturated ester containing 1,4-dihydroquinoline products with high enantioselectivities (up to 99% ee). In addition, the subsequent organocatalytic intramolecular Michael reaction of the α,β-unsaturated ester containing 1,4-dihydroquinoline adducts is applied for the formation of the chiral tricyclic-fused dihydroquinolines.



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발표코드: **ORGN.P-787**
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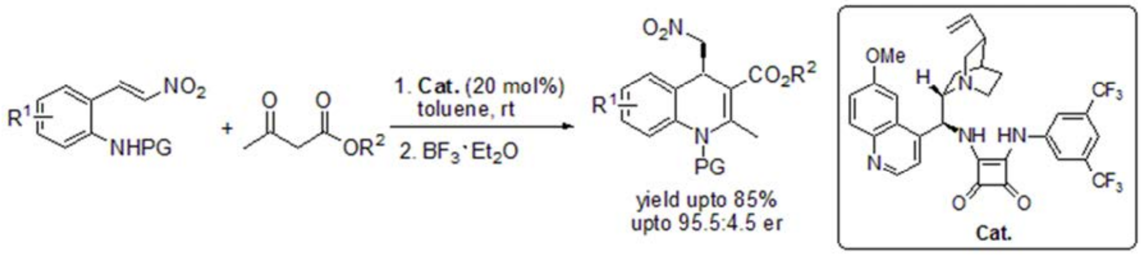
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective synthesis of functionalized 1,4-dihydroquinolines via a one-pot Michael/aza-cyclization domino reaction and dehydration sequence

김한나 김성곤*

경기대학교 화학과

The synthetic methodology of chiral highly functionalized 1,4-dihydroquinolines has been developed based on the organocatalytic enantioselective Michael/aza-cyclization cascade reaction of β-keto esters with *N*-protected-2-amino-β-nitrostyrenes followed by dehydration. The asymmetric catalytic reactions using quinine-derived squaramide as an organocatalyst have produced the desired products in good yields and with excellent enantioselectivities.



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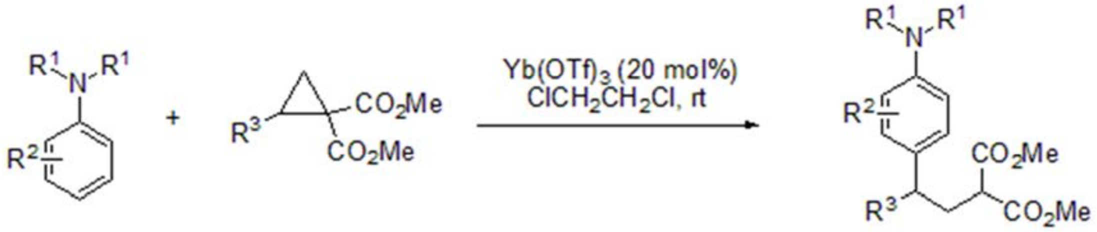
Catalytic Friedel—Crafts alkylation of donor—acceptor cyclopropanes with electron-riched benzenes

김아름 김성곤*

경기대학교 화학과

A Lewis acid catalyzed Friedel?Crafts alkylation of donor?acceptor cyclopropanes with electron-riched benzenes is descried. The reactions using Yb(OTf)$_3$ as a catalyst have produced desired Friedel?Crafts products in good yield for a broad range of functional groups and substitution patterns. This synthetic approach allows the construction of complex benzylic carbon stereogenicity.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of cargo exchange through collision

최은성 유자형[1,*]

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) 나노생명화학공학부

In drug delivery system, diverse kinds of materials were developed through the researches. Among them, block copolymer micelles have been promising vesicles to carry hydrophobic molecules. Among many kinds of block copolymers, amphiphilic micelles consisting of PEG and PDLLA, are effective drug carriers due to its outstanding biocompatibility of the hydrophobic group. It degrades into acid in the cell. Another advantage is high aqueous solubility of hydrophobic drugs in hydrophobic cores surrounded by hydrophilic coronas. In this work, Forster resonance energy transfer (FRET) is applied to identify the release of hydrophobic drug molecules. As a model of drugs, FRET pairs, DiI as an acceptor and DiO as a donor, were encapsulated into self-assembled polymeric micelles in water as drug molecules are encapsulated in nanocarriers. To demonstrate the idea, we vary the ratios of hydrophilic and hydrophobic group so that the thickness of hydrophilic surface is adjusted. Depending on the different FRET efficiency of each type of micelles, cargo release through micelle-micelle collision will be investigated. Through this work, we demonstrate how drug molecules are released from polymeric micelle system.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Push-Pull Porphyrin Dyes Conjugated with Donor and Acceptor for Dye-Sensitized Solar Cells

김호준 김희준*

금오공과대학교 응용화학과

With advantages of low cost, low weight, coloring, and easy processing, dye-sensitized solar cells(DSSCs) are prospective alternatives for future devices for the conversion of solar energy. Inspired by the important role that porphyrins play in natural photosynthesis, researchers have tested numerous derivatives of this substrate class as sensitizers for DSCs, but conversion efficiencies obtained so far have largely remained below 8%. Recently porphyrin dyes for dye-sensitized solar cells have been synthesized system of electron donor-Porphyrin-electron acceptor (D-π-A). The best performed zinc porphyrin(YD2-o-C8) with organic dye efficiency of 12.3% was reported in 2011. We designed and synthesized porphyrin dyes with a new acceptors of 2,1,3-benzothiadiazole (BTD).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Campothecin containing self assembling short peptide-drug conjugate for cancer cells, a pH dependent study

최후연 MANAYATHTHEKKEYILJEENA[1] 유자형[2,*]

울산과학기술대학교(UNIST) Chemistry [1]울산과학기술대학교(UNIST) 나노생명화학공학부 [2]울산과학기술대학교(UNIST) 자연과학부 화학과

There has been a great deal of research over past few decades towards improving the selective delivery and cellular uptake of anti cancer drugs via the use of macromolecular based delivery vehicles, such as liposomes, micelles, hydrogels etc. However, delivery based on covalent conjugation presents a facile and yet effective approach towards cancer drug delivery owing to their high stability and pre mature leakage. The cell penetrating peptide based drug conjugate have explored as a molecular vector to anti cancer drugs to improve drug's water solubility and cellular uptake. Among them, self assembling peptide-drug conjugates, called prodrugs, are promising antitumor efficacy and to reduce the toxicity of anti cancer drugs. As a simple and facile approach, here in, we present tripeptide based self assembling, water soluble anti cancer pro drug. Our molecular structure includes short peptide sequence Lys-Cys-Lys conjugated to campothecin via disulfide bond. In the cancer cell environment, in the presence of GSH, di sulfide bond will cleave to release campothecin and can serve as an anticancer drug. To study the pH dependence on cellular uptake, we had modified the Lys-Cys-Lys-ss-CPT with succinic anhydride, maleic anhydride and methyl maleic anhydride. Moreover the peptide drug conjugate exhibit various self assembly in water so that showed difference in the cellular uptake. Our molecule can serve as a tool for basic understanding of pH and morphology dependent cellular uptake of anticancer drugs.Key words: Prodrug, Lys-Cys-Lys-ss-CPT, Self assembly, pH dependence

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발표분야: 유기화학
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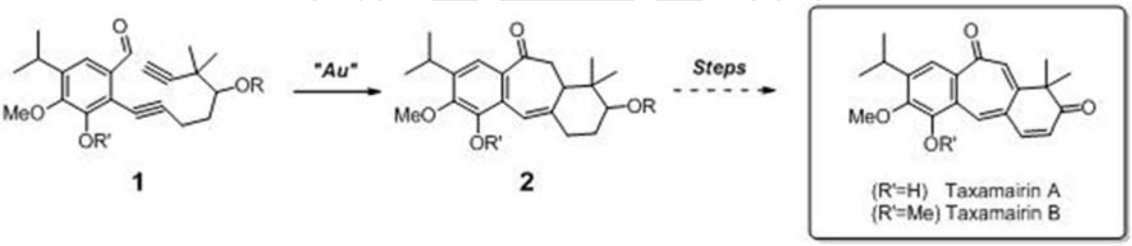
Synthetic study of Taxamairin B

이영주 고은비 오창호*

한양대학교 화학과

Taxamairins (A, B), extracted from Taxus are one of the bioactive natural products having an antitumor activity. The characteristic core skelectone of Taxamairins is a [6.7.6] tricycle. We have designed a suitable substrate 1 for synthesis of Taxamairin based on the accumulated results on polycycle syntheses. We will report some of our preliminary results on the total synthesis of Taxamairin B.



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발표코드: **ORGN.P-793**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of high Tg hole transport layer materials based on spiro derivatives for OLEDs

양두리 임효[1] 김후희[2] 김보미[3] 채규윤[3,*]

원광대학교 바이오나노화학과 [1]원광대학교 바이오나노화학부 [2]원광대학교 바이오 나노 화학부 [3]원광대학교 화학과

In this study, the novel hole transport layer (HTL) materials with high glass transition temperature values based on spiro derivatives were synthesized by Suzuki-Miyaura reaction. these novel compounds were characterized by FT-IR, TGA, DSC, UV and CV. Our preliminary results showed that these novel HTL materials exhibited good photophysical properties to be used as hole transporting materials for fabrication OLED device.Keyword : Hole transport layer(HTL), spiro derivatives, OLED, Suzuki coupling

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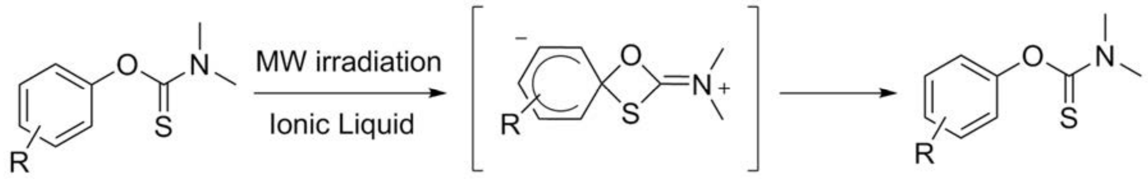
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Mild Newman-Kwart rearrangement of O-Aryl Thiocarbamates: Microwave Synthesis in Ionic Liquid Medium

강민경 염현석[1,*] 류재욱[1,*]

서강대학교 화학과 [1]한국화학연구원 친환경신물질 연구센터

The Newman-Kwart rearrangement (NKR) is a useful synthetic tool for converting phenols to thiophenols via their *O*- and *S*-thiocarbamates. Indeed, such is the utility that other sulfur-containing functional groups have been readily accessed through this methodology, including thioethers, (homo-chiral) sulfoxides, sulfones and sulfonic acids. Alternatively, this approach can be used to access particular aromatic substitution patterns without the phenol/sulfur function, starting from the many widely available phenols, and de-sulfurizing the hydrolysed thiol once the desired transformations are complete. Consequently, the NKR has seen wide application in synthesis, medicinal chemistry, materials and supramolecular chemistry, agrochemicals and dyes. The NKR proceeds via an *O*- to *S*-aryl migration, which has high activation energy, so that high temperatures (200?300oC) are required to access the strained 1,3-oxathietane transition state. Not only do such high temperatures present issues in terms of practicality and safety, but they can also induce “charring” and other undesired side reactions, meaning that fragile substrates are not amenable to the harsh reaction conditions. Nevertheless, thermally induced NKR by microwave or conventionally is commonly referred and recently, Pd-catalyzed NKR in moderate temperature have been reported by Moseley and co-workers. They have also studied the solvent effect for NKR, the reaction rate fits the relative order of solvent polarity. Encouraged by this initial result and explored a range of solvent to can more stabilize polar transition state. Interestingly, in the ionic liquid medium, reaction rate was dramatically improved without undesired side product and microwave was more efficient than thermal heating unlike a result of Moseley. Herein we present ionic liquid effect for the Newman-Kwart rearrangement and a tolerance of substituent on aromatic ring.


MW irradiation
Ionic Liquid
O
N
S
R
N+

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Lithocholate-based Glyco-Amphiphiles (LCGAs) for Membrane Protein Study

DASMANABENDRA 채필석[1,*]

한양대학교 bionano engineering [1]한양대학교 생명나노공학과

Intrinsic membrane proteins play important roles in controlling the flow of molecules and information across lipid bilayers. Structural and functional characterization of these bio-macromolecules generally requires extraction from the native membranes and purification with an assistance of an amphipathic agent such as conventional and synthetic detergents. In this study, we synthesized several lithocholate-based glyco-amphiphiles (LCGAs) and characterized their micelles in terms of critical micelle concentrations (CMCs) and micelle sizes. These agents will be evaluated for their efficacy in solubilization and stabilization on a few membrane proteins

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Mechanisms and Applications of Cyclometalated Pt(II) Complexes in Photoredox Catalytic Trifluoromethylation

최원준 유영민[1,*]

성균관대학교 에너지과학과 [1]이화여자대학교 화학신소재공학부

Lately, one notable example spotlighting the value of photoredox catalysis is trifluoromethylation. However, a limited understanding of the mechanism and molecular parameters that control the catalytic actions has hampered the full utilization of the photoinduced trifluoromethylation. To address this challenge, we evaluated and investigated the photoredox catalytic trifluoromethylation reaction using a series of cyclometalated Pt(II) complexes with characteristically varied ligand structures. The Pt(II) complexes were capable of catalyzing the trifluoromethylation of non-prefunctionalized alkenes and heteroarenes in the presence of CF3I under visible light irradiation and displayed high yields and functional group tolerance. Spectroscopic measurements, including nanosecond laser photolysis and transient photoluminescence experiments, were performed to identify the catalytic intermediates and directly monitor their conversions. The mechanistic studies provided compelling evidence that the catalytic cycle selects the oxidative quenching pathway, and that electron transfer during each step of the cycle strictly adheres to the Marcus normal region behaviors. Finally, quantum yields exceeding 100% strongly suggested that radical propagation significantly contributes to trifluoromethylation. These findings establish molecular strategies for designing trifluoromethyl sources and catalysts in an effort to enhance catalysis performance.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Sensing and Antibacterial Activity of Imidazo-lium-Based Conjugated Polydiacetylenes

이송이 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Every year, over 2 million children are reported to have been killed due to bacterial infections. Furthermore, antibiotic-resistant bacteria have emerged as a major threat to public health worldwide. Thus, there is an urgently need to develop novel classes of antibacterial compounds that can overcome the antibiotic resistance of bacteria including MRSA (methicillin-resistant Staphylococcus aureus), VRSA (vancomycin-resistant Staphylococcus aureus) and ESBL-EC (extended-spectrum β-lactamase-producing Escherichia coli). PDAs (polydiacetylenes) belong to an unique family of conjugated polymers with non-fluorescent blue color, which can shift to a fluorescent red color upon environmental stimuli, such as metal ions or proteins. Sensors based on the fluorogenic properties of PDAs have been actively studied since 2005. Schmuck et al. have shown that the PDA containing oligo-lysine groups and naphthalic acid functions as a fluorescent turn-on sensor for the detection of bacterial lipopolysaccharides (LPS), in which the four-lysine residues with positive charges exhibited a strong affinity to the negative-charged LPS.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Two-Photon Fluorescent Probes for Imaging OCl? Production in cells and tissues

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이화여자대학교 유기화학 [1]아주대학교 에너지시스템학부 [2]이화여자대학교 화학·나노과학과

Hypochlorite (OCl?) is one of the prominent member of reactive oxygen species (ROS) in living system. Detection of OCl- by fluorescence probe is useful to understand the physiological and pathological roles of OCl- at the cell, tissue, and organism levels. Therefore, we designed and synthesized the imidazoline-2-thiones containing OCl- probes, PIS and NIS. The probes show highly selective and sensitive fluorescence turn-on responses to OCl-. We demonstrated that PIS can be employed to image OCl? generation in macrophages in a co-culture system with Hella cell. More importantly, PIS can be combined with two-photon microscopy to image OCl- in live cells and tissues.

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발표분야: 유기화학

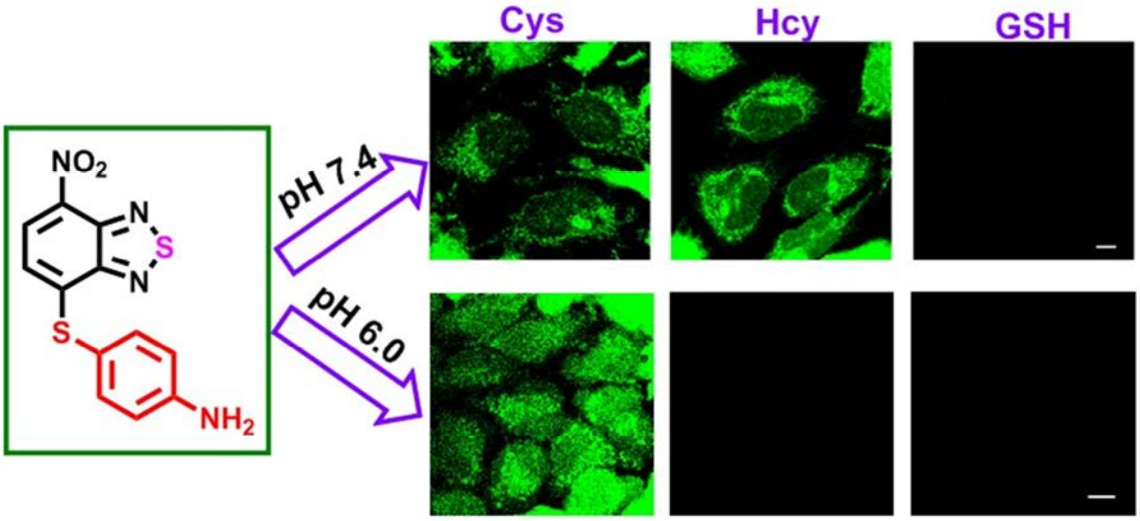
발표종류: 포스터, 발표일시: 수 16:00~19:00

The fluorescent detection of cysteine and homocysteine using aryl-thioether substituted nitrobenzothiadiazole

이다영 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

The aryl-thioether substituted nitrobenzothiadiazole (NBD) was synthesized as a fluorescent turn-on probe for detection of cysteine and homocysteine in living cells. In pH 7.4, both cysteine (Cys) and homocysteine (Hcy) promote an enhancement of the fluorescence intensity of the probe. In weakly acidic solution (pH 6.0), however, only Cys promotes fluorescent enhancement of the probe. Moreover, because of its good water solubility, cell-penetration ability and biocompatibility, it acts as a fluorescent probe to monitor Cys and Hcy in living cells. According to these results, the aryl-thioeter substituted NBD probe will be useful to understand biology related to Cys and Hcy.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluoride Sensing Using Triaryl Boron Complex

Hu Ying 윤주영[1,*]

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Due to the considerable significant role of fluoride to health, environment and industrial processes, a number of chemosensors for fluoride anion have been developed. Inorganic fluorides have markedly different physical properties than their halogen congeners owing to the small size and extraordinary electronegativity of fluorine atoms. Fluorescent sensing is a powerful technique that has been used to detect and image the location of a wide variety of anions both qualitatively and quantitatively, for this reason, our research group has designed triaryl boron complex for sensing fluoride.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Nondestructive readout fluorescence memory based on a gallium(III) corrole complex and photochromic *cis*-1,2-dithienylethene

강지준 유영민[1,*]

성균관대학교 에너지과학과 [1]이화여자대학교 화학신소재공학부

Photochromic modulation of energy transfer between a fluorophore and photochrome provides a viable principle to creation of all optical molecular memory. One essential requirement for successful operation of the molecular memory is ability for non-destructive readout, for which photoexcitation for fluorescence emission should not interfere with the photochromic processes. Gallium(III) corrole complexes with large Stokes shifts outfit the requirement, permitting photoexcitation at the optical window where the photochromism of *cis*-1,2-dithienylethene is not executed. To demonstrate the capability for fluorescence memory, we prepared poly(methyl methacrylate) films doped with a gallium corrole complex and *cis*-1,2-dithienylethene. The memory cycle comprising fluorescence readout and reversible photochromic switching of the fluorescence emission is fully reversible without suffering from fatigue during repeated operation. Spectroscopic measurements based on time-correlated single photon counting techniques revealed effective trafficking of energy transfer by the reversible photochromism.

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Fluorescence turn-on sensor detecting peroxynitrite

박진희 오진록 홍종인*

서울대학교 화학부

Peroxynitrite (ONOO?), a strong oxidant found in biological system, causes oxidation of biomolecules involved in a variety of physiological and pathological processes. Many reports suggest that ONOO- is related to many diseases, immune responses and redox regulation of signaling pathways. However, the effects of ONOO- are not clearly understood because of its short half-life (

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-803**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure-recognition relationship of chiral bis(Zn(II)-DPA) complexes toward phosphate-containing molecules

오진록 홍종인*

서울대학교 화학부

Phosphate-containing biomolecules are recognized as important molecules in a living system because of their roles involved in signal transduction, energy currency and control of metabolic processes and so on. Also, many of these processes are usually conducted with a concomitant release of pyrophosphate by the enzymatic reactions of NTPs using kinases. For this reason, it is important to develop a fluorescent chemosensor that can distinguish pyrophosphate from NTPs.Recently, Hong et al developed several pyrophosphate probes which show moderately selective behavior against various nucleotides, such as ATP. Because the natural recognition of nucleotide is occurred in highly stereoselective manner, we anticipated that a chiral host molecule can show better selectivity over nucleotides. Here, we report a synthesis of chiral bis(Zn(II)-DPA) complexes and their discriminatory ability of pyrophosphate and nucleotides.

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발표코드: **ORGN.P-804**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrostatics-driven pyrophosphate recognition by using graphene oxide-probe conjugate

이동남 홍종인*

서울대학교 화학부

A variety of probes have been developed using intermolecular interactions (hydrogen bonding, pi-pi interactions, metal-ligand coordination) and chemical reactions (electrophilic/nucleophilic reaction, reduction/oxidation and enzymatic reaction) with analytes, respectively. Introduction of graphene oxide (GO) sheets to the molecular recognition system of a probe and a target analyte is expected to exert different intermolecular forces on probe itself and probe-analyte supramolecular complex. We report highly selective detection of pyrophosphate (PPi) by modulating the electrostatic interaction between negatively charged GO and Zn^{2+}-coordinated synthetic probe (1) before and after PPi recognition. A dramatic change in fluorescence intensity of 1 occurred when PPi was added to the electrostatically attractive patch (GO-1), which originates from charge inversion in probe 1 upon binding the highly complementary target (PPi), concomitantly resulting in Columbic repulsion between GO and 1-PPi. Ionic strength modulation of a solution further gives rise to subtle changes of binding constants and increases the PPi selectivity over nucleotide triphosphates.

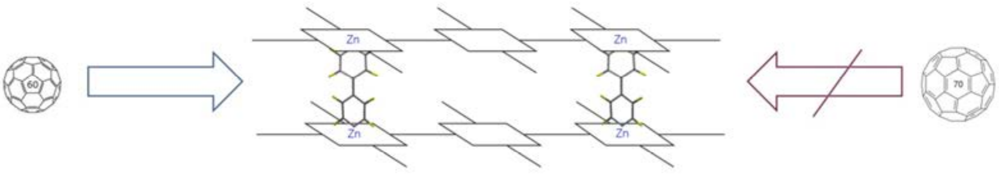
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-805**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Binding and Easy Separation of C_{60} by 3D-nanosized supramolecular architectures

이재철 백경수* 박연실 구혜린

숭실대학교 화학과

The self-assemblies of copillar[5]arene 1, tetracationic porphyrin guest 2, and dipyridyl bridges 3 into 3D-nanosized supramolecular architectures via quadruple hydrogen bondings, cation-π interactions, and metal-ligand coordination were investigated by ^{1}H-NMR and 2D-NOESY experiments. These self-assembled architectures display a remarkable selectivity for the complexation of C_{60} over C_{70} within its inner hole, which was confirmed by ^{13}C-NMR, UV-Vis spectrometer, and HPLC experiments. Especially, polar-solvent addition disrupts these 3D architectures and allows easy recovery of C_{60} and recycling of the receptor by only filtration without tedious procedures.



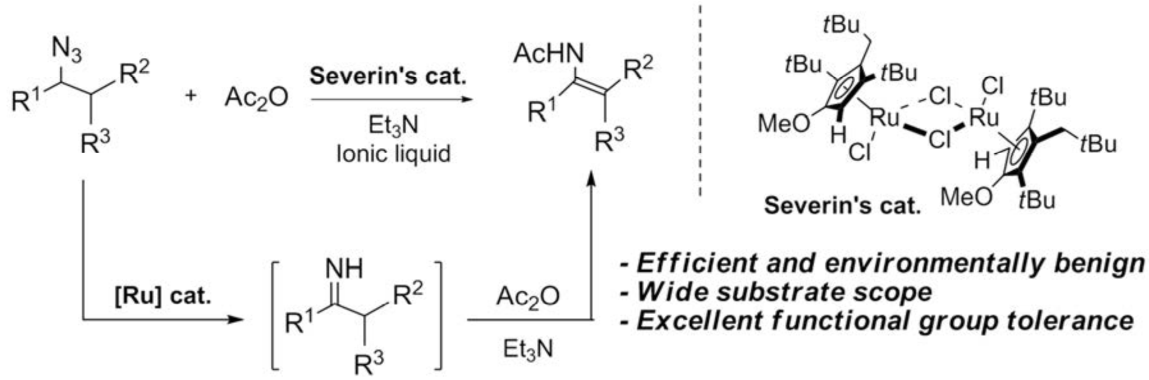
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-806**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Enamides by Ru-Catalyzed Reaction of Alkyl Azides with Acyl Anhydrides in Ionic Liquid

박한규 이영호* 박재욱*

포항공과대학교(POSTECH) 화학과

Enamides are key functional groups in numerous natural products and drug candidates, and serve as versatile intermediates in organic synthesis. A number of methods have been devised for the synthesis of enamides. Conventional ones include the addition of Grignard reagents to nitriles followed by the reaction with acyl donors, transition metal catalyzed cross coupling reaction of vinyl electrophiles with amides, direct condensation of amides with ketones, and reductive acylation of ketoximes. However, these methods frequently suffer from functional group tolerance, difficulty in preparing substrates, low yield, and/or requirement of stoichiometric reductants or additives. As an alternative to these methods, we recently presented a new synthesis of enamides using alkyl azides and acid anhydrides, which is based on the Ru-catalysis to transform alkyl azides to N-H imines under illumination of fluorescent light. However, the synthetic methods involving the intermediacy of N-H imines would suffer from the side reactions of unstable N-H imine intermediates such as rearrangements and self-condensation reactions. From the search for new catalyst systems that can overcome the limitation, we found an unexpected activity of the Severin's diruthenium complex ([Cp^RuCl2]2: Cp^ = 1-methoxy-2,4-di-tert-butyl-3-neopentylcyclopentadienyl) for the transformation of alkyl azides to the corresponding N-H imines in ionic liquids. Here in, we report novel potential of Severin's diruthenium complex in the synthesis of enamides from organic azides and acetic anhydride. The one-pot one-step synthetic process is much more convenient than previous ones and highly efficient to afford a wide range of enamides containing various functional groups from primary azides as well as from secondary azides. A large scale reaction was demonstrated in uninflammable ionic liquid to diminish the concern of using organic azides as substrates for safety.



- Efficient and environmentally benign
- Wide substrate scope
- Excellent functional group tolerance

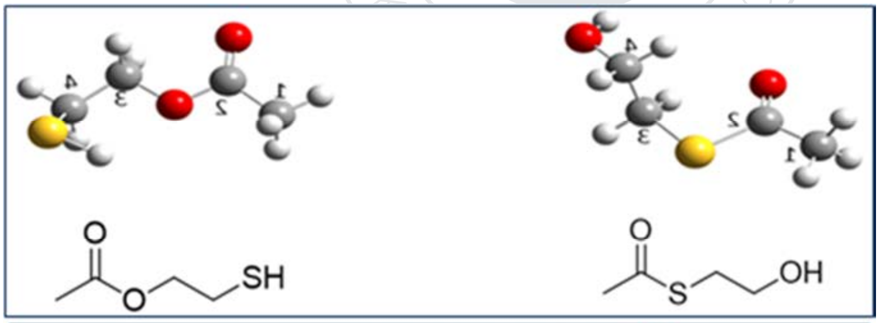
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-807**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

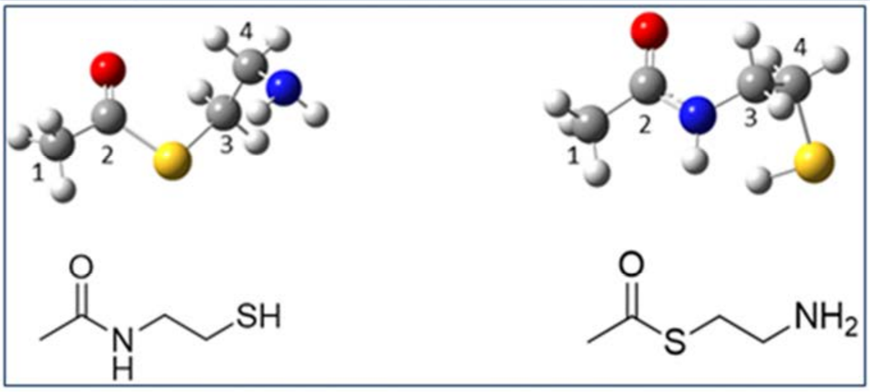
The Mechanistic Study of Chemoselective OAcylation of βMercapto Alcohol and NAcylation of βMercaptoamine with Acid Chloride Derivatives

김미형 안철진*

창원대학교 화학과

The chemoselectivity in O-acylation of β-mercaptoalcohol and N-acylation of β-mercaptoamine are synthetically important to prepare the organic compounds with free-SH. In this paper, the investigation to the chemoselective O-acylation of β-mercaptoalcohol and N-acylation of β-mercaptoamine with acid chloride derivatives and mechanistic study are reported.





일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-808**

발표분야: 유기화학

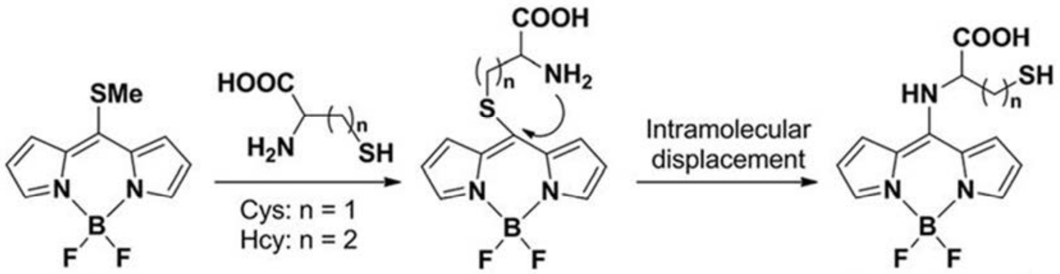
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ratiometric fluorescent probe for the detection of cysteine and homocysteine through mimicking the native chemical ligation

전용웅 안교한*

포항공과대학교(POSTECH) 화학과

Biological thiols or biothiols such as glutathione (GSH), cysteine (Cys), and homocysteine (Hcy) play essential roles in maintaining the redox balance of biological systems.1 For example, glutathione (GSH) is the major endogenous cellular antioxidant and it prevents cellular damage. Deficiency of Cys is associated with diseases such as haematopoiesis decrease, leukocyte loss, psoriasis, slowed growth, liver damage, skin lesions, hair depigmentation and edema.2 Also, the concentration of Hcy is associated with various diseases or clinical conditions, which include Alzheimer's disease, schizophrenia, end-stage renal disease, osteoporosis, and type II diabetes.3 Therefore, the selective and efficient detection of these biothiols has become an important subject of current research interest.The native chemical ligation has emerged as a promising strategy for the selective sensing of biothiols. Here in, a new type of the native chemical ligation approach toward a ratiometric sensing system for cysteine and homocysteine is disclosed. The probe 1, an 8-MeS-BODIPY, was found to selectively sense cysteine and homocysteine over glutathione and other amino acids, exhibiting a ratiometric fluorescence response through a chemical conversion that mimics the native chemical ligation. Under physiologically relevant concentrations of biothiols, the ratiometric fluorescence response to homocysteine became minor. The probe was thus applied to the imaging of biothiols in different organs of zebrash, using confocal microscopy.1. Schulz, J.; Lindenau, J.; Seyfried, J.; Dichgans, J. Eur. J. Biochem. 2000, 267, 4904.2. Shahrokhian, S. Anal. Chem. 2001, 73, 5972.3. Mills, J. L.; McPartlin, J. M.; Kirke, P. N.; Lee, Y. J.; Conley, M. R.; Weir, D. G.; Scott, J. M. Lancet, 1995, 345,149.



Probe **1**

Product **2**: n = 1
Product **3**: n = 2

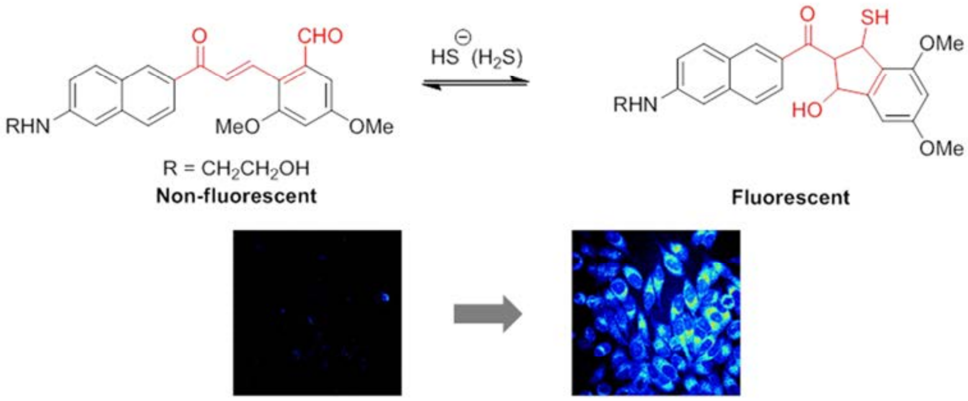
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-809**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Pragmatic Two-Photon Probe for Hydrogen Sulfide

김혜림 안교한*

포항공과대학교(POSTECH) 화학과

Hydrogen sulfide has been generated as an exciting endogenous gasotransmitter besides nitric oxide and carbon dioxide. Non-invasive detection methods for hydrogen sulfide are required for studying its diverse roles in biological systems. Fluorescent probes for hydrogen sulfide thus have received great attention in recent years.[1] A useful fluorescent probe for bioimaging of hydrogen sulfide should be selective, sensitive, fast-responsive, biocompatible, observable in the biological optical window, and capable of deep-tissue imaging. However, these sensing properties are extremely difficult to achieve at the same time. We herein introduce the two-photon fluorescent probe that meets all of these criteria to a practically useful level.[2] The probe belongs to a known Michael acceptor system, which raised a serious selectivity issue over the competing biothiols such as cysteine and glutathione. We have addressed the selectivity by optimizing the electronic and steric interactions between biothiols and the probe, in addition to achieving very high sensitivity, fast-response, and tissue-imaging capability. Also, the sensing mechanism suggested in the literature was revised. The probe enables us to image the endogenously produced hydrogen sulfide with negligible interference from other biothiols in live cells and tissues of mouse and zebrafish. Furthermore, we have detected a significant increase in the hydrogen sulfide level in various organs for an injury-induced mouse model for the first time, using the probe. The excellent sensing properties of the probe combined with its capability of deep tissue imaging thus make it a practically useful tool for further studying biological roles of hydrogen sulfide including its protective role against injury-induced oxidative stress.References[1]Chan J, Dodani SC, Chang CJ, *Nat. Chem.* 2012, 4, 973-984[2]Singha S, et al. *Anal. Chem.* 2015, 87, 1188-1195.



Two-photon imaging of endogenous H_2S in cells

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-810**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Substituted 3,4-Dihydro-*2H*-[1,4]-Oxazines from Rhodium-Catalyzed Reaction of 2,3-epoxy alcohol with *N*-Sulfonyl 1,2,3-Triazoles

고영옥 이상기[1,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학/나노과학과

We have described a novel method for the preparation of substituted 3,4-dihydro-*2H*-[1,4]-oxazine derivatives, found in a number of biologically active natural products. In past years, the various approach to α-imino rhodium (II) carbene species was made. The [1,4]-oxazine structure was formed by the O-H insertion of 2,3-epoxy alcohol to rhodium (II) azavinyl carbene species and the epoxide ring-opening, activated by catalytic amount of Lewis acid. This study shows a new and meaningful way to prepare 3,4-dihydro-*2H*-[1,4]-oxazines, hard to synthesize from the known synthetic routes.

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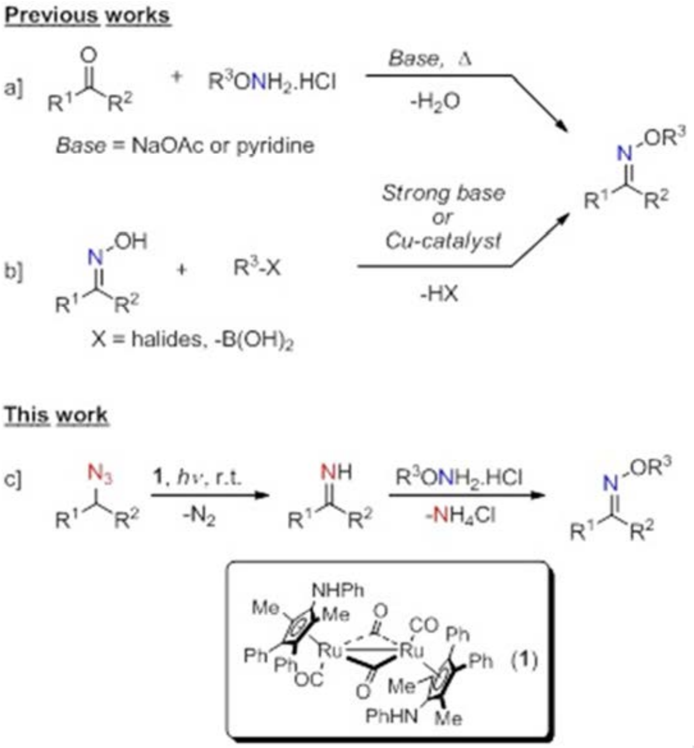
장소: 일산 KINTEX
발표코드: **ORGN.P-811**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fast and Complete Synthesis of O-Alkyl Oximes from N-H Imines

김용진 이영호* 박재욱*

포항공과대학교(POSTECH) 화학과

O-alkyl oxime has been recognized as an important functional group which is frequently found in numerous bioactive compounds such as fluvoxamine, oxiconazole, roxithromycin. Traditional approach for the preparation of O-alkyl oximes principally deals with the condensation reaction of aldehydes or ketones with O-alkylhydroxylamine hydrochloride salts in the presence of excess amount of base. Theoretically, the condensation of amines and carbonyl compounds is reversible in nature. Therefore, for complete conversion, such transformations frequently require excess amount of amines, high temperature and long reaction time. Recently, the approach of dynamic covalent chemistry (DCC) with the full reversibility of the C=N linkage of imines by transimination reaction has shown the great advantage. Since, such transformation takes place without disruption of the C=N bond into free amines and carbonyl components and does not include the intervention of water as a third constituent, the equilibrium mostly shifts towards the more stable adduct in anhydrous organic solvents.Herein, a new synthetic method for O-alkyl oximes is developed by combining the Ru-catalyzed transformation of alkyl azides into N-H imines and transimination reaction with O-alkylhydroxylamine hydrochloride. Various O-alkyl oximes are synthesized in high yields at room temperature in short reaction time. Another notable advantage of our method is demonstrated by the chemoselective transimination reaction in the presence of carbonyl functionality.


Previous works
a]
R1 R2
R3ONH2.HCl
Base, Δ
-H2O
Base = NaOAc or pyridine
N-OR3
R1 R2
b]
N-OH
R1 R2
R3-X
Strong base
or
Cu-catalyst
-HX
X = halides, -B(OH)2
This work
c]
N3
R1 R2
1, hν, r.t.
-N2
NH
R1 R2
R3ONH2.HCl
-NH4Cl
N-OR3
R1 R2
NHPh
Me
Me
Ph
Ph
OC
Ru
O
CO
Ru
Ph
Ph
O
Me
PhHN
Me
(1)

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-812**

발표분야: 유기화학

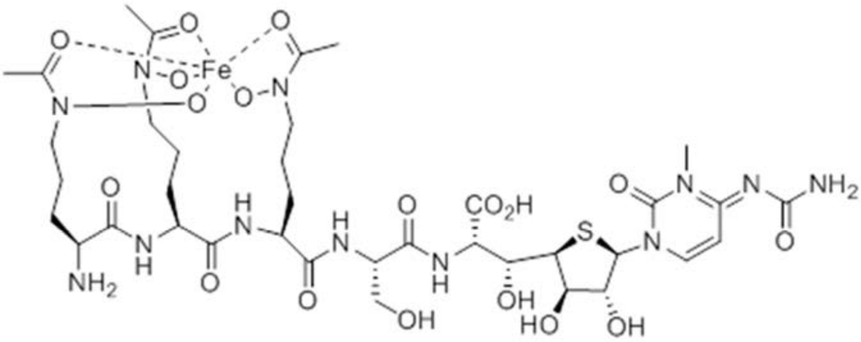
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies toward total synthesis of albomycin δ2

안진수 송운영 김학중*

고려대학교 화학과

Albomycins are Trojan horse antibiotics consisting of a modified seryl thionucleoside compound, SB-217452, and a ferrichrome-like siderophore. Mechanistically, the nucleoside portion of albomycins were found to act as an inhibitor of bacterial seryl-tRNA synthetase, a crucial enzyme for protein biosynthesis, once taken up by bacteria through a siderophore uptake machineries, of which events lead to the growth inhibition of treated pathogens. Structurally, albomycin δ2 contains a few uncommon functionalities such as the thiofuranose ring and N4-carbamoyl group at the cytosine base. Intrigued by such unique structural features, we decided to pursue total synthesis of albomycin δ2. In addition, we are also planning to investigate the origin of its excellent antimicrobial activity as well as biosynthesis mechanisms of the thionucleoside formation. Initially, we tried to synthesize the seryl thionucleoside compound, SB-217452, based on conventional chemical methods. Our synthesis commenced with commercially available L-arabinose to establish the correct stereochemistry. The first key step to install the cytosine moiety onto the cyclic thioether intermediate could be accomplished by Pulmmer-type. Then, the C-terminal end featuring the anti-2,3-aminohydroxy carboxylate could be stereoselectively implemented by adopting Barbas anti-selective direct aldol chemistry.



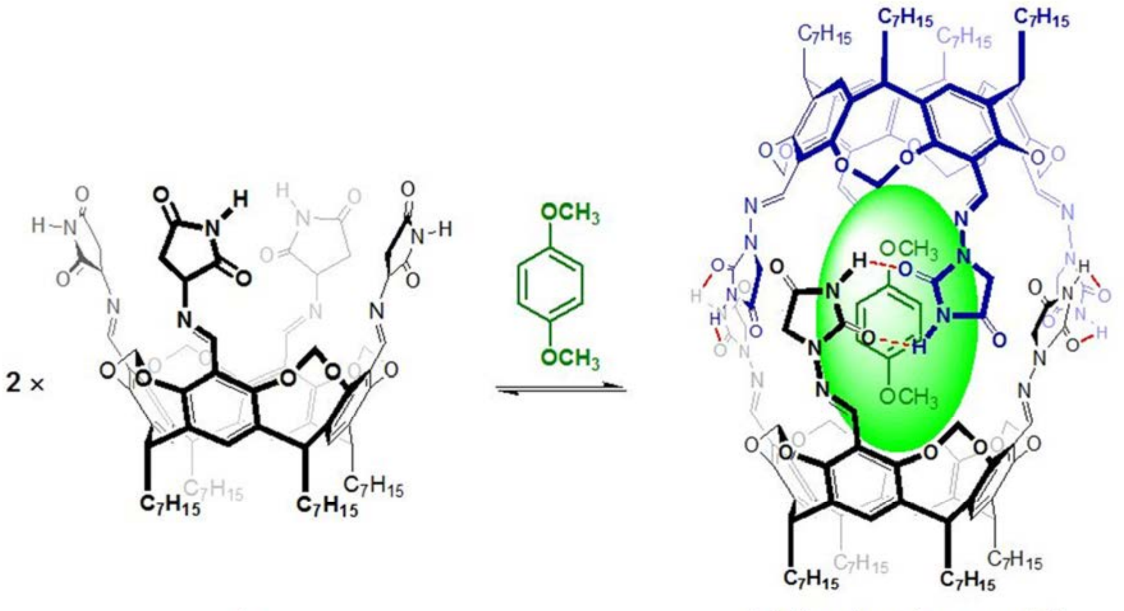
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-813**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembled molecular capsule formation of a resorcin[4]arene-based hydantoinyliminocavitand

김조원 유선호 박연실 백경수[*]

숭실대학교 화학과

Resorcin[4]arene-based tetrakis(N-hydantoinylimino)cavitand 1 forms a stable molecular capsule in the presence of suitable neutral guests such as 1,4-dimethoxybenzene. Molecular capsule G@1_2 is stabilized by the eight intermolecular imide N-*H*…O=C hydrogen bondings, two from each four paired hydantoinyl units on two cavitands. The formations of molecular capsules were confirmed by solvent titration, VT ^{1}H-NMR, 2D-NOESY, and 2D-DOSY NMR.



1

1,4-dimethoxybenzene@**1**$_2$

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-814**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium catalyzed (Ullmann-type) reductive homocoupling of Blaise reaction intermediate

XUAN ZI 이상기[1,*]

이화여자대학교 화학.나노학과 [1]이화여자대학교 화학/나노과학과

Biaryl compound is of great importance for many agrochemicals, pharmaceuticals, nature product as well as many asymmeric catalysts. The general method to prepare symmeric or unsymmetirc biary compound is Ullman reaction, a reductive homocoupling of aryl halids under copper catalyst. However, this reactionrequires high reaction temperature (> 200℃) and stoichiometricamount of copper reagents. Improvements to this method emerged by using transitiom metal catalysts involving Pd, Ni and Co with additional reductive agent such as hydrogen donor or electron source to regenerate catalyst active species. As part of our studies on the use of Blaise reaction intermediate, we found that Blaise reaction intermedate which starts from aryl halide nitriles can provide homoumcoupling product under 7.5 mol% of palladium catalyst withount any auxiliary reducing agent with effective yield. More expansion to our homocoupling biaryl compound of Blaise reaction intermediate is currently underway.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium-Catalyzed Diastereoselective *N*-Sulfonyl Aminoalkenylation of Azulenes from Terminal Alkynes and Azides through *N*-Sulfonyl-1,2,3-triazoles

용우순 서보람 이필호*

강원대학교 화학과

Azulenes, which are known to be a class of nonbenzenoid aromatic hydrocarbons, have attracted notable attention because of their significance as natural products, biologically active compounds, and molecular materials. Thus, development of efficient synthetic methods of these compounds from readily available starting materials has been in continuous demand. Although Hafner and co-workers reported a novel synthetic approach of azulene in one pot, introduction of valuable substituents onto azulene have limitations due to its unusual reactivity caused by the polarized π-electron system. For this reason, synthetic strategies of azulene through an introduction of a new functional group and its transformation are extremely desirable for the preparation of azulene derivatives. Herein, we report diastereoselective introduction of an enamine functionality on the azulenes from terminal alkynes and azides via *N*-sulfonyl-1,2,3-triazoles.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-816**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of *N*-Alkylated Azetidine Derivatives

이효준 조창우*

경북대학교 화학과

3,3-Dinitroazetidine (DNAZ) derivatives constitute an important class of energetic materials, with inherently high energies resulting from their strained ring systems and nitrogen contents. Recently, considerable efforts have been devoted to the development of new energetic plasticizers having lower glass transfer temperature and higher thermal decomposition temperature to increase the performance of composite explosives. Therefore, we deemed azetidine applicable to key skeleton of new energetic plasticizers because of its ring strain. In order to develop the new energetic plasticizer having azetidine as key skeleton, we planned to control structural regularity of azetidine via *N*-alkylation of azetidine to afford *N*-alkylated azetidine derivatives. Here, we report the synthesis and physical properties of *N*-alkylated azetidine derivatives.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-817**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

In Situ Generation of Phosphoryl Alkylindiums and Their Synthetic Application to Arylalkyl Phosphonates via Palladium-Catalyzed Cross-Coupling Reactions

김철의 서보람 이필호*

강원대학교 화학과

Organophosphonate is an essential functional group in synthetic as well as biological chemistry. In synthetic chemistry, it is a starting material for the preparation of alkenes via the Horner-Wadsworth-Emmons reaction. In biological chemistry, their distinctive structure and polarity provide them a significant function in pharmaceuticals and agrochemicals. Therefore, a wide range of synthetic intermediates and precursors and biologically active compounds require introduction of a phosphonate group to the molecule. To date, the most conventional approaches for the formation of the P-C (sp^3) bond are the Michaelis-Arbuzov and Michaelis-Becker reactions. Despite its prevalence, the trivalent phosphorus compounds employed in the Michaelis-Arbuzov reaction have normally low stability and effuse a repulsive odor. The Michaelis-Becker reaction occasionally needs long reaction times and a strong base. Thus, we envisioned that if organometallic reagents having a phosphonate group can be successfully prepared, it will be an efficient synthetic method of functionalized organophosphonates via C-C bond-forming reaction. We have developed in situ preparation of phosphoryl alkylindiums from the direct insertion of indium with bromoalkyl phosphonates in the presence of CuCl. The Pd-catalyzed cross-coupling reaction of the phosphoryl alkylindium reagents with a number of aryl iodides, bromides, and triflates and vinyl bromide proceeded smoothly to provide the functionalized arylalkyl phosphonates in good to excellent yields. A wide range of functional groups, including ester, ketone, aldehyde, nitrile, nitro, trifluoromethyl, chloride, methoxy, hydroxy, and amino, are tolerable in the cross-coupling reactions. Upon increasing the chain length between the bromide and the phosphoryl group, the directing effect by the phosphoryl group is observed.

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Organocatalytic Stereoselective Aza-Michael Reactions: Synthesis of Chiral Pyrazoles

이수정 조창우*

경북대학교 화학과

Pyrazole is important skeleton that exhibit a variety of interesting biological activities and thus have found application in the development of pharmaceuticals such as Celebrex and Zoniporide. However, the use of pyrazole as the *N*-centered heteroaromatic nucleophile remains almost unexplored in organocatalytic asymmetric reactions, in spite of the importance of pyrazole as optically pure *N*-heteroaromatic pharmacophores in biologically active natural products. Here, the use of pyrazoles as the *N*-centered heteroaromatic nucleophiles in the organocatalytic asymmetric aza-Michael reactions of enones will be presented.

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Cinchona-Based Primary Amine-Catalyzed Asymmetric Aza-Michael Reactions: Synthesis of Chiral Pyrroles

성언선 조창우*

경북대학교 화학과

Pyrroles are an important class of heterocycles that display a variety of remarkable biological activities and thus have found application in the development of pharmaceuticals. In organocatalytic asymmetric reactions, the use of pyrroles as N-centered heteroaromatic nucleophiles remained unexplored in contrast to the widely studied *C*-centered nucleophiles. However, recently, we reported the chiral prolinol trimethylsilyl ether-catalyzed asymmetric aza-Michael reactions of pyrroles as the *N*-centered heteroaromatic nucleophiles to α,β-unsaturated aldehydes. As the expansion of the organocatalytic asymmetric aza-Michael reactions with pyrroles as the *N*-centered heteroaromatic nucleophiles, we report the cinchona-based primary amine-catalyzed asymmetric aza-Michael reactions of pyrroles to α,β-unsaturated aldehydes.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal-Free, Brønsted Acid Mediated Synthesis of Coumarin Derivatives from Phenols and Propiolic acids

최혁 이구연*

강원대학교 생명건강공학과

Coumarin and its derivatives are one kind of important natural products in plants and show a wide range of biological activity. To date, various synthetic methods for coumarins have been developed. However, these most of synthetic methods require metal Lewis acid catalysts. In this study, we report a simple synthetic route to coumarin from phenols and propiolic acid using trifluoromethanesulfonic acid (TfOH) without metal catalyst in chlorobenzene at 100 °C.

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Asymmetric Synthesis of Chiral Azetidine Derivatives

장덕호 조창우*

경북대학교 화학과

3,3-Dinitroazetidine (DNAZ) derivatives are of interest to aerospace and defense industries due to their inherent energetic characteristics which come from a strained ring system with high nitrogen content. Recently, considerable efforts have been devoted to the synthesis of 3,3-dinitroazetidine derivatives and their application to the synthesis of biologically active lead molecules in medicinal chemistry. However, asymmetric synthesis of chiral 2-substituted-3,3-dinitroazetine derivatives remain unexplored in spite of the importance of 3,3-dinitroazetidine as the potential pharmacophore. Here, we report the stereoselective synthesis of chiral 2-substituted-3,3-dinitroazetines via diastereoselective aza-Henry Reactions with *N*-sulfinylimines.

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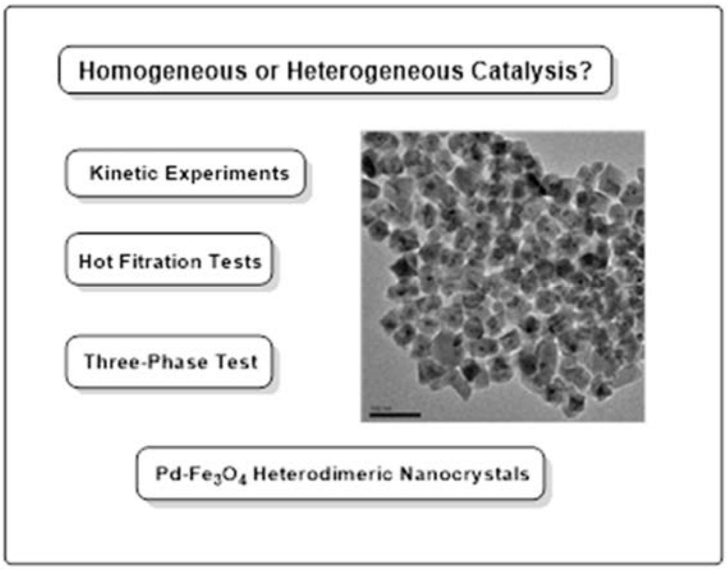
Mechanistic studies on the organic reactions catalyzed by Pd?Fe3O4 heterodimeric nanocrystals

변상문 김병문*

서울대학교 화학부

Recently, we have reported several useful catalytic reactions using Pd?Fe3O4 heterodimeric nanoparticles as novel magnetically recyclable catalysts. Successful applications of the nanocrystals toward various organic reactions such as Heck, Suzuki, and Sonogashira coupling reactions, direct C?H activation reaction, and Wacker oxidation have been reported. However, detailed mechanistic studies of these reactions have not been delineated. It has been unclear whether these reactions proceed through a heterogeneous or homogeneous mechanism. Herein, we report our detailed mechanistic investigations on the Suzuki coupling reaction and Wacker oxidation as two representative heterogeneous reactions employing the Pd-Fe3O4 catalysts. Hot filtration tests, general kinetic studies and three-phase tests were performed for the two reactions. The results of our investigation led us to believe that these reactions most likely proceed through the use of a solution-phase Pd species.



Homogeneous or Heterogeneous Catalysis?

Kinetic Experiments

Hot Fitration Tests

Three-Phase Test

Pd-Fe_3O_4 Heterodimeric Nanocrystals

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Synthesis of Fluorenes *via* Tandem Copper-Catalyzed [3 + 2] Cycloaddition and Rhodium-Catalyzed Denitrogenative Cyclization in a 5-*exo* Mode from 2-Ethynylbiaryls and *N*-Sulfonyl Azides in One Pot

서보람 김성화 이필호*

강원대학교 화학과

Fluorenes have attracted a great deal of attention due to their optical and electronic properties and their function as π-conjugated materials. They have been widely used as significant privileged structure in a myriad of areas such as optical agents, dyes, organic transistors, and light-emitting devices. Hence, an efficient synthesis of fluorene and its derivatives from easily available compounds has been continuously required. Especially, it is very important to prepare selectively unsymmetrically substituted fluorene derivatives and to introduce substituents at the C-9 methylene bridge of the fluorene moiety without use of base.In this paper, we report an efficient synthetic method of a wide range of unsymmetric fluorenes having enamine moiety at C-9 methylene bridge from *N*-sulfonyl-4-biaryl-1,2,3-triazole derivatives *via* Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode. Rh-catalyzed denitrogenative cyclization followed by catalytic hydrogenation produces the aminomethyl-substituted fluorenes in a one-pot. Moreover, fluorenes are prepared *via* tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode starting from 2-ethynylbiaryls and *N*-sulfonyl azides in a one-pot. In addition, fluorene was selectively produced in 99% yield in a 5-*exo* mode from triazole possessing 1-naphthyl group without the formation of 3,4-fused dihydroindoles *via* intramolecular dearomatizing [3 + 2] annulation in a 6-*exo* mode.1 Herein, we report a synthetic approach of fluorenes from *N*-sulfonyl-4-biaryl-1,2,3-triazoles *via* Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode.

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Application of Alkynyldimethylaluminum Reagents and Aluminum-amide Reagents prepared from Trimethylaluminum

정성수 이상협*

대구가톨릭대학교 생명화학과

Organoaluminum reagents have proven as remarkable reagents in organic synthesis due to their inherent reactivity, wide range of applicability, low cost and commercial availability. Organoaluminum compounds can easily react with various heteroatoms in organic molecules, particularly with oxygen and nitrogen, even with carbon to form a strong coordinate complex (1:1). As a latter example, Micouin et al. developed the alkynyldimethylaluminum reagent from the reaction of alkynes with trimethylaluminum using a catalytic amount of Et3N. This reagent has been utilized in a wide range of organic transformations, such as alkynylative ring opening of activated epoxides or oxazolidines, Pd-catalyzed cross-coupling reaction, addition reaction with acid chloride to form α,β-alkynyl ketones, and in the synthesis of aluminoisoxazoles, and pyrazoles, etc. One widely used reagent of note is dimethylaluminum amide, derived from the reaction between trimethylaluminum and corresponding amine. This reagent has been utilized in the direct conversion of ester or acid to amide, carbamate to urea and nitrile to amidine. As a part of ongoing research on development of new organic synthetic methods, we have utilized alkynyldimethylaluminums for the synthesis of N,N-disubstituted 3-amino-1,4-diynes and 3-amino-1-ynes (Scheme 1), α,β-alkynyl ketones (Scheme 2), N-substituted propiolamides (Scheme 3), N-aryl substituted, five- and six-membered azacycloalkanes, isoindoles and tetrahydroisoquinolines (Scheme 4).

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Synthesis of Mono, Di and Tri substituted Amidines from Amides using AlMe3

RAMACHANDRAN 이상협[1,*]

대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

Amidines are the valuable precursors for the synthesis of a wide variety of heterocyclic ring systems. They are representing an important pharmaphore in drug discovery and have been indicated as potential agents for the treatment of Alzheimer’s disease, malaria, and as inhibitors of acid-sensing ion-channels, platelet aggregation and serine protease. In addition, they have employed in the field of material science, catalyst design and also shown its capacity to fix carbon dioxide. Accordingly, a number of synthetic methods have been developed for the preparation of amidines. Typically, they are prepared by pinner reaction and modified pinner reaction that involves the addition of amine to an activated nitrile or imidate moiety which employ as common protocols for synthesizing amidines. Among the organometallic species, organo-aluminum motifs are more significant reagents due to their low cost, high selectivity and considerable stabilities. Owing to these advantages of organo aluminum moiety, it has been applied in various organic transformations. Traditionally, garigipati introduced AlMe3 in the synthesis of unsubtitituted amidines from nitriles and later by many others. We herein report the simple procedure for synthesis of mono, di and tri substituted amidines from primary, secondary and tertiary amides.

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Synthesis of Trifluoroethylated Alkynes by Pd Catalyst

임정아 김한성 황진일 이선우*

전남대학교 화학과

A trifluoroethylation of alkynes through apalladium-catalyzed decarboxylative coupling reaction wasdeveloped. When alkynyl carboxylic acids and ICH_2CF_3 wereallowed to react with $[Pd(\eta^3\text{-allyl})Cl]_2$/XantPhos and Cs_2CO_3in *N*,*N*-dimethylformamide (DMF) at 80 °C for 1 h, the desiredproducts were formed in good yields. This catalytic system showed high functional group tolerance.

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Copper-catalyzed One-pot Synthesis of Diketones

최진섭 이선우*

전남대학교 화학과

Benzil derivatives such as diaryl 1,2-diketones are synthesized via the direct decarboxylative coupling reaction of aryl propiolic acids and their oxidation. The optimized condition is that the reaction of aryl propiolic acids and aryl iodides is conducted at 140 ℃ for 6 h in the presence of 10 mol% CuI/Cu(OTf)$_2$ and Cs_2CO_3, and then HI (aq) is added and further reacted. It showed good functional group tolerance toward ester, aldehyde, cyano and nitro groups. In addition, symmetrical diaryl 1,2-diketones are obtained from aryl iodide and propiolic acid in the presence of palladium and copper catalyst.

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Synthesis of Alkynyl Amides using Palladium-Catalyzed Oxidative Aminocarbonylation via Decarboxylative Coupling

김한성 황진일 이선우*

전남대학교 화학과

Alkynyl amides were synthesized from palladium-catalyzed coupling reactions of alkynyl carboxylic acid and amines under carbon monoxide atmosphere. The reaction was conducted with palladium(II) acetate (5 mol%) and silver(I) oxide (1.0 equiv) in acetonitrile at 80 ^{o}C for 1 h. This method showed good to moderate yield and good functional group tolerance towards ketone, ester and nitrile groups.

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Phosphaannulation of Phosphonic Acids with Unactivated Alkenes through Palladium-Catalyzed C-H Activation/Cyclization Reaction

손정유 김선웅 이필호*

강원대학교 화학과

An efficient phosphaannulation via Pd(II)-catalyzed C-H activation/oxidative cyclization by 6-*endo* mode is reported for the synthesis of 3-substituted phosphaisocoumarins from the reaction of aryl phosphonic acids with unactivated alkenes under aerobic conditions. Also, α,α-disubstituted benzyl phosphonic acids were phosphaannulated with unactivated alkenes, producing phosphaisochromanones having (Z)-alkylidenyl groups via anti-phosphoryoxypalladation by 6-*exo* mode.

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Alkenylation of Phosphacoumarins via C-H Activation and Their Synthetic Application to Fluorescent Benzophosphacoumarins

김철의 손정유 이필호*

강원대학교 화학과

For several decades, organophosphorus compounds have received attention due to applications in diverse fields such as coordination and materials chemistry, homogeneous catalysis, pharmaceuticals, agrochemicals, additives for polymers, and flame retardants. We were attracted to developing a streamlined method for the synthesis of a myriad of phosphacoumarins and bezophosphacoumarins with the aim of making useful chemical libraries and probes. In addition, the importance of cross-dehydrogenative coupling reactions on Pd-catalyzed direct C-H alkenylation of heteroarenes has been rapidly increased. Herein, we have developed an oxidative alkenylation from the reaction of phosphacoumarins with a wide range of activated as well as non-activated alkenes via aerobic oxidative Heck reactions. Moreover, 3-alkenylphosphacoumarins undergo inverse electron demand Diels-Alder reaction with enamines in situ generated from ketone and pyrrolidine followed by 1, 2-elimination and a dehydrogenation, affording fluorescent benzophosphacoumarins.

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Synthesis of the novel hole transport layer materials for OLED

김미진 김보미[1] 정성훈[2] 채규윤[1,*]

원광대학교 화학 [1]원광대학교 화학과 [2]원광대학교 바이오나노화학과

In this study, the novel hole transport layer (HTL) materials with high glass transition temperature values based on carbazole and triphenylamine moieties were synthesized by Suzuki coupling reactions. Our preliminary results showed that these novel HTL materials good photophysical properties (PL, Tg, HOMO/LUMO, band gap, UV) to be used as hole transporthing materials for fabrication OLED device.

Keyword: Hole transport layer(HTL), carbazole, triphenylamine, OLED, Suzuki coupling

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Synthesis and fluorescence properties of rhodamine B derivatives containing 2-carboxybenzaldehyde

최재영 장승현*

대구대학교 화학과

In this research, we synthesized new kinds of fluorescent sensors by rhodamine B derivatives. Compound 1 was synthesized from compound 3 and 2-carboxybenzaldehyde. Compound 2 was synthesized from compound 4 and 2-carboxybenzaldehyde. These synthesized compounds were confirmed by measurement of ^{1}H-NMR and GC-Mass. These compounds were found selectivity for metal cation by fluorescence titration using various metal cations.

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Rhodium-Catalyzed Reaction of 2*H*-Azirines with *N*-Sulfonyl 1,2,3-Triazoles: Synthesis of Pyrazines

신서현 백용현 이필호*

강원대학교 화학과

Development of a new synthetic method for azaheterocyclic compounds is highly significant in the investigation for new medicines, active pharmaceutical ingredients (API), and fine chemicals. In particular, pyrazine is one of the most representative privileged azaheterocyclic scaffolds, which show cytostatic, antifungal, and antitumor properties and are broadly present in flavorings and alarm pheromones. Accordingly, access to pyrazines from easily available starting materials is highly required. we report herein an efficient synthetic route to a wide range of trisubstituted pyrazines is developed from Rh-catalyzed reaction of 2*H*-azirines with *N*-sulfonyl-1,2,3-triazoles through the elimination of nitrogen molecule and arylsulfinic acid. The present reaction proceeds through formation of in situ generated dihydropyrazines.

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The synthesis and fluorescence properties of rhodamine 6G derivatives containing fluorene-2-carboxaldehyde

박성호 장승현*

대구대학교 화학과

In this research, we synthesized fluorescent sensors from fluorene-2-carboxaldehyde and rhodamine 6G derivatives. The synthetic routes for rhodamine 6G derivatives containing fluorene-2-carboxaldehyde was outlined at scheme 1. The structures of new compounds were confirmed by ^{1}H-NMR and Mass. The compounds were confirmed to selectivity about Fe^{3+} by fluorescence titration using various metal cations. The binding analysis using the job’s plot suggested the compounds formed a 1:1 complex with Fe^{3+}.

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Porphyrin을 포함하는 conjugated microporous polymer의 합성 및 특성 연구

조진희 박경철 이창연[1,*]

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Conjugated microporous polymers(CMPs)는 building block 들이 π-conjugation 에 의해 연결된 다공성 물질로 기공도가 높고, 큰 표면적을 가진다는 특징이 있다. CMP 는 유사 다공성 소재인 Metal-organic frameworks (MOFs) 의 약한 금속-리간드 의 배위결합 대신 강한 공유결합을 사용 하기 때문에 기존 MOFs 가 가지고 있던 화학적 불안정성을 해결한 신소재로 주목 받고 있다. 또한 CMPs 는 building block, 합성방법 등을 선택함으로써 골격과 pore 의 크기, 표면적을 조절할 수 있다는 장점이 있어 가스 흡착, 촉매, light emitting, light harvesting, 전기에너지 저장 등에 많은 연구가 이루어지고 있다. 본 연구에서는 porphyrin 과 여러 광감응제 (Boron dipyrromethenes 혹은 pyrene)를 사용하여 여러 탄소-탄소 결합 반응을 통해 CMPs 를 합성하였다. 합성된 CMPs 는 FT-IR, NMR, N2 isotherm 등을 통해 특성을 파악하였으며 광학적 특성을 UV-Vis 과 Fluorescence spectrum 을 사용하여 관찰하였다.Acknowledgments : This work was supported by the Korea Foundation for the Advancement of Science & Creativity(KOFAC), and funded by the Korean Government(MOE).

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Unprecedent Desilylative Allyl Rearrangement of Homoallylic α-Silylamines

정욱 박재욱* 이영민* 이영호*

포항공과대학교(POSTECH) 화학과

Desilylative allyl rearrangement of homoallylic α-silylamines in the presence of acid has been discovered. This transformation represents formal [1,3]-sigmatropic rearrangement. Interesting diastereoselectivity and chirality transfer was also noted. Mechanistic rationale with the result of computational study will be discussed.

일시: 2015년 4월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-837**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Diastereoselective One-pot Synthesis of Cyclic cis-1,2-Aminoalcohols from trans-1,2-Azidoalcohols

김동길 정욱 박한규 박재욱* 이영호*

포항공과대학교(POSTECH) 화학과

Cyclic 1,2-aminoalcohol is an important building block for numerous biomolecules and chiral ligands. Thus, stereocontrolled synthesis of cyclic 1,2-aminoalcohol is an interesting topic in organic chemistry. Herein, a stereodivergent route to cyclic 1,2-aminoalcohol will be introduced. Ru-catalyzed generation and reduction of *N*-unprotected α-alkoxy ketimine afforded desired cyclic *cis*-1,2-aminoalcohol in one pot manner with excellent diastereoselectivity in good yield. Direct reduction of the cyclic 1,2-azidoalcohol afforded the cyclic *trans*-1,2-aminoalcohol as well. Notably, the synthetic utility of this novel approach will be also demonstrated by the stereodivergent synthesis of 3,4,6-trideoxy-3-aminosugars (D-desosamine derivatives).

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-838**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct C-5 arylation of [1,2,4]-triazolo[1,5-a]pyridine derivatives using a Pd catalyst

이미정 박진규*

부산대학교 화학과

[1,2,4]-Triazolo[1,5-a]pyridines constituted an important class of heterocyclic compounds. They have frequently been found in pharmaceuticals, fluorescent brighteners, complexing agents, herbicides, and electronic materials. Especially, C-5 substituted [1,2,4]-triazolo[1,5-a]pyridines are useful structures as DNA-dependent protein kinase, stabilizing agents for photographic emulsions, antibacterial agents, selective adenosine receptor antagonists and several inhibitors, such as PDE inhibitors, selective JAK1 inhibitors, and TGFβ receptor inhibitors. In spite of their usefulness, installation of an aryl group at the C-5 of triazolopyridine can only be achieved via multi-step reactions, such as Suzuki coupling reaction. From the perspective of green chemistry, the development of direct C-5 arylation would be attractive for rapid and systematic generation of useful heterocycles, however, which remains elusive so far. Herein, we describe Pd-catalyzed regioselective C-5 arylations of [1,2,4]-triazolo[1,5-a]pyridine derivatives. Further details will be provided in the presentation.

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장소: 일산 KINTEX
발표코드: **ORGN.P-839**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-catalyzed direct C-7 arylations of pyrazolo[1,5-a]pyridine derivatives

오경환 김성민 박진규*

부산대학교 화학과

In view of atom economy and sustainable chemistry, direct CH activation of aromatic compounds has been deeply investigated over the past 10 years and considered as an efficient synthetic method with broad applications. Especially, Pd-catalyzed regioselective CH arylations of heteroaromatic compounds have become alternatives to the traditional coupling reactions because many heteroaromatic organometallic reagents are quite unstable. Since we recognized that fused heterocycles have been used as the privileged backbones of many pharmaceuticals and electronic materials, we were interested in pyrazolo[1,5-a]pyridine derivatives and developed the direct C-7 arylation with aryl halides using a palladium catalyst. We expect this highly regioselective reaction to be quite promising for the preparation of a variety of useful pyrazolo[1,5-a]pyridines that are used in bioactive compounds and electronic materials. Further details will be provided in the presentation.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-840**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Discrimination of α/β-Amino Saccharide Anomers by Cucurbit[7]uril

장윤정 이영민* 김기문*

포항공과대학교(POSTECH) 화학과

The stereoisomer discrimination is important and challenging in chemistry and pharmaceutical research. Recently, we have reported that CB[7] can distinguish anomers of protonated amino saccharides including D-galactosamine (GalN), D-glucosamine (GlcN), and D-mannosamine (ManN), with high preference being for the α-anomers in water. Understanding how the anomer selection is achieved with CB[7] in a detailed manner will be crucial as a further guidance for the designing of new classes of binding systems especially for biological applications. This motivated us to investigate the underpinning mechanism of such selective host-guest interactions. By molecular dynamics (MD) simulations, we therefore, calculated the double binding free energy differences of the α- and β-anomers of protonated amino saccharides to the cavity of CB[7]. The simulations illustrated the consistent preferences for the α-anomers of all three saccharides with 2.4 ? 7.0 kJ/mol larger binding free energies over their β-counterparts. The relative solvation free energy calculations demonstrated that the desolvation process of amino saccharide had a governing effect on the selective encapsulation of α-anomers. Moreover, we successfully determined the X-ray crystal structure of the host-guest complex between CB[7] and GlcN, which confirmed the six membered ring of the α-anomer of GlcN is included deep inside the CB[7] cavity, consolidating the optimized lowest energy geometries of amino saccharide complexed CB[7].

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-841**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Isoindolinones from 2-Chlorobenzoic Acid using Copper iodide

GABRIELCHARLESEDWINRAJA 이선우*

전남대학교 화학과

we report an efficient one-pot method for the synthesis of isoindolinones from the 2-chlorobenzoic acid, aryl aryl propiolic acid and ammonium acetate by using copper iodide as a catalyst and cesium carbonate as a base. The employment of 2-chlorobenzoic acid provides easy accessible tool for the synthesis of isoindolinones. In addition, use of copper catalyst in the absence of a ligand, instead of an expensive palladium catalyst, allows the process to be cost effective.

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장소: 일산 KINTEX
발표코드: **ORGN.P-842**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence detection of Lewisite simulant by a disulfide bond receptor

이두희 이동남[1] 홍종인[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Currently growing international concern over terroristic attack using chemical warfare agents has led to the development of affordable and accurate detection of the toxic gases. Despite several decades of research, intense efforts have been mainly directed toward the detection of nerve agents. Lewisite, an organoarsenic compound, is classified as a blister agent, and causes severe skin, eye and mucosal pain and irritation. During World War II, British biochemists found that British anti-Lewisite (BAL; dimercaprol = 2,3-dimercaptopropanol) formed a stable chelate with Lewisite, thus reduced its toxicity. Mimicking the structure of BAL, we chose a disulfide bond as a binding site to recognize arsenic trichloride (ATC) which is a Lewisite simulant. A coumarin moiety was introduced as a fluorescence signaling unit. The addition of ATC resulted in change in the fluorescence intensity of coumarin, which was ascribed to the heavy atomic effect and/or photo-induced electron transfer mechanism owing to the coordination of the arsenic metalloid to a phenoxy oxygen and two sulfur atoms in the probe.

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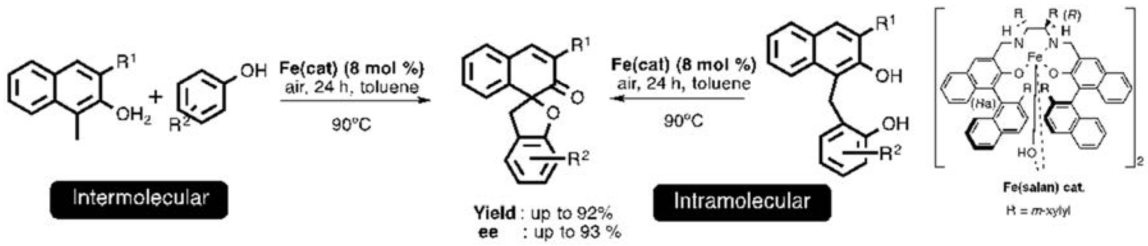
장소: 일산 KINTEX
발표코드: **ORGN.P-843**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Iron(salan)-Catalyzed Inter- and Intramolecular Asymmetric Oxidative Dearomatization for the Synthesis of Enantioriched Spirocyclic Compounds

KIM Chungsik OGUMA Takuya[1] FUJITOMO Chisaki[1] UCHIDA Tatsuya[2,*] KATSUKI Tsutomu[3]

International Institute of Carbon-Neutral Energy Research(I2CNER), Kyushu University [1]Graduate School of Science, Faculty of Arts and Science, Kyushu University [2]International Institute of Carbon-Neutral Energy Research(I2CNER), Kyushu University, Graduate School of Science, Faculty of Arts and Science, Kyushu University [3]International Institute of Carbon-Neutral Energy Research (I2CNER), Kyushu University, Institute for Advanced Study, Kyushu University

Asymmetric construction of spirocyclic compounds, which are found in various biologically active reagents and chiral auxiliaries, has attracted enormous attention. Recently, we found that optical active iron(salan) complex is an efficient catalyst for the formation of carbon quaternary center with good to high enantioselectivity via aerobic oxidative nucleophilic dearomatization of 1-methyl-2-naphthol derivatives with nitroalkane. Based on these results, we considered that methylenebis(arenol) derivatives also could proceed intermolecular nucleophilic dearomatization and obtain the corresponding spirocyclic (2H)-dihydrobenzofurans. Based on the consideration, we started investigation of iron(salan)-catalyzed asymmetric oxidative construction of spirocyclic compounds and achieved highly enantioselective formation of spirocyclic (2H)-dihydrobenzofurans. Under the iron(salan)-catalyzed aerobic conditions, in situ generated or separately synthesized methylenebis(arenol) derivatives could convert to corresponding spirocyclic (2H)-dihydrobenzofurans with good to high yields (up to 92 %) and enantioselectivities (up to 93 %).


R^1
OH$_2$
+
OH
R^2
Fe(cat) (8 mol %)
air, 24 h, toluene
90°C
Intermolecular
R^1
O
O
R^2
Yield : up to 92%
ee : up to 93 %
Fe(cat) (8 mol %)
air, 24 h, toluene
90°C
R^1
OH
OH
R^2
Intramolecular
R
R (R)
H
N
N
H
O
Fe
O
(Ra)
R
R
HO
2
Fe(salan) cat.
R = m-xylyl

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-844**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regio- and Stereoselective Synthesis of α-Vinylated γ-Oxo-β-Amino Esters involving Rh-Carbene Promoted [3,3]-Sigmatropic Rearrangement

정다정 전현지 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

The development of concise catalytic methods for stereocontrolled synthesis of non-natural amino acid derivatives is a continuing challenge in organic synthesis. Due to the multi-functionality enabling further synthetic elaborations, γ-oxo amino esters have drawn considerable interest.Herein we report the first catalytic one-pot synthesis of highly functionalized α-vinylated γ-oxo-β-amino esters starting from readily available 1-alkynes, sulfonyl azide, and γ-hydroxy-α,β-unsaturated esters, in which copper(I) and rhodium(II) catalysts sequentially assembled the starting molecules to generate allylic (Z)-amino vinyl ether, which then rapidly undergoes deconjugative [3.3]-sigmatropic rearrangement to result in target non-natural amino acid derivatives in high yields with high levels of diastereoselectivity.

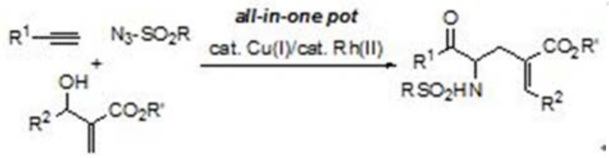
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-845**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Multi-funtionalized Non-Natural Amino Acid Derivatives involving Rhodium-Carbenoid Promoted Claisen Rearrangement

전현지 정다정 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

Amino acids play a vital role in living systems,and represent an under-utilized inventory of building blocks for protein engineers, medicinal chemists, and materials scientists.Given this significance, the development of succinct catalytic methods for synthesis of non-natural amino acid derivatives is a continuing challenge in organic synthesis.Herein, we present a new tandem one-pot catalytic method to access highly functionalized d-oxo-r-amino esters starting from 1-alkynes, sulfonylazides, and Morita-Baylis-Hillman adduct by using copper(I) and rhodium(II) catalysts, in which the rhodium carbenoid-promoted Claisen rearrangement is involved as a key reaction.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-846**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Phytochemical constituents from the flower of Robinia psudoacacia

홍성수

(재)경기과학기술진흥원 천연물연구팀

Robinia psudoacacia extract was suspended in distilled water and partitioned with solvent to give EtOAc, and n-BuOH. The purification of each fraction by column chromatography separation and HPLC analysis. Consequently, eight known compounds, resacetophenone (1), 2,4-dihydroxybenzaldehyde (2), 3,4-dihydroxybenzaldehyde (3), norathyriol (4), 3,8,9,10-tetrahydroxyurolithin (5), 3,8,9-trihydroxyurolithin (6), catechin lactone A (7), and bis(2-ethylhexyl) phthalate (8) were isolated from the flower of R. psudoacacia. The identification and structural elucidation of compounds were based on 1D and 2D NMR spectroscopic data analysis and MS data.

일시: 2015년 4월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-847**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal Precursors Having Novel Aminoalcohol Ligands for MOCVD and ALD

이가연 전동주[1,*] 정택모[2] 김창균[3] 박보근[3]

고려대학교 화학과 [1]한국화학연구원 화학물질연구단 [2]한국화학연구원 화학소재연구단 [3]한국화학연구원 화학소재연구본부

Semiconductor is composed of a number of processes, many materials are being used. In recent years, Vacuum technology such as metal organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD), one of the key processes, and the materials used in the process are attracting a lot of attention, especially, metal precursor has become a major concern. The role of ligand is important precursor in order to have the property suitable for the process. we have successfully developed excellent metal precursors, especially containing amino alcohol-type ligands and adopted them to deposit metal and metal oxide thin films using CVD and ALD for advanced electronic devices. Here we will discuss our recent results on new metal precursors synthesized novel amino alcohol-type ligands by molecular design. The compound was characterized using NMR spectroscopy, FT-IR and Elemental Analysis.

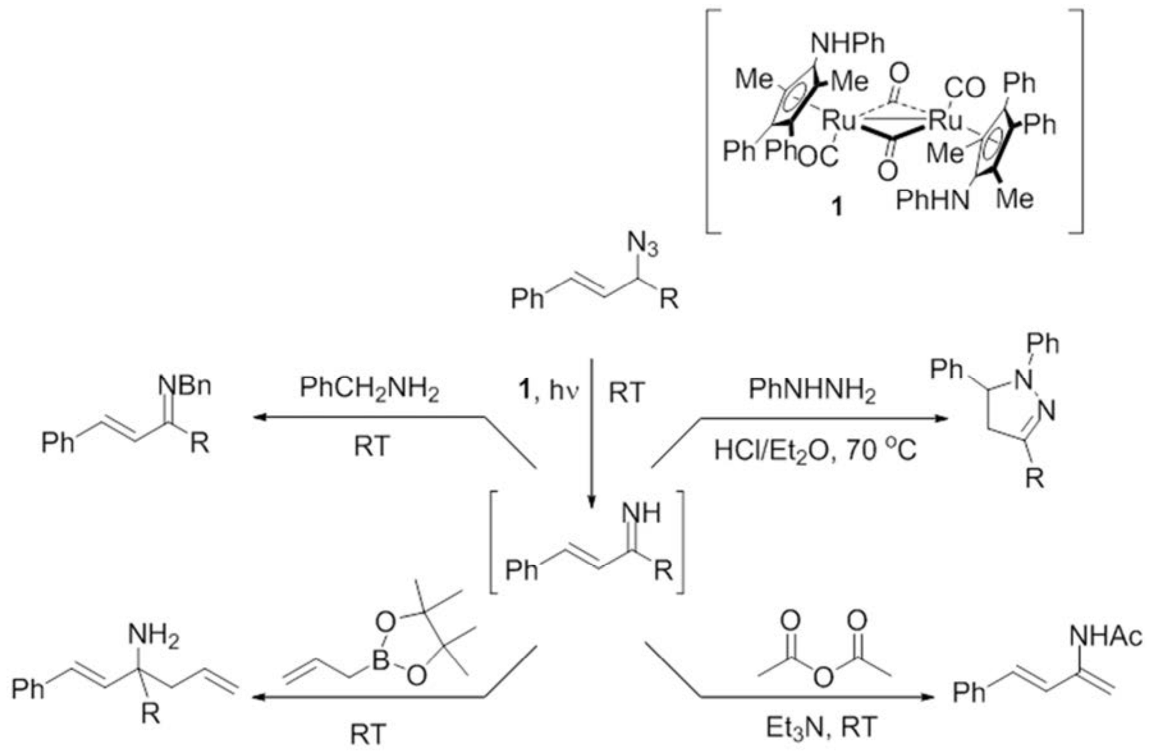
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-848**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1-H-azadienes from allylic azide and its utilizations in various organic transformations

권예랑 이영호* 박재욱*

포항공과대학교(POSTECH) 화학과

1-H-azadienes are valuable building blocks for the synthesis of various nitrogen-containing compounds, because they act as electrophiles in 1,2-addition and Michael-type 1,4-addition reactions as well as N-nucleophiles. They were also used in cycloaddition reactions as heterodienes to generate heterocyclic compounds. We synthesized various 1-H-Azadienes from allylic azides by a ruthenium catalysis under mild and neutral conditions. The 1H-azadines were characterized by IR and NMR spectroscopy, and utilized in organic transformations to afford N-substituted 1-azadiens, pyrazolines, tertiary carbinamines, N-acetyl dienamides, N-cyclohexenylacetamides and pyridine derivatives.


NHPh
Me
Me
O
CO
Ph
Ru
Ru
Ph
Ph
Ph
OC
O
Me
1
PhHN
Me
N3
Ph
R
NBn
PhCH2NH2
1, hν
RT
PhNHNH2
Ph
N
Ph
R
RT
HCl/Et2O, 70 °C
N
R
NH
Ph
R
NH2
O
O
NHAc
O
B
O
O
Ph
Ph
R
RT
Et3N, RT

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-849**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Reverse Phase Transfer Catalyst Based on Calix-[4]-Arene for Nucleophilic Fluorination

최원실 김진관 임재욱 정현진 김동욱*

인하대학교 화학과

The calixarenes (1) comprise an extensively studied class of macrocyclic, polyphenolic compounds that are usually strongly associated with host-guest chemistry. Remarkable applications of calixarene derivatives have been discovered, which include their use as platforms for shape-selective catalysts, efficient sensors, highly selective extractants, enzyme mimics, precusors of capsules, molecular glue for multimetal assembly, building blocks for nanoporous materials, and sophisticated auxiliaries in separation science (2).We have prepared calix-[4]-arene substituted tert-alcohol that can act as highly efficient multifunctional organic promoter to increase the reactivity of CsF significantly in nucleophilic fluorinations and provide the required fluorination product in excellent yield.This calix-[4]-arene substituted tert-alcohol system could not only enhance the reactivity of CsF significantly but also reduce the formation of byproducts. Further studies on the development of more efficient calix-[4]-arene substituted tert-alcohol through its structural modifications and the applications of these unusual promoter to other chemical transformations as well as the rapid 18F labeling for radiopharmaceuticals with PET are currently underway.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-850**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Synthetic Method of heterobiaryls through Sequential N-H Functionalizations

이동진 신진환 유은정*

강원대학교 화학과

Our laboratory have reported reaction of rhodium(II) azavinyl carbene, generated from 1-sulfonyl-1,2,3-triazole, with N-containing compounds. Given the recent interest in the characteristic exhibited by this carbene species, we envisioned their application to synthesize C-N-coupled heterobiaryls. In this symposium, synthetic route for C-N-coupled heterobiaryls will be presented. Various 9*H*-carbazoles are stereoselectively inserted into the rhodium(II) azavinyl carbene species to afford (*Z*)-carbazolated enamide, which cyclizes to indole by palladium-catalyzed C-H amination. Owing to the compatibility of this method with various substrates, the novel construction of unprecedented C-N-coupled heterobiaryls is possible.

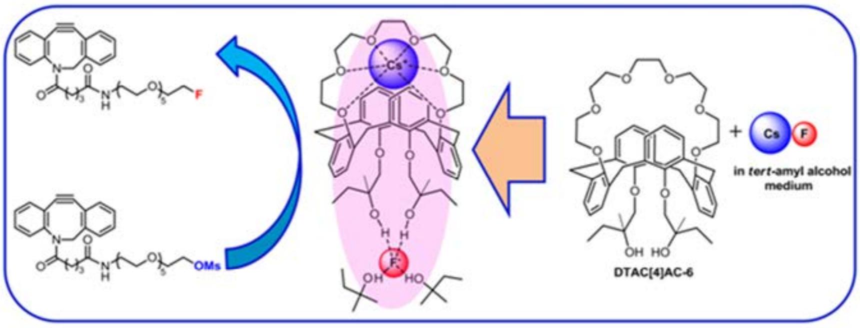
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-851**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hexaethylene Glycol Bridged Dicatioic Ionic Liquids: Significantly Enhanced Reactivity of KF in Nucleophilic Fluorination as Organic Promoter

최원실 정현진 김진관 임재욱 김동욱*

인하대학교 화학과

The calixarenes (1) comprise an extensively studied class of macrocyclic, polyphenolic compounds that are usually strongly associated with host-guest chemistry. In particular, calix[4]arene was the simplest representative of this family of compounds, which is easily accessible in large quantities, is a very convenient building block (find refs), there have been many reports on the complexation properties of calix[4]arene derivatives as a potential ionophores with metal ions (3). In recent years, the synthesis of fluorinated biomolecules has attracted much attention from the scientific community as a result of the importance of these compounds in pharmaceutical science and radiological applications involved with positron emission tomography (PET) studies. we have designed and synthesized highly efficient PTC di-tert-alcholic-calix[4]arene crown-6 (DTAC[4]AC-6) for nucleophilic fluorination using KF. This DTAC[4]AC-6 significantly enhanced the reactivity of KF, and well as selectivity of nucleophilic fluorinations. Furthermore, by their synergistic effect, the combination of DTAC[4]AC-6 and tert-amyl alcohol media system showed tremendous efficiency in the fluorination of base-sensitive substrates.


F
OMs
Cs⁺
F⁻
+
Cs
F
in tert-amyl alcohol medium
DTAC[4]AC-6

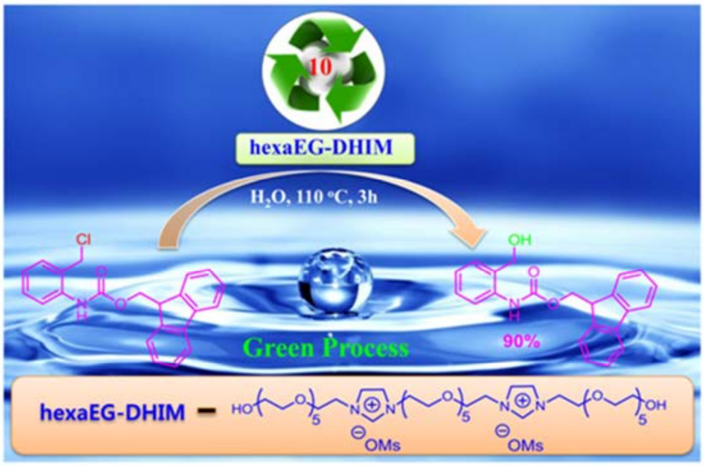
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-852**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hexaethylene Glycol Bridged Di-catioic Ionic Liquid: Significantly Enhanced Reactivity of water in Eco-Friendly Nucleophilic Hydroxylation

김진관 정현진 최원실 임재욱 김동욱*

인하대학교 화학과

The interest in di-cationic ionic liquids (DCILs) was mainly due to their additional properties such as several combinations of cations, anions, and linker explored the opportunity to design their structures to achieve significant properties according to specific chemical task, high melting points, and exhibited a thermal stability and volatility higher than that of mono-cationic ILs. Water is the most vital element among the natural resources, and is a “universal solvent” where most elements and compounds can dissolve in its powerful molecular structure. We have designed and prepared well-tailored hexa-ethylene glycol bridged DCIL hexaEG-DHIM as multifunctional organic promoter for nucleophilic hydroxylations using water at 110 oC. This hexaEG-DHIM could enhance the reactivity of H2O significantly in nucleophilic fluorinations. Furthermore, chemoselective hydroxylation of base sensitive substrate by hexaEG-DHIM was achived in excellent yield, In addition, the recyclability and stability of hexaEG-DHIM was also studied, the hexaEG-DHIM could be reused repeatedly (10 times-run) in the hydroxylation using water without loss of its activity and decomposition.


10
hexaEG-DHIM
H2O, 110 °C, 3h
Cl
O
N
H
O
OH
Green Process
90%
hexaEG-DHIM
HO
O
5
N
N
OMs
OH

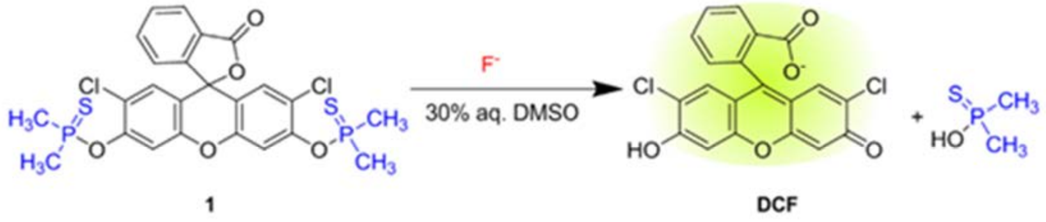
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-853**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric and fluorogenic signaling of fluoride ions by thiophosphinated dichlorofluorescein

장인정 이상훈 장석규*

중앙대학교 화학과

A new fluoride-selective chemosignaling probe based upon thiophosphinated dichlorofluorescein has been developed. Prominent chromogenic and fluorogenic signaling is realized by employing fluoride-selective cleavage of the latent thiophosphinated probe in mixed aqueous media. The signaling process is confirmed by the UV-vis, fluorescence measurements as well as ^1H and ^{31}P NMR spectroscopy. Possible interferences from Hg^{2+} and Cu^{2+} ions are readily suppressed by using diethylenetriaminepentaacetic acid as a masking agent. With the aid of the masking agent, the probe also shows potentially useful sensing ability for the determination of fluoride ions in practical samples of tap water and simulated wastewater. The limit of the fluoride detection by probe 1 is 9.8 nM.



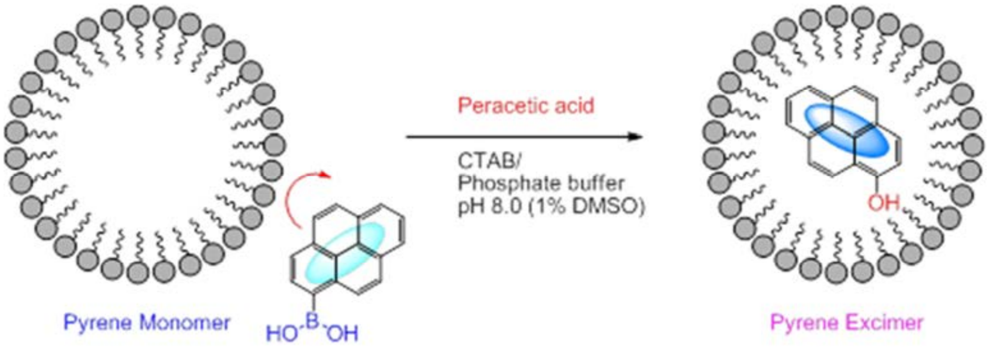
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-854**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Micelle-assisted signaling of peracetic acid by pyreneboronic acid via monomer-excimer switching

조민정 이효진 장석규*

중앙대학교 화학과

A simple fluorescent probe for the industrial oxidant peracetic acid (PAA) has been investigated. The signaling behavior of PAA is due to PAA-assisted oxidative conversion of 1-pyreneboronic acid into 1-hydroxypyrene. Pyreneboronic acid is found to display selective signaling behavior, being more responsive to PAA than to other commonly used practical oxidants such as H_2O_2 and HOCl. The changes in pyrene monomer fluorescence to excimer are used in the ratiometric analysis of PAA. When using the surfactant cetyltrimethylammonium bromide (CTAB) as a micellar additive, the ratiometric signaling of PAA is markedly enhanced. Selective fluorescence signaling of PAA by 1-pyreneboronic acid with a detection limit of 1.5 x 10^{-6} M in aqueous environments is successfully achieved.



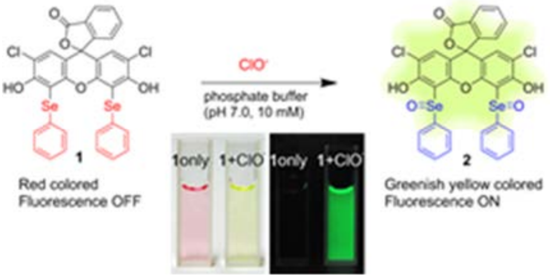
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-855**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual signaling of hypochlorite by selective cleavage of selenated dichlorofluorescein and its application in tap water

박현지 정연욱 장석규*

중앙대학교 화학과

A new hypochlorite selective signaling probe based on a selenated dichlorofluorescein has been developed. Hypochlorite-assisted oxidation of selenyl ether group of the probe **1** into selenoyl group resulted in prominence colorimetric and turn-on fluorescence signaling. The signaling shows no appreciable changes for other widely used practical oxidants (such as H_2O_2, O_2^-, *tert*?butyl hydroperoxide, percarbonate, and perborate), and proceeds rapidly within 5 min. The signaling of hypochlorite is not affected by the presence of commonly encountered relevant metal ions and anions except bromide and iodide ions. The detection limit for the determination of hypochlorite is 4.87 x 10^{-7} M in pH 7.0 phosphate buffer solution. As practical application of the probe, visualization of hypochlorite in tap water was tested.



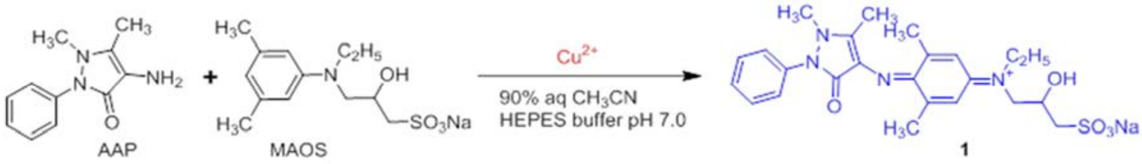
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-856**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric signaling of Cu^{2+} ions by oxidative coupling of anilines with 4-aminoantipyrine

홍자민 정용애 장석규*

중앙대학교 화학과

A new Cu^{2+}-selective signaling system by oxidative coupling of anilines with 4-aminoantipyrine (AAP) has been investigated. Cu^{2+}-assisted reaction of *N*-ethyl-*N*-(2-hydroxy-3-sulfopropyl)-3,5-dimethylaniline (MAOS) with AAP resulted in pronounced colorimetric signaling of Cu^{2+} ions by color change from colorless to blue. The signaling is possible without any extra oxidants, such as hydrogen peroxide, and proceeds rapidly within 5 min. Signaling is not affected by the presence of common metal ions as background. The detection limit for the determination of Cu^{2+} ions is 4.0 x 10^{-6} M in 90% aqueous acetonitrile. Applications as a convenient chromogenic test strip for the practical samples of industrial wastewater or synthetic urine are tested.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-857**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Conformaional Study of A Series of Depsipeptides Containing Unnatural Building Blocks

장근혁 최수혁*

연세대학교 화학과

Within the past decade, the folding properties of several types of foldamers with unnatural backbones have been explored. At this point, We will discuss a new helical secondary structures of depsipeptides. Depsipeptides containing one or more ester bonds in addition to the amide bonds have emerged as an important source of biomedical compounds. In this study, We incorporated unnatural residues into a depsipeptide, then studied on the conformational behavior of depsipeptides.

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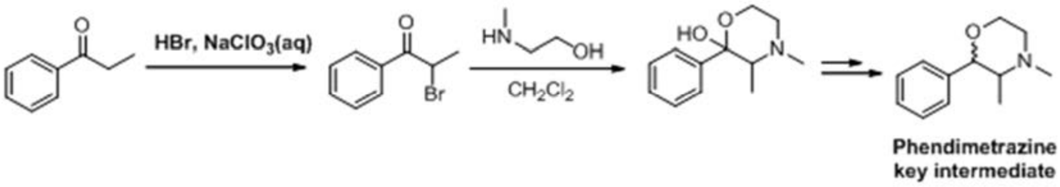
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Key Intermediates of an active stimulant obesity drug Phendimetrazine tartrate Using Eco-friendly and Economical Bromination Method

고성현 반재영 정유리 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Phendimetrazine tartrate is used as an appetite suppressant to treat obesity. The known syntheses of this drug include the exothermic pathways and toxic reagents or byproducts. Therefore, we focused on the development of a more reliable process for its synthesis and were successful to develop the key steps using cheap, easy to handle and eco-friendly reagents and conditions specifically for bromination.



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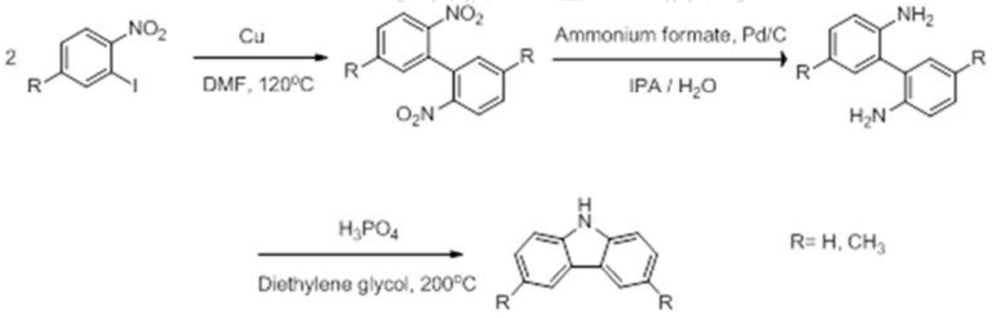
장소: 일산 KINTEX
발표코드: **ORGN.P-859**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient and Economical synthesis of carbazoles by using Ullmann Coupling reaction, reduction and consecutively processing Tauber carbazole synthesis

백정현 반재영 shabbir saira[1] 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Carbazole derivatives are widely employed in Organic Light-Emitting Diodes that offer significant promise for reducing energy usage in lighting and display technology. Typical key intermediates of carbazole derivatives are expensive; therefore, we investigated the synthesis of carbazoles by efficient and economical process. We synthesized carbazoles economically using Ullmann Coupling reaction, reduction and Tauber carbazole synthesis with good yields.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-860**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal Precursors Synthesized by Novel amide-type Ligands for MOCVD and ALD

남지현 전동주[1,*] 박보근[2,*] 정택모[3,*] 김창균[2,*]

고려대학교 화학과 [1]한국화학연구원 화학물질연구단 [2]한국화학연구원 화학소재연구본부 [3]한국화학연구원 화학소재연구단

New precursors for metal and metal oxide thin films have been required continuously for diverse applications to electronic devices. In vacuum technology such as metal organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) the development of metal precursors having desirable properties such as high vapor pressure and thermal stability is most important and so design and preparing suitable organic ligands is indispensable. so I have tried to synthesize ligand to get a suitable precursor as a result I synthesized the ligand of the amide type further more I attempt to synthesize precursor using to ligandIn the synthesis of new ligands through FT-IR, 1H NMR, 13C NMR, EA (elemental analysis) determine the synthesis and further synthesizes the new precursor to evaluate and apply to the process

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발표코드: **ORGN.P-861**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stable helical structures of α/β-peptides for 12/10- and 11/9- mixed helices

김유진 최수혁*

연세대학교 화학과

Peptidic foldamers consisting of α- and β-amino acid residues adopt a variety of helical secondary structures. Oligopeptides containing D-Alanine and cis-ACHC have been reported to exhibit a high propensity to form 11/9 helical structures. Also cis-ACHC residues afforded 12/10 helix formation with alternating backbone configuration. From this information, we designed α/β-peptides forming stable 12/10- and 11/9-mixed helices. In this study, the torsion angle of 3rd residue of pentapeptides had an important role in the stability and handedness of the helix. 5 kinds of different β-amino acid were replaced at the 3rd residue of pentapeptides to observe stable conformation and it confirmed by X-ray crystallography.

일시: 2015년 4월 15~17일(수~금) 3일간
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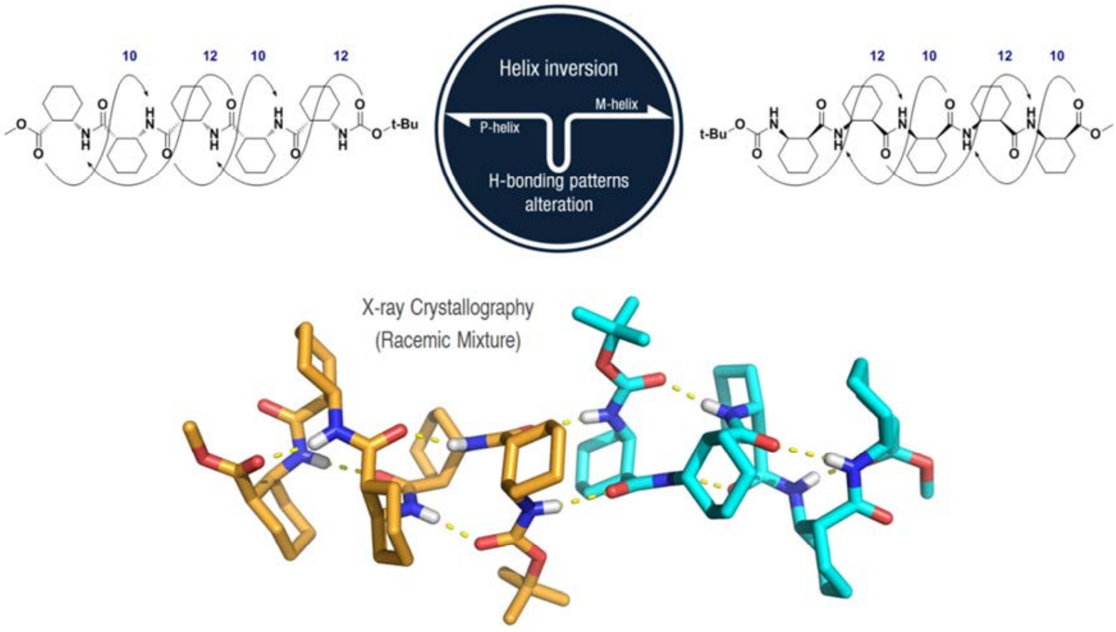
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrogen bonding patterns alteration for helix inversion

신선호 최수혁*

연세대학교 화학과

We synthesized β-peptide oligomers consisting of (1S, 2R)-Aminocyclohexanecarboxylic acid (ACHC) and (1R, 2S)-ACHC. The ACHC has two stable chair conformations. Using this character, we altered hydrogen bonding patterns and induced a helix inversion. We expected that these β-peptides will adopt 10/12-helix conformation, and we modified compounds through various methods in order to alter H-bonding patterns. In some cases, we confirm helix inversions by using Circular dichroism and X-ray crystallography.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-863**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of α/β peptide oligomers containing cis-APiC and change of helix propensity using various cis-APiC`s substitution compound

최성림 최수혁*

연세대학교 화학과

Generally, we can study various helical secondary structures for synthesis of many peptide oligomers containing various residues. This research focus on α/β-peptides oligomers containing 6-membered ring β-residues because , from the previous study, we researched that α/β-peptides oligomers containing cis-ACHC and L-Ala have two intramolecular hydrogen bonds: C=O(i) ... H-N(i+3) and C=O(i) ... H-N(i-1).This research shows that α/β-peptides oligomers` helical structure is changed by transformation form cis-ACHC to some 6-membered ring β-residues such as cis-APiC. And then, by so changing substituents to nitrogen in piperidine ring from cis-APiC, change of α/β-peptides oligomers` conformational characterization is researched.

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장소: 일산 KINTEX
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Diketopyrrolopyrrole Based Copolymer for OTFTs

장용주 이다현 SHAIK BAJI 박민주 송동진 강훈민 이상경*

경상대학교 화학과

Synthesis and physical properties of a novel organic thin film transistors (OTFTs) material containing thiophene and diketopyrrolopyrrole derivative was studied. Stille coupling reaction was used for the synthesis of this material at the final step. The obtained compound was confirmed by Mass, FT-IR, 1H-NMR, 13C-NMR spectroscopy and elemental analysis. The thermal properties of the compound were analyzed by thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC). Optical and electrochemical properties of the compound were analyzed by UV-vis absorption spectroscopy and cyclic voltammetry.

일시: 2015년 4월 15~17일(수~금) 3일간

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발표코드: **ORGN.P-865**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of nitrogen-rich heterocycle compound for Organic Light Emitting Diodes (OLEDs)

이다현 장용주 박민주 송동진 강훈민 **SHAIK BAJI** 이상경*

경상대학교 화학과

Nitrogen-rich heterocyclic molecules have been focusing for development of electron transporting materials (ETMs). Because nitrogen have lone pair electrons, leading high electron mobility. So nitrogen-rich heterocycle compound was synthesized by Suzuki and Stille coupling. The obtained compound was confirmed by ^{1}H-NMR and ^{13}C-NMR. Thermal stability was characterized by TGA and DSC. TGA showed the decomposition temperature (T_d) corresponding to 5% weight loss at 482 ℃. DSC showed the glass transition temperature (T_g) at 150 ℃. Physical properties were characterized by UV, PL spectra. Based on the absorption edges in the UV-Vis absorption spectrum, the optical energy gap (E_g) was calculated to be 3.05 eV. Electrochemical stability was characterized by CV. From the CV data HOMO level calculated from the onset of oxidation potential was -5.64 eV. LUMO level was calculated from the HOMO value and the energy gap (3.05 eV) was -2.59 eV. Electron transporting ability was measured by EOD (Electron-Only Device), which showed 40 mA/cm^2.

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장소: 일산 KINTEX
발표코드: **ORGN.P-866**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of trans-Cyclopently Tadalafil from L-Tryptophan

박민주 이다현 장용주 SHAIK BAJI 송동진 강훈민 이상경*

경상대학교 화학과

Tadalafil is known for the treatment of pulmonary hypertension, and its analogues possess two stereogenic chiral centers at C-6 and C-12a positions in the tetra cyclic scaffold, and have four stereomers with (6R,12aR), (6R,12aS), (6S,12aS) and (6S,12aR)-configurations. Recently, (6S,12aR) stereomer is focused on. Many similar tetracyclic compounds, that possess different configurations of both chiral centers, exhibited various other biological activities, or can be used as intermediates in the pharmaceutical synthesis. Here, the synthesis of trans-Cyclopently Tadalafil from L-tryptophan was described. The title compound was synthesized via six steps starting from the L-tryptophan methyl ester hydro chloride. trans-Cyclopentyl tadalafil can be expect to exhibit good pharmacological effect. So, will be researched for biological test in the future.

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발표코드: **ORGN.P-867**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of nitorogen hetrocycle material related with OLED

강훈민 장용주 이다현 박민주 송동진 SHAIK BAJI 이상경*

경상대학교 화학과

A nitorogen containing heterocycle materials, which have been widely used for development of electron transporting materials (ETMs). Because nitorogen containing heterocycle materials have high electron mobility. The compound was synthesized by suzuki and Stille coupling. The obtained material was confirmed by ^{1}H-NMR and ^{13}C-NMR. The thermal stability of material was measured by thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). The compound was shown the decomposition temperature(T_d) at 5% weight loss at 481℃ and the glass transition temperature (T_g) at 164 ℃. Electrochemical stability was characterized by CV. The HOMO energy level of the compound was determined to be -5.62 eV. The LUMO energy level of the compound, calculated from the obtained HOMO level and optical energy gap (E_g = 3.1 eV), was -2.52 eV. Optical properties were characterized by UV absorption and photoluminescence (PL) spectra. Electron-only device (EOD) was measured to know Current density-voltage, which showed 15 mA/cm^2.

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발표코드: **ORGN.P-868**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Transitor Properties of Asymmetric Oligothiophenes:Relationship between Molecular Structure and Device Performance

송동진 장용주 이다현 박민주 강훈민 SHAIK BAJI 이상경*

경상대학교 화학과

A series of three thiophene-naphthalene-based asymmetric oligomers-5 - decyl-2,2': 5',2'':5'',2'''-quaterthiophene (DtT), 5-decyl-5''-(naphthalen-2yl)-2,2':5',2''-terthiophene (D3TN), and 5-(4-decylphenyl)-5'-(naphthalen-2yl)-2,2'-bithiophene (DP2TN) - was synthesized by Suzuki cross-coupling reactions. The long alkyl side chains improved both the solubility of the oligomers in solvent and their tendency to self-assemble. UV/Vis absorption measurements suggested that DtT, D3TN, and DP2TN from H-type aggregates with a face-to-face packing structure. In addition, the three oligomers were found to adopt vertically aligned crystalline structures in films deposited on substrates, as revealed by grazing-incidence wide-angle X-ray scattering. These oligomers were used as the active layers of p-type organic field- effect transistors, and the resulting devices showed field-effect mobilities of 3.3×10-3 cm2V-1s-1 for DtT, 1.6×10-2 cm2V-1s-1 for D3TN, and 3.7×1.6×10 -2 cm2V-1s-1 for DP2TN. The differences in transistor performances were attributed to the degree π overlap and the morphological differences determine d by the molecular structures.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-869**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Donor-Acceptor Based OTFT Material containing Benzoselenadiazole as Acceptor

SHAIK BAJI 장용주 이다현 이상경*

경상대학교 화학과

OTFTs composed of donor-acceptor based compounds have shown significant charge mobility. The selenium containing benzoselenadiazole as an acceptor has not much studied. The benzoselenadiazole as an acceptor material was synthesized by the dehydration of 1,2-phenylenediamine in the presence of selenium dioxide. The compound coupled with donor group to construct the donor-acceptor material. The synthesized compound was characterized by the IR, NMR and mass spectra. The thermal properties were analyzed by TGA and DSC analysis. The electrochemical properties were analyzed by cyclic voltammetry analysis. The optical properties were analyzed by UV-visible absorption and PL emission spectroscopy. The compound has shown good thermal stability. The OTFT characterization is under process.

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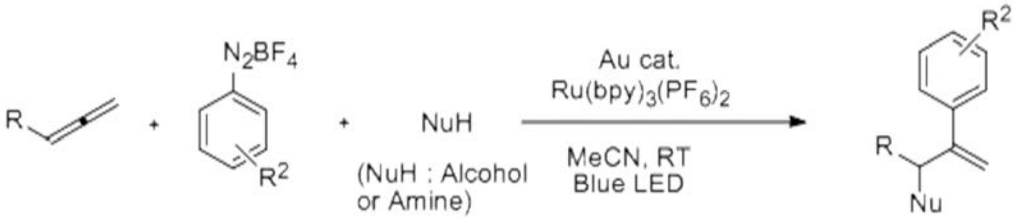
발표코드: **ORGN.P-870**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Three-Component Aryl Alkoxyation of Allenes under the Dual Gold and Photoredox Catalysis

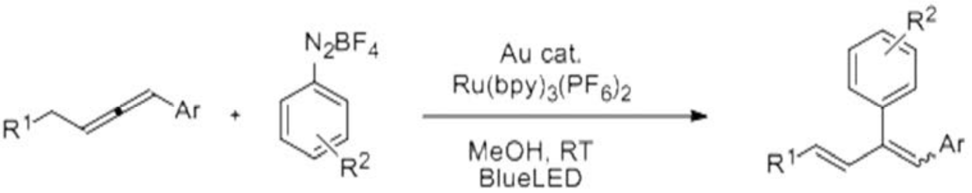
<u>윤호근</u> 신승훈*

한양대학교 화학과

Gold-catalyzed hydroalkoxylation or hydroamination of allene occurs intra- and intermolecularly, leading to allyl ethers or allylamines, respectively.1,2 Herein, we developed three-component coupling of alcohols, allenes and aryl diazonium salt by dual catalysis of gold and Ru-photocatalyst (Eqs. 1 and 2). Proposed mechanism involves auroalkoxylation followed by photoredox coupling of the vinyl gold species with arene diazonium salts. In the case of 1,3-di-substituted allenes, in the place of the desired, 2-diaryl-1,3-dienes were obtained as a major product. Progress on the scope and the mechanism of these transformations will be presented.



(1)



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Synthetic studies towards spliceostatin E

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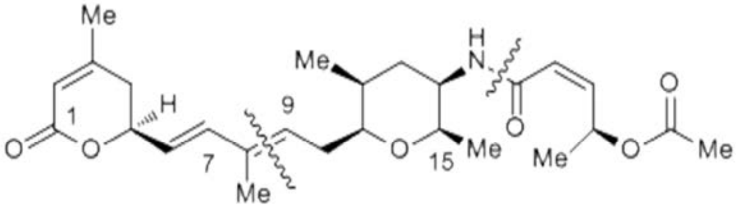
Splicesome is a ribonucleoprotein which is associated in splicing step during the gene expression. Removal of intrones (noncoding sequences) followed by ligation of exones (coding sequences) takes place in this event. Splicing inhibitors exhibit their activity by binding to the subunit of splicesome. Spliceostatins that shows splicing inhibitory activity are structurally complex molecules with implications of anticancer drug development. Spliceostatin E, structure of which is shown below, is one of structurally related compounds that belong to spliceostatins. We have been interested in the synthesis of spliceostatin E. Our efforts to synthesize the C1-C7 part and the C9-C15 core tetrahydropyran ring part will be presented.



Spliceostatin E

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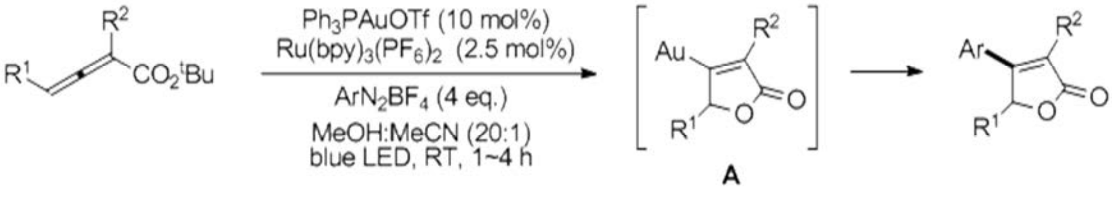
Combining Gold and Visible-light Photoredox Catalysis for Cross-Coupling of Allenoates with Aryl Diazonium Salts

PATILDILIPVITTHAL 신승훈*

한양대학교 화학과

Over the past decade, gold catalysis has evolved into an indispensable tool for organic transformations, allowing access to complex structures in short steps. In majority of these transformations, C(sp2)-Au or C(sp3)-Au species undergo simple proto-demetallation. Cross-coupling of these intermediates will significantly expand the utility of gold catalysis. However, the application in the cross-coupling chemistry is limited due to the reluctance of Au(I) to undergo two-electron oxidation. Recently, single-electron transfer (SET) redox property of Au(I) has been highlighted in the photoredox catalysis, enabling cross coupling of C(sp3)-Au with arene diazonium salts.1 We hypothesized that this SET condition could lower down the barrier of oxidation of Au(I), enabling cross-coupling with C(sp2)-Au species. We found that a vinyl gold obtained from the cyclization of tert-butyl allenoate underwent an efficient coupling with arene diazonium salts in the present of Au and Ru catalyts under the irradiation of blue LED. Control experiments indicated that the reaction occurred via a dual pathway, i.e. either initial Au(I) oxidation, then cyclization or initial cyclization, then Au(I) oxidation. Surprisingly, cross-coupling of the isolated A occurred in the absence of light and photocatalyst, indicating both two-electron and SET pathways are operative.



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Investigation of total synthesis of fimsbactin A and a preliminary evaluation of its siderophore function

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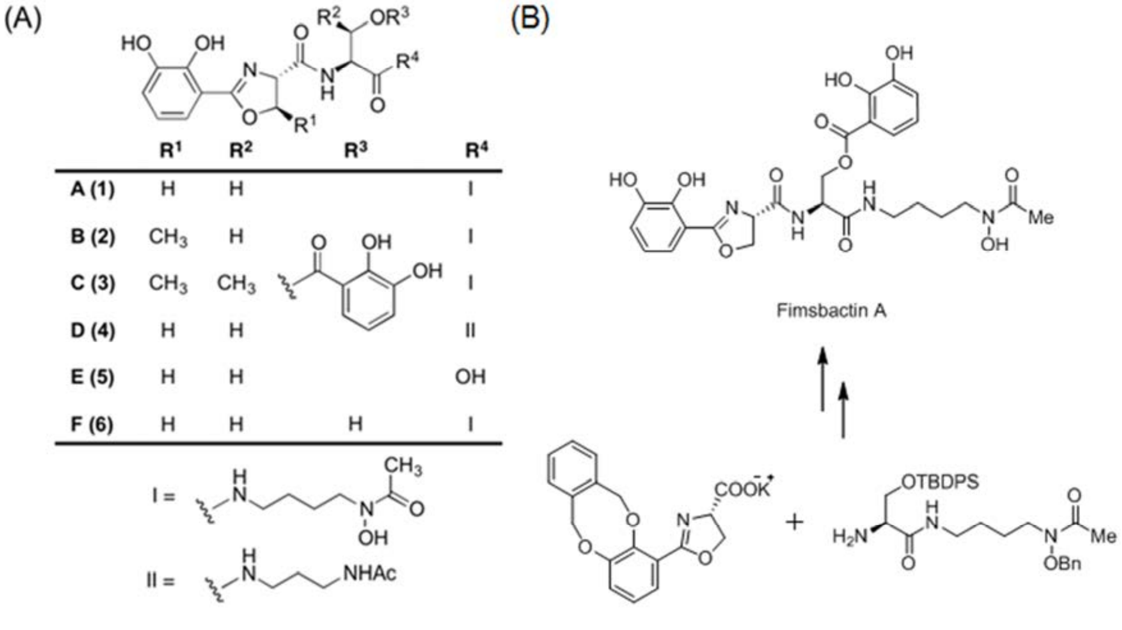
고려대학교 화학과

The iron is crucial for the survival of bacteria as it is involved in in many fundamental cellular processes. Despite its abundance in the earth, the aqueous solubility of iron is extremely low under aerobic conditions. Thus, bacteria need to possess a strategy for obtaining iron. Indeed, they accomplish this goal by utilizing small molecular Fe(III) chelators called siderophores. Once siderophores are excreted from the cell, it chelates Fe(Ⅲ), and shuttled back into bacteria.Acinetobacter baumannii is one of the most notorious Gram-negative pathogens with high resistance of multi-drug. For a while, A. baumannii has been known to produce acinetobactin as its sole siderophore. However, the latest study identified an alternative set of siderophores named fimsbactin A-F (Figure (A)), which were isolated from A. baumannii in addition to non-pathogenic Acinetobacter baylyi ADP1. In contrast to acineobactin, the physicochemical and biological properties of these fimsbactins have yet to be well understood.Previously, we were able to synthesize fimsbactin B, and evaluate its siderophore function revealed that it was incapable of delivering the iron inside the A. baylyi ADP1. To better understand this unexpected observation, we are currently trying to synthesize fimsbactin A, the major isolate from A. baylyi ADP1. As delineated in Figure (B), the synthesis of fimsbactin A could be accomplished by amide coupling between a catechol-containing oxazolyl carboxylate (I) and a serine derivative containing the protected hydroxamate moiety (II). With fimsbactin A and other fimsbactin isoforms in hands, we are investigating their structure-function relationship to identify which is the genuine siderophore for Acinetobacter species.


(A)
HO
OH
N
NH
O
R^2
OR^3
R^4
R^1
R^1 R^2 R^3 R^4
A (1) H H I
B (2) CH$_3$ H I
C (3) CH$_3$ CH$_3$ I
D (4) H H II
E (5) H H OH
F (6) H H H I
I =
II =
NHAc
(B)
Fimsbactin A
COOK
OTBDPS
H$_2$N
Me
OBn
+

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Direct Amide Bond Formation of Aldehydes via Metal-Free Aerobic Oxidative Amidation in the Presence of Cyanide

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고려대학교 화학과

ABSTRACT: The one-pot protocol for the direct synthesis of amide bonds from aldehydes and primary amines via metal-free aerobic oxidative amidation in the presence of cyanide was described. Various aromatic aldehydes were applicable to this protocol and the desired amide products were obtained in good to high yields. Mechanistic studies suggest that this aerobic oxidative amidation might proceed via the addition of cyanide to imines, followed by the proton transfer leading to the benzylic carboanions of α-aminonitriles, and subsequent oxidation with molecular oxygen in air.

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General Procedures for meta-Functionalization of Arene boronic acid using a boronic acid moiety as a blocking group in EAS reactions

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고려대학교 화학과

Hydroxyl group of phenol works as strong direction group in electrophilic aromatic substitution reaction. Hydroxyl group ortho or para-position was substituted for electrophile in common EAS of phenol. For this reason, it is impossible to introduce electrophile directly for substitute meta-position of hydroxyl group. We assumed boron derivatives worked as the blocking group to prevent the introduction of the electrophile in the para-position, and it can be introduce in the ortho-position. After that, finally, we can obtain meta substituted phenol by oxidation of boronic acid. At this moment, by using variable functional group that gives para-position electron donating groups and various electrophiles, we can extend that research area and suggest diversity. This protocol can be applied to natural products synthesis.

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Enantioselective Synthesis of ß-aryl amines via chiral phosphoric acid-catalyzed asymmetric reductive amination

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고려대학교 화학과

Over the past decade, chiral phosphoric acid catalysis has become one of the most rapidly growing fields in asymmetric catalysis. Among the various asymmetric reactions that involve chiral phosphoric acid catalyst, asymmetric reduction of ketimines with organic hydride sources has become one of the most popular reactions in enantioselective phosphoric acid catalysis. A number of examples of the synthesis of chiral amines through chiral phosphoric acid-catalyzed asymmetric reduction of imines have been limited to the synthesis of chiral α-aryl amines via enantioselective reduction of ketimines derived from alkyl aryl ketones. Thus, we have developed a new method for the synthesis of chiral ß-aryl amines via chiral phosphoric acid-catalyzed asymmetric reductive amination of benzyl methyl ketone using Hantzsch ester as an organic hydride source. A variety of substrates from aromatic ketone to heteroaromatic ketone as benzyl methyl ketone derivatives, are applicable to this protocol and afforded the desired chiral ß-aryl amines in high yields and good enantioselectivity.

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Determination of Polyphenols from A. rugosa Using Liquid Chromatography-Tandem Mass Spectrometry

DestaKebedeTaye 신성철*

경상대학교 화학과

A. rugosa, commonly called Banga in Korea, is a perennial plant which belongs to 6000 species of the Labiatae family. A total of eighteen polyphenols were characterized on the basis of their [M-H]- and MS/MS fragmentation pattern from flower, leaf, stem and root parts of A. rugosa (Labiatae). Except for rosmarinic acid isomers, all of them were identified for the first time for A. rugosa. The total polyphenol contents were found to be 8371.334 ± 9.05, 6091.67 ± 11.89, 3156.99 ± 4.03, and 2123.37 ± 4.45 mg kg-1in leaf, flower, stem, and root of A. rugosa.

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Enantioselective One-Pot Synthesis of Tetrahydroquinolines via Aerobic Oxidation and Hydride Transfer/Ring Closure

서창원 김대영*

순천향대학교 화학과

Enantioselective organocatalytic synthesis of tetrahydroquinolines has been achieved via an aerobic oxidation and a 1,5-hydride transfer/cyclization sequence. The feature of this research is a one-pot transformation of 3-arylprop-2-en-1-ol derivatives into tetrahydroquinolines using a Ru(VII)-catalyzed aerobic oxidation and highly efficient internal redox reactions. The synthetically useful ring-fused tetrahydroquinoline derivatives are obtained in moderate yields and high levels of enantioselectivity.

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Catalytic Asymmetric Michael Addition of α-Fluoro β-Ketoesters to Nitroalkenesin the Presence of Nickel Complexes

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순천향대학교 화학과

Chiral fluorine-containing organic molecules are interesting and important materials with uses in medicinal and biological chemistry. The catalytic enantioselective conjugate addition reaction of α-fluoro β-ketoesters to nitroalkenes promoted by chiral nickel complexes is described. Treatment of α-fluoro β-ketoesters with nitroalkenes under mild reaction conditions afforded the corresponding Michael adducts containing fluorinated quaternary stereogenic center with excellent enantioselectivity (up to >99% ee).

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Organocatalytic enantioselective addition of diphenyl phosphite to ketimines derived from isatins

장희승 문진수 김대영*

순천향대학교 화학과

Oxindoles are widely present in natural products and bioactive molecules, and oxindoles bearing 3-aminated quaternary stereogenic center are structural motifs that have important applications in the pharmaceutical industry. A highly enantioselective addition of diphenyl phosphite to ketimines derived from isatins has been achieved using a bifunctional organocatalyst, quinine-derived squaramide catalyst. This method works efficiently with several ketimines to produce the corresponding 3-amino-2-oxoindolin-3-yl-phosphonates in excellent yields with high enantioselectivity .

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Organocatalytic enantioselective Michael addition of pyrazolin-5-ones to nitroalkenes

이민영 윤지희 김대영*

순천향대학교 화학과

Pyrazolone derivatives have been used to synthesize many drugs such as complexes of aminoantipyrine with barbiturate. An efficient chiral squaramide-catalysed enantioselective Michael addition of pyrazolin-5-ones to nitroalkenes has been developed. This reaction afforded the chiral pyrazol-3-ol derivatives in high to excellent yields with high enantioselectivities for most substrates under mild conditions. This catalytic asymmetric reaction provides valuable and easy access to chiral pyrazol-3-ol derivatives, which possess potential pharmaceutical activity.

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Enantioselective Fluorination of β-Ketoamides Catalyzed by Chiral Palladium Complexes

권수진 김대영*

순천향대학교 화학과

Fluorinated molecules have attracted increased interest in pharmaceutical and material science because of their utility as medicines, agrochemicals, and functional materials. A facile and powerful enantioselective construction of C-F containing molecules was successfully developed through asymmetric fluorination of β-ketoamides catalyzed by chiral palladium complexes. The present catalytic system exhibited excellent enantioselectivity and a broad substrate scope for indanone-derived β-ketoamides under mild conditions.

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Synthesis of Furan and Thiophene from the Decarboxylative Copper Catalylsed coupling Reaction of Arylalkynyl Carboxylic Acid with H_2O or Na_2S

IRUDAYANATHANFRANCISMARIARAJ 이선우*

전남대학교 화학과

2,5-Diaryl-substituted furans were synthesized from the copper-catalyzed decarboxylative coupling reaction of aryl-subsituted aryl propiolic acid in the presence of H_2O. The homocoupling of alkynyl carboxylic acid provided the 1,4-diaryldiyne, and then reacted with with H_2O to give the desired furan through the cyclization. We found that copper was a key catalyst and ligand increased the yield of products in both homocoupling and cyclization. In addition, thiophenes were obtained when the reaction was conducted in the presence of Na_2S.

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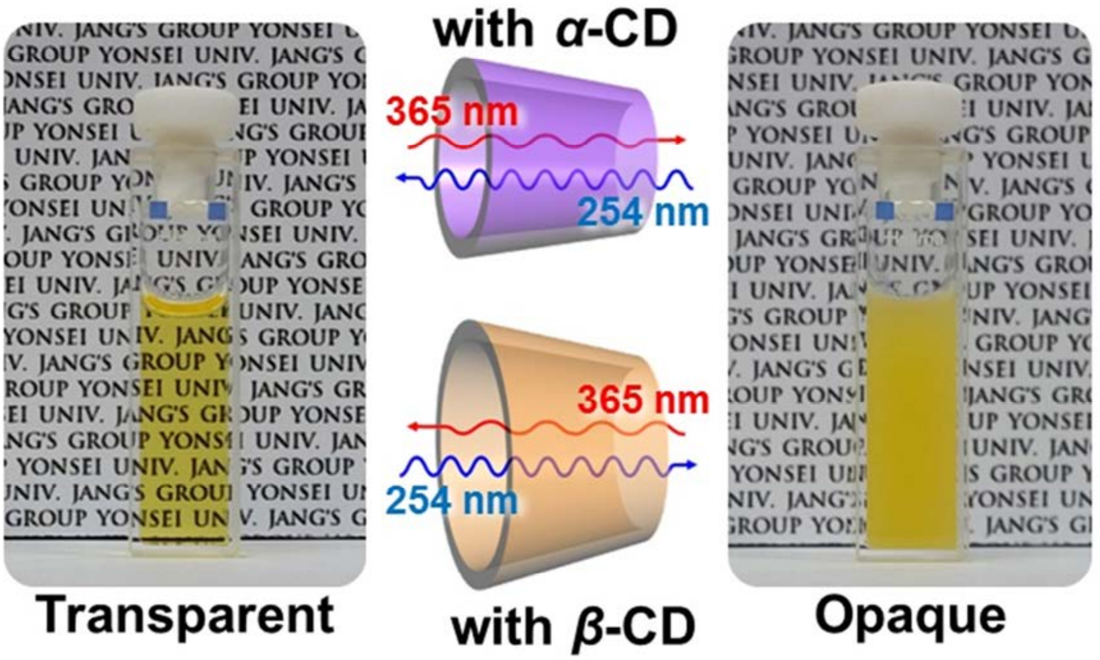
Molecular logic gates using multimodal stimuli-responsive poly(2-isopropyl-2-oxazoline)-azobenzene hybrid

김주호 구은혜 주상용* 장우동*

연세대학교 화학과

We investigated the hybrid system with thermo-poly(2-isopropyl-2-oxazoline) for thermo-responsiveness and azobenzene moieties as end groups (Az-POx-Az) for photo-responsiveness and applied for multimodal logic circuit. Az-POx-Az solution in PBS (pH 7.4) underwent reversible photoisomerization between *cis* and *trans* form by irradiation of 365 nm and 254 nm UV light. ^{1}H-NMR spectra of Az-POx-Az for each state were measured. Azobenzene groups are known to bind with cyclodextrins (CDs) via host-guest interaction. Thermo-responsive behaviors of Az-POx-Az without CD, with α- or β-CD were observed. The *cis* form Az-POx-Az rather than the *trans* form, and samples with CDs rather than without CD exhibited higher lowest critical solution temperature (LCST). However, the *cis* form of Az-POx-Az with α-CD exhibit lower LCST than the trans form, because *cis*-azobenzene could not bind with α-CD.


with α-CD
365 nm
254 nm
365 nm
254 nm
with β-CD
Transparent
Opaque

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Fibrous Supramolecular polymers formed from artificial light harvesting porphyrin dendrimers

이호수위 김주호 장우동*

연세대학교 화학과

Artificial light harvesting multiporphyrin dendrimers ($P_{Zn}P_M$, M=H, Cu) and multipyridyl porphyrins (PyP_M, M=H, Cu) assembled to supramolecular polymers through coordination interactions of pyridyl groups to zinc porphyrins. UV/Vis titration and Job's plot indicated 1:1 binding stoichiometry and the association constant between $P_{Zn}P_{FB}$ and PyP_{FB} which was measured through isothermal titration calorimetry (ITC) was strong enough to form fibrous polymer assemblies. Atomic force microscopy (AFM) and transmission electron microscopy (TEM) images indicated fibrous assemblies. The intramolecular energy transfer among multiporphyrin dendrimers was changed to intermolecular energy transfer by the formation of polymer assemblies, which was indicated from the fluorescence emission measurements.

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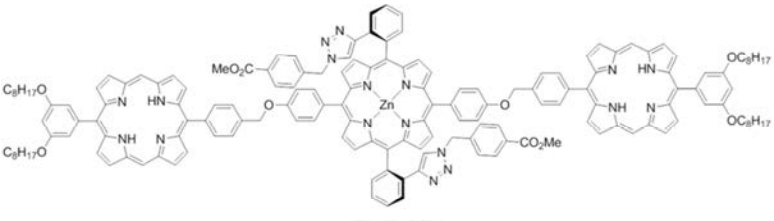
Guest-induced Energy Transfer Control in a Porphyrin Triad

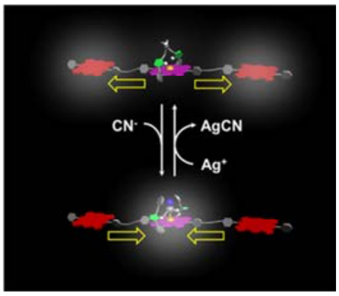
임다정 성주영 김동호* 장우동*

연세대학교 화학과

Natural photosynthetic light-harvesting systems have not only high efficient in energy transfer but also continuous conversion of light energy to other forms. Natural light-energy conversion is initiated by photon absorption of complex molecular assemblies called light-harvesting antenna complexes (LHC). Well-ordered three-dimensional multiporphyrin arrays in LHC facilitate effective photon capture and energy migration to the reaction center, which is composed of a non-covalently associated pair of chromophore units. Based on the process of natural photosynthetic systems, many chemists have reported highly efficient energy transfer. However, few studies have been conducted to control energy transfer pathway by guest binding.Triazole-bearing porphyrin triad (**P$_{Zn}$Tz-2P$_{FB}$**) consists of central zinc porphyrin (**P$_{Zn}$**) and two freebase porphyrin wings (**P$_{FB}$**). **P$_{Zn}$Tz-2P$_{FB}$** exhibited unique photoluminescence switching phenomena by guest binding. As a result of fluorescence spectroscopy, **P$_{Zn}$Tz-2P$_{FB}$** exhibited the emission of **P$_{FB}$** regardless of excitation wavelength, and this result suggests that effective energy transfer takes place from **P$_{Zn}$** to **P$_{FB}$**. After the addition of CN$^-$, emission spectrum of **P$_{Zn}$Tz-2P$_{FB}$** was consistent with the emission of CN$^-$ complex of **P$_{Zn}$** whether **P$_{FB}$** or **P$_{Zn}$** excitation.



P$_{Zn}$Tz-2P$_{FB}$



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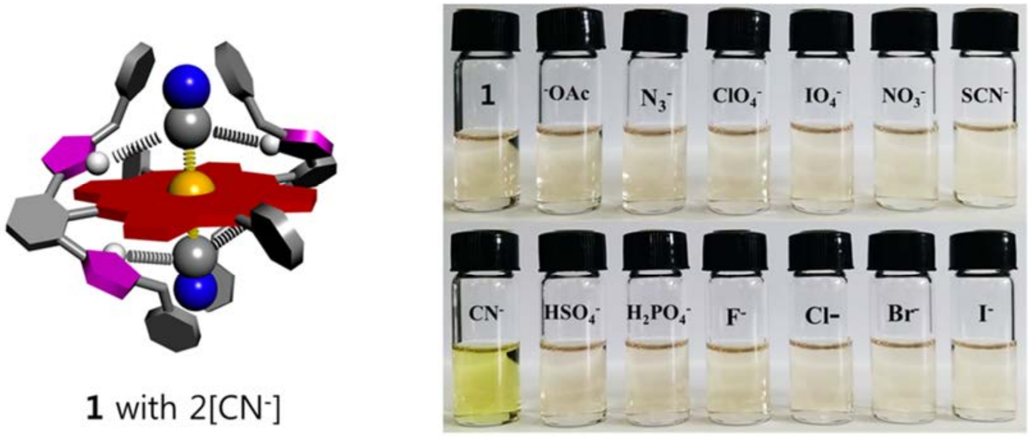
Sensor for Cyanide using Triazole-Based Picket Fence Nickel Porphyrinvia Positive Allosteric Binding

홍경임 장우동*

연세대학교 화학과

Allosteric effect is the most important and essential regulation mechanism in biological system. The first guest binding induces a conformational change in the host protein, which influences the binding affinity of additional guests. Such phenomena are of great interest for the design of functional materials. We synthesized triazole-based picket fence type nickel(II) porphyrin(1). Triazole groups enhance anion binding affinity through hydrogen bonds. Although 1 is weaker Lewis acid than Zn(II) porphyrin, 1 could recognize cyanide anion selectively with color change. Nickel porphyrin is known to accommodate two axial ligands to form hexa-coordination state. Therefore, we can expect 1:2 binding formations between 1 and cyanide ions. And this hypothesis is proved with continuous variation method (Job`s plot) and ^{1}H-NMR spectra. Detailed aspect of this system will be reported in the symposium.



1 with 2[CN^-]

Figure 1. **1** with [CN^-] and the color change of **1** (6 μM) upon addition of various anions (50 eq) in 0.5% H_2O/Acetonitrile.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-888**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

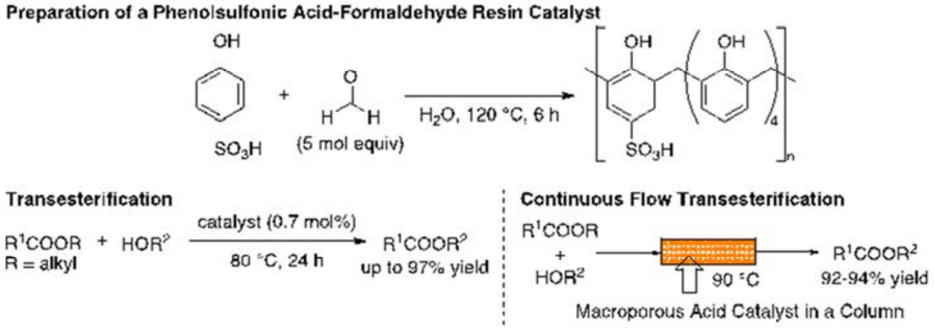
Transesterification of Various Alcohols and Esters with a Porous Phenol-Sulfonic Acid Resin

Heeyoel Baek Maki Minakawa Yoichi M. A. Yamada[*] 한진욱[1] Yasuhiro Uozumi[2,*]

RIKEN Center for Sustainable Resource Science [1]한양대학교 화학과 [2]RIKEN Center for Sustainable Resource Science, Institute for Molecular Science (IMS)

We previously reported a novel macroporous polymeric acid catalyst that was prepared by the condensative polymerization of p-phenolsulfonic acid and formaldehyde (5 mol equiv) at 120 °C, and its catalytic application to direct esterification under solvent-free conditions.[1] Herein, the heterogeneous acid catalyst with 0.7 mol% SO_3H was applied to the transesterification of various esters (R^1COOR) and alcohols (R^2OH) at 80 °C without removal of alcohol (ROH), affording the corresponding esters (R^1COOR^2) in up to 97% isolated yield. The continuous flow transesterification was achieved by using a column-packed macroporous acid catalyst under mild conditions without removal of alcohol, lasting for 7 days without loss of catalytic performance.

1. Minakawa, M.; Baek, H.; Yamada, Y. M. A.; Han, J. W.; Uozumi, Y. Org. Lett. 2013, 15, 5798.


Preparation of a Phenolsulfonic Acid-Formaldehyde Resin Catalyst
OH
SO3H
+
O
H H
(5 mol equiv)
H2O, 120 °C, 6 h
OH
OH
SO3H
4
n
Transesterification
R1COOR + HOR2
R = alkyl
catalyst (0.7 mol%)
80 °C, 24 h
R1COOR2
up to 97% yield
Continuous Flow Transesterification
R1COOR
+
HOR2
90 °C
R1COOR2
92-94% yield
Macroporous Acid Catalyst in a Column

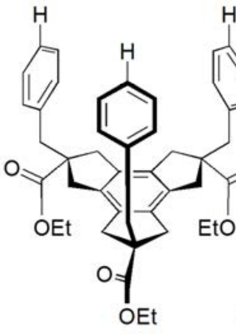
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-889**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Improved synthesis of C_{3v} -symmetric scaffolds for Anion sensors;*cis,cis,cis*-2,5,8-tris(*p*-substituted benzyl)trindane-2,5,8-tricarboxylate

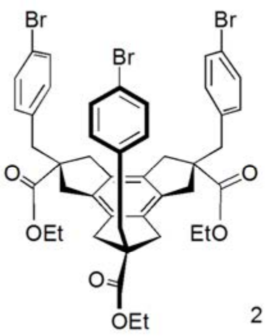
김기동 최홍진*

경북대학교 응용화학과

Design and synthesis of artificial receptors for selective recognition of anions have been received considerable interest recently. Receptor molecules with preorganized binding motifs are useful for the effective and selective binding of guest species. Most anions interested in biological, environmental measurement are F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, HSO_4^-, NO_3^-, HCO_3^- ions which have C_3-symmetric element. We have developed a $H_2PO_4^-$ selective anion receptor that has C_{3v}-symmetric scaffold; *cis,cis,cis*-2,5,8-tribenzyltrindane (1). As shown in compound 1, molecular planes of three phenyl groups in C_3-symmetric trindane molecule parallels to the principal molecular axis each other such that the molecule 1 has C_3-symmetric vase-like shape, which is a promising aspect for recognition of C_{3v} symmetric guest species.Compound 1 was synthesized from mesitylene in seven consecutive step; chloro-methylation, benzylic bromination, cyclization with malonate, ester-hydrolysis, decarboxylation and esterification to trindane tricarboxylate, and then benzylation. Each reaction step requires three-fold reaction so that the reaction requires very high efficiency to afford high yield. We have optimized each reaction conditions for further divergent C_3-symmetric scaffolds as shown below.



1



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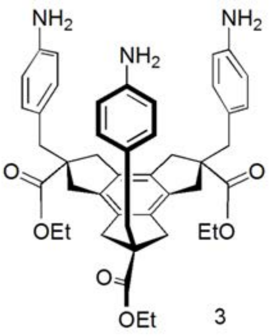

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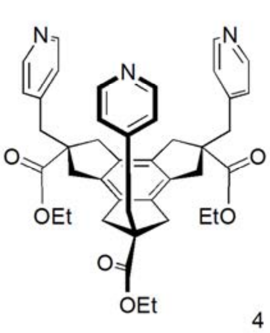


4

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-890**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot multi-component radical reaction for the synthesis of secondary amines

김지혜 장두옥*

연세대학교 화학과

Secondary amine functionality is found in many natural bioactive products such as alkaloids, amino acids, nucleic acids, pharmaceuticals, and agrochemicals. Secondary amines have also been used as building blocks for nitrogen-containing organic compounds. A multi-component reaction involving aldehyde, benzhydrazide, alkyl iodide, triethylborane and diphenylsilane in the presence of $Yb(OTf)_3$ was developed to synthesize secondary amines. The present one-pot radical addition reaction to C=N bond offers mild, efficient reaction conditions to result in high yields of various aromatic and aliphatic secondary amines.

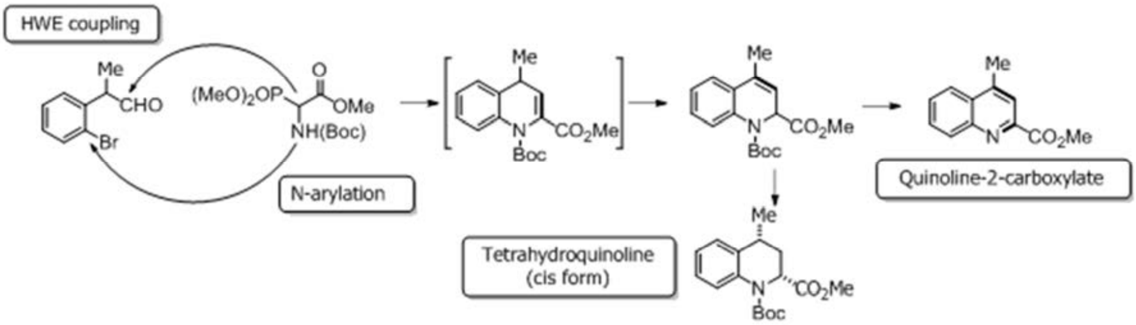
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-891**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Dihydroquinoline-2-Carboxylates via a Sequential HWE Coupling and Pd-catalyzed N-arylation

박경용 이진용 허정녕[1] 임환정[1,*]

충남대학교 신약전문대학원 [1]한국화학연구원 의약화학연구센터

Quinoline- and quinolone-2-carboxylates have been received much attention in medicinal and organic chemists because of their potent biological activities and utilities as an intermediate of ligands. Sequential Horner-Wadsworth-Emmons (HWE) coupling and Pd-catalyzed N-arylation reaction under microwave irradiation enable us to prepare the target molecules in good yields.



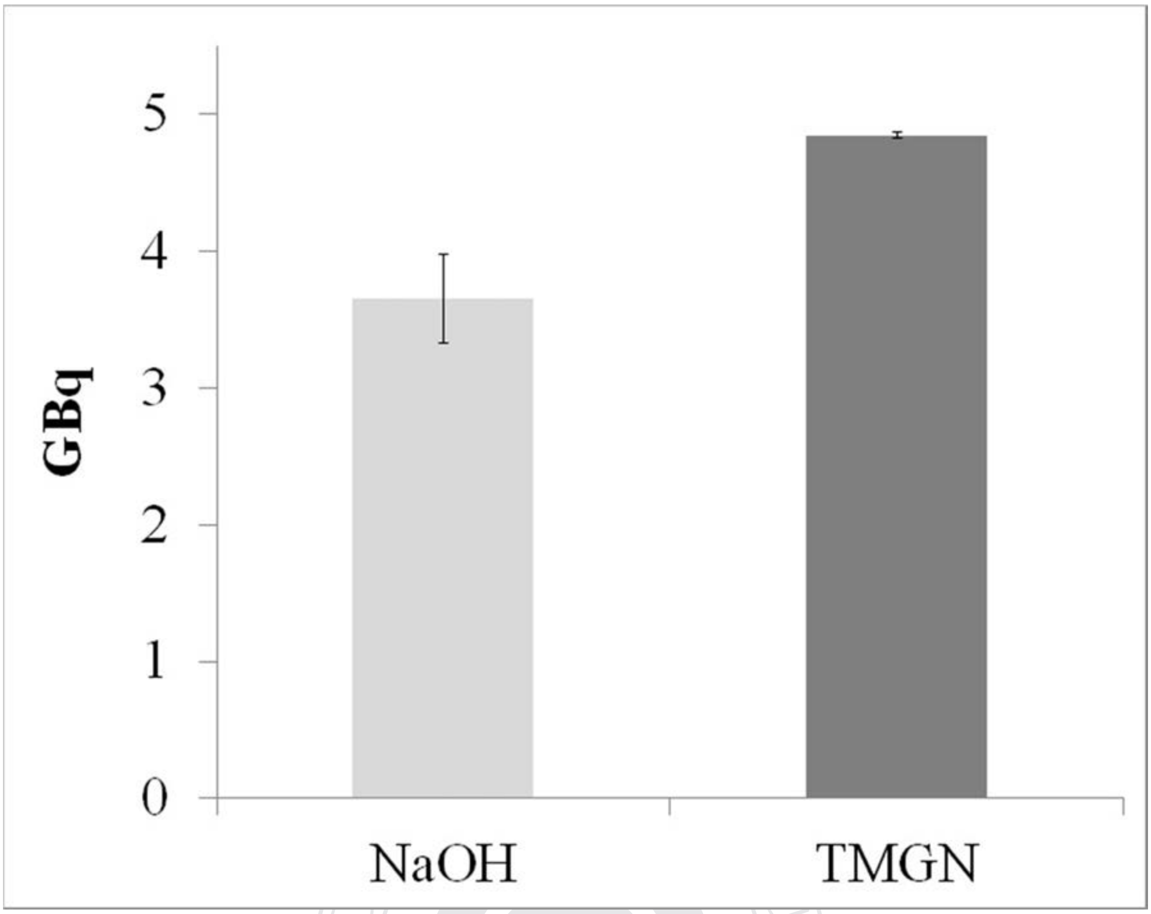
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-892**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The novel approach for [C-11]radiolabeling with uniformed high radiochemical yield: utilization of a strong organic base for phenolic O-[^{11}C]mehylation

이상윤

가천대학교 메디컬캠퍼스 보건과학대학/방사선학과

The strong inorganic bases (NaOH, KOH, NaH etc.) basically has been employed for C-11 methylation of phenolic alcohols ([^{11}C]raclopride, [^{11}C]DTBZ, etc), but they are not perfectly dissolved in reaction media which cause lowering solubility of precursors, (S)-O-desmethylraclopride and 9-O-Desmethyl-DTBZ and gives erratic trends of radiochemical yields. The novel approach is here introduced that 1,8-bis(tetramethylguanidino)naphthalene (TMGN), an organic base (relatively strong base, pKa=25.1 in ACN) can provides enhance the solubility of labeling precursors and reaction yields with the precursors include phenolic alcohols. The radiochemical yields from two different bases were 3.65±0.33 (n=10) and 4.85±0.03 (n=3) GBq for NaOH and TMGN respectively (Figure, Left). Total synthesis time with NaOH was 30 minute longer than that with TMGN (30 min). This method showed the higher average radiochemical yield compared to traditional one and shorter synthesis time as well.



GBq
5
4
3
2
1
0
NaOH
TMGN

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-893**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Asymmetric 3-Membered Ring Formation with Diazo Compound and Acrolein Compound

심수용 김재연 정현실 백은희 김태형 신성호 강병철 강기태 **JINMINGYU** 류도현*

성균관대학교 화학과

Cyclopropane rings are often found in various natural products and biologically active compounds. Natural and synthetic cyclopropanes with simple or complex structure have a broad spectrum of biological properties, including enzyme inhibition and insecticidal, antifungal, herbalcidal, antimicrobial, antibiotic, antibactierial, antitumour, and antiviral activities. A number of effective cyclopropanation procedures have been described in recent years. However, the examples of asymmetric cyclopropanation of α,β-unsaturated aldehyde with diazoesters are uncommon. In this research, we found the catalytic condition for diazoacetate to provide regio- and stereoselective cyclopropanes.

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-894**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Multifunctional and Water-Soluble Polyglycerol Dendrimers via One-Pot, Orthogonal Chemical Reactions

노형주 양시경*

전남대학교 화학교육과

The synthesis of a water-soluble polyglycerol dendrimer with two orthogonal functional groups at the core is reported. The two groups, an azide and amine group, are highly reactive towards alkyne and activated ester moieties, respectively. The orthogonality of the two chemical reactions is demonstrated by the ability to conjugate quantitatively either group, independent of the other and in either order. The orthogonal functionalization of the azide- and amine-cored dendrimer can be accomplished in a stepwise or a one-pot synthetic protocol. All resulting bifunctional dendrimers are fully soluble in water as the water-soluble dendritic scaffold decorated with 48 hydroxyl groups on the surface successfully solubilizes both the hydrophobic fluorophore and targeting group.

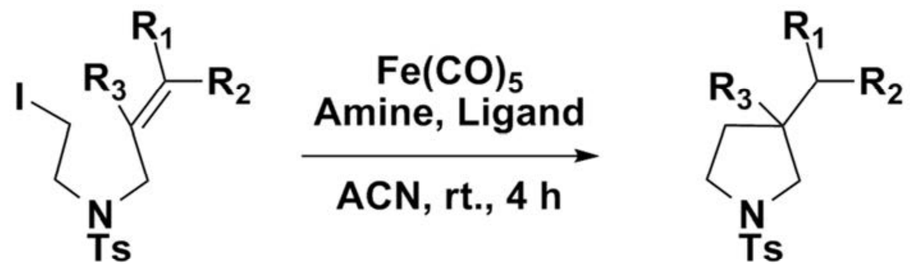
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-895**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

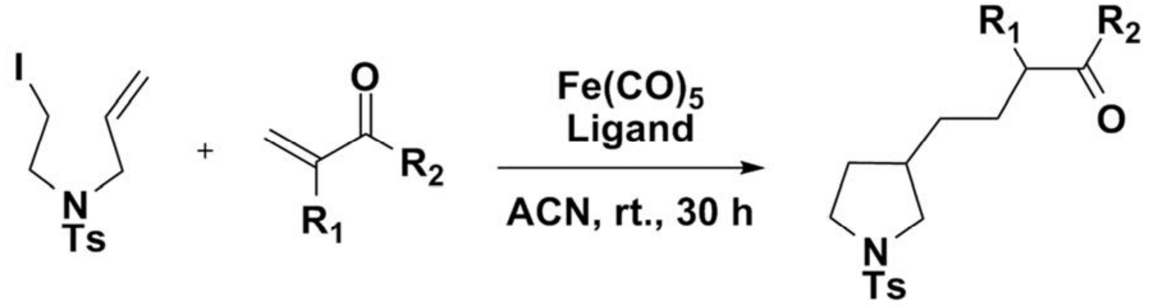
New Radical Cyclization Strategy: Iron(0) Carbonyl Complex-Mediated Reaction of Terminal Iodoalkene for Heterocycle Synthesis

황준영 강은주*

경희대학교 응용화학과

Fe(CO)5-mediated radical cyclization of alkyl iodides is reported. We describe the identification of reaction conditions under which metal-ligand complexes can be utilized to form radicals from unactivated alkyl iodide substrates. The generated radicals undergo reduction via hydrogen atom abstraction or reductive cyclization. The reaction protocol utilizes only inexpensive reagents, occurs under mild reaction conditions. This process appears to be a ligand-accelerated reaction, and iron(0) pentacarbonyl compound gives single-electron to alkyl iodides by SET mechanism. Furthermore, tandem radical cyclization was achieved by α,β-unsaturated carbonyl compounds


R1
R3
R2
I
N
Ts
Fe(CO)5
Amine, Ligand
ACN, rt., 4 h
R1
R3
R2
N
Ts


I
N
Ts
+
O
R2
R1
Fe(CO)5
Ligand
ACN, rt., 30 h
R1
R2
O
N
Ts

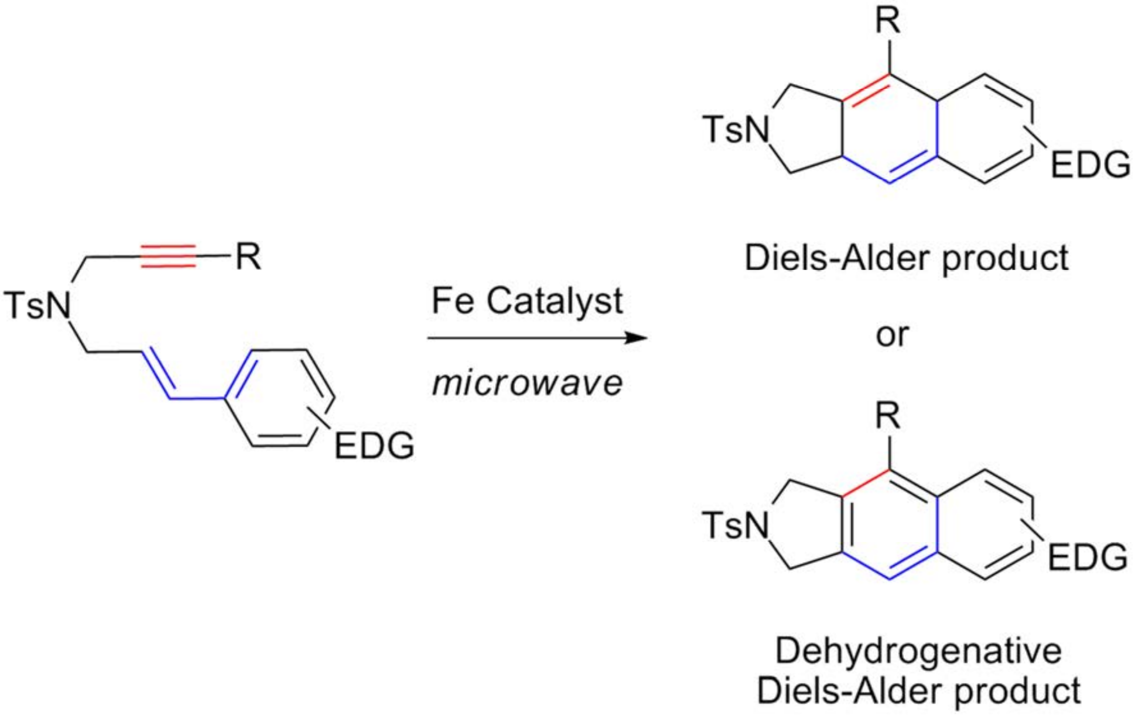
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-896**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fe-catalyzed Dehydrogenative Diels-Alder Reaction

문현진 강은주*

경희대학교 응용화학과

The Diels-Alder reaction is undoubtedly one of the most fundamental and useful reactions available to organic chemists. It is used widely to form carbocyclic and heterocyclic frameworks as precursors for constructing complex organic molecules such as natural products. Also naphthalene derivatives are synthesized by dehydrogenative Dies-Alder reaction of diene in the form of a styrene moiety and dienophile in the form of an alkyne moiety. In this study, dehydrogenative Diels-Alder reactions are shown with iron salt catalyst and various substrates contained electron donating group at styrene moiety.



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-897**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

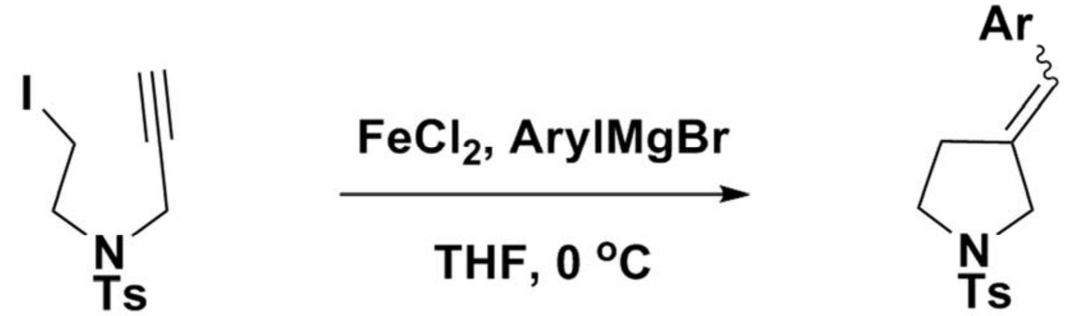
Iron(II)-catalyzed Kumada-type Radical Cyclization and Cross-coupling Reaction of Iodoalkyne with Grignard Reagents

김재곤 백종화 강은주*

경희대학교 응용화학과

Carbon-carbon bond formation via radical reactions is one of the most important synthetic steps in the construction of organic molecules. Recently, we have found that intramolecular radical cyclization reaction of 6-halo-1-hexyne derivatives has been carried out by means of alkyl Grignard reagent. Furthermore, N-(2-iodoethyl)-4-methyl-N-(prop-2-ynyl)benzenesulfonamide also afforded 5-exo tandem radical cyclization and cross-coupling reaction upon treatment with aryl Grignard reagent under iron(II) chloride catalysis.

R = H, CH_3, TMS, Ar
X = NR or O



일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-898**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Cytotoxic Secobutanolides

정현실 남동국 JINMINGYU 강병철 신성호 강기태 심수용 김태형 백은희 류도현*

성균관대학교 화학과

A stereoselective synthesis of (Z)-β-iodo Morita-Baylis-Hillman ester has been developed through a multi-component coupling reaction using lewis acid catalyst and TMS-I. Iodine catalyzed photo reaction or thermal rearrangement provided a geometric isomer, (E)-β-iodo Morita-Baylis-Hillman ester without racemization. The synthesis of cytotoxic secobutanolides was accomplished after organocuprate coupling reaction and ozonolysis.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-899**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Chiral Seven-membered ring via Sigmatropic Rearrangement

김태형 김재연 강병철 강기태 신성호 심수용 **JINMINGYU** 정현실 백은희 류도현*

성균관대학교 화학과

Seven-membered ring skeleton is frequently found among the natural products; such as, occidenol, miscandenin, dictyoxepin, clavubicyclone, etc. These compounds can exhibit a wide range of bioactivities such as anti-tumor, anti-HIV, anti-bacterial, and anti-inflammatory.One of the powerful tools used for the construction of seven-membered ring is sigmatropic rearrangement of cyclopropane moiety. In 2011, our research group reported the synthetic method for highly enantioselective cyclopropane. We were able to anticipate optically active cyclopropanes to be useful precursors for chiral seven-membered ring through rearrangement. Additionally, we are expecting this synthetic methodology to be useful for synthesis medicines or natural products which contain seven-membered rings.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-900**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Roskamp Reaction using Lewis Acid Catalyst

<u>신성호</u> JINMINGYU 강병철 강기태 심수용 백은희 김태형 정현실 류도현*

성균관대학교 화학과

We have developed catalytic asymmetric Roskamp reaction with aldehydes. Stereoselective reduction is proceeded sequentially to produce alpha-aryl-beta-hydroxy amide in good yields and good enantioselectivities which can be used for various acyl derivative synthesis. This two-steps reaction gives another method of asymmetric aldol product synthesis.

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-901**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Synthesis the Cyanohydrin Compounds Catalyzed by a Chiral Lewis Acid

JINMINGYU 정현실 **JINHUI** 김승태 강기태 강병철 신성호 심수용 김태형 백은희 류도현*

성균관대학교 화학과

One of the most useful C-C bond-forming reaction is addition of trimethylsilyl cyanide (TMSCN) to carbonyl compound. The asymmetric cyanohydrins are useful intermediates for pharmaceuticals, including alpha-hydroxy carbonyl compounds, alpha-hydroxy amines, beta-amino acid derivatives.1 This research describes an enantioselective synthesis the cyanohydrins catalyzed by a Chiral Lewis Acid,2 the reaction proceeded in excellent yield with excellent enantioselectivity. Further experimental and calculation studies should be performed to broaden the utilities of this new catalytic system.

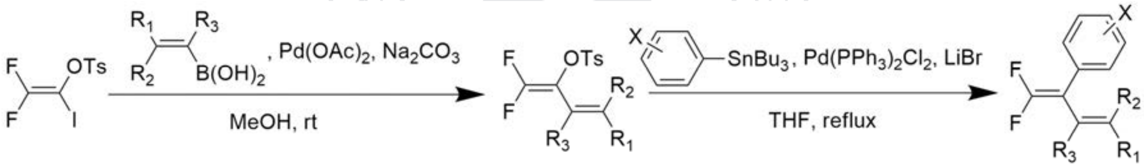
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-902**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient preparation of 2-aryl-1,1-difluoro-1,3-butadienes

김수진 안혜진 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

Suzuki coupling reaction of 2,2-difluoro-1-iodoethenyl tosylate 1 with alkenylboronic acids in the presence of Pd(OAc)2 and Na2CO3 in MeOH at room temperature afforded 1,1-difluoro-1,3-butadienes 2 in excellent yields. Stille coupling reaction of 2 with arylstannanes in the presence of Pd(PPh3)2Cl2 and LiBr in THF at reflux temperature provided 2-aryl-1,1-difluoro-1,3-butadiene 3 in good yields. The scope and limitation of these reactions will be presented.



1 **2** **3**

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-903**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Novel Hab mutases from database search

조새롬 이혁[1,*]

과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]한국화학연구원 의약화학 연구 센터

Biotransformation using enzymes or whole-cell catalysts has been emerging as one of major synthetic tools in organic synthesis. As a biocatalyst, Hab mutase has been known to convert hydroxylaminobenzene to aminophenol regioselectively. Recently we have found a novel Hab mutase through High-throughput screening of metagenomics libraries, and developed a new synthetic pathway from nitrobenzenes to aminophenols. Based on this result, database search using BLASTp found 62 organisms that have similar sequence to the original HabM. Among these 62 Hab Mutase-like proteins, 30 proteins with 25-80% sequence identity were selected and phylogenetically compared using Clustal W2. Finally, 17 Hab Mutase-like proteins with least sequence similarity among each other were selected, and their gene synthesized for recombinant expression in Escherichia coli. Then we checked Hab Mutase activities of those proteins by testing the biotransformation of hydroxylaminobenzene to 2-aminophenol, and 5 novel Hab Mutases were identified.

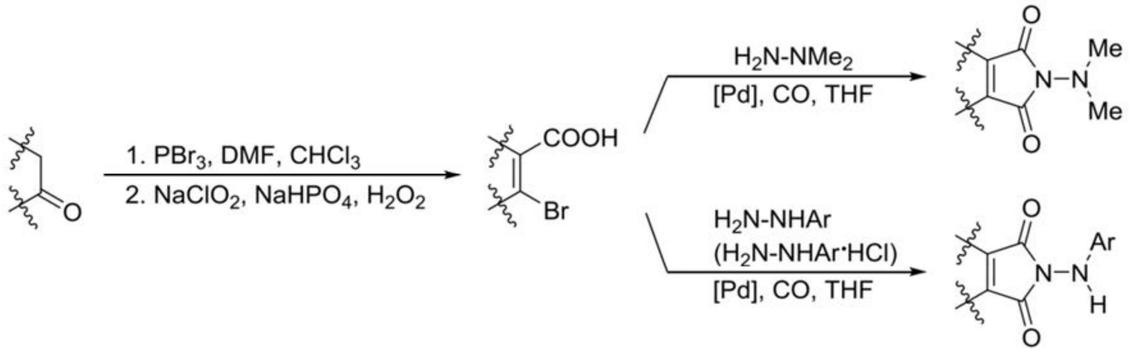
일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-904**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Carbonylative Cyclization of β-Bromo-α,β-unsaturated Carboxylic Acids with Hydrazines Leading to 1-Amino-1H-pyrrole-2,5-diones

윤일철 양병우 유재명 조찬식*

경북대학교 응용화학과

β-Bromo-α,β-unsaturated carboxylic acids are carbonylatively cyclized with hydrazines under carbon monoxide pressure in THF in the presence of a catalytic amount of a palladium catalyst along with a base to give 1-amino-1H-pyrrole-2,5-diones.



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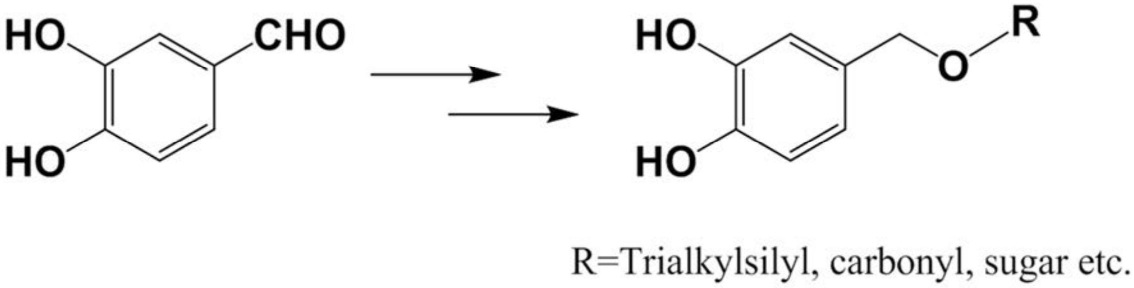
Synthesis of new CO_2-soluble catechol derivatives and its evaluation as a metal chelating agent in $scCO_2$

yan xinhao 오유리* 윤호준[1,*] 이송호[1,*] 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

In present study, new CO_2-soluble catechol derivatives containing nonfluorous ether, trialkylsilyl ether and carbonyl groups had been designed and synthesized from 3, 4-dihydroxybenzaldehyde by simple chemical modifications for the CO_2-phlic chelating agent. Their solubilities and metal ion extraction ability in supercritical carbon dioxide ($scCO_2$) have been tested and the relationship between structure and CO_2-solubility has been proposed. All synthesized catechol derivatives would show high solubilities in $scCO_2$ and good or moderate extraction efficiencies for metal ions, Sr^{2+} and Cs^+ etc.



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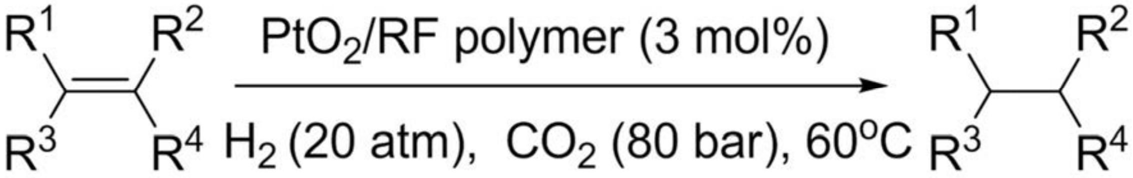
RF-Polymer supported PtO_2-catalyzed hydrogenation of alkenes in sc-CO_2

<u>안소연</u> 유종성[1,*] 김학원[2,*]

경희대학교 화학과 [1]대구경북과학기술원(DGIST) 에너지시스템공학과 [2]경희대학교 응용화학과

The hydrogenation of olefins has been considered as a key synthetic method for research and industrial processes. Supercritical carbon dioxide ($scCO_2$), considered as a green solvent (non-toxicity, availability at low cost and easy recycling) and completely miscible with gas (e.g. hydrogen), has been investigated as one of alternative media for both homogeneous and heterogeneous catalytic hydrogenations, because a low solubility of gaseous hydrogen in conventional organic liquid solvents results in a slow reaction rate in a gas-liquid system. In the present research, hydrogenation of alkenes with a newly synthesized polymer-supported metal nanoparticle catalyst has been investigated in organic solvents and supercritical carbon dioxide. Resorcinol-formaldehyde(RF)-polymer supported Pt nanoparticles are prepared by reacting resorcinol, formaldehyde and H_2PtCl_6 in aqueous ammonia-ethanol solution hydrothermally at 100℃. In non-polar organic solvent, PtO_2/RF polymer catalyst shows low reactivity, but in $scCO_2$ solvent, PtO_2/RF-polymer-catalyzed hydrogenation shows remarkably enhanced reactivity compared with one in nonpolar organic solvent.



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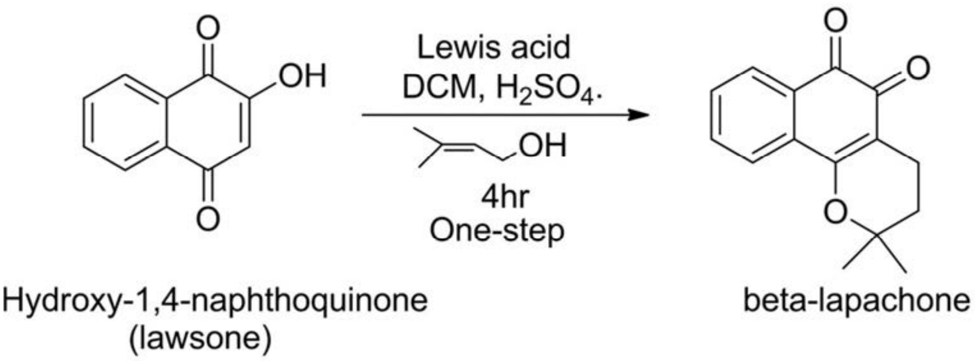
An improved regioselective, one-step synthesis of β-Lapachone from 2-hydroxy-1,4-naphtoquinone

이현진 한태동* 김학원*

경희대학교 응용화학과

β-Lapachone (β-LAPA), is a chemotherapeutic agent derived from the bark of the South American Lapacho tree, has recently emerged as a potent antitumor, anti-virus, anti-parasitic, and anti-inflammatory agent *in vitro*, and *in vivo*.Several synthetic approaches toward to β-LAPA have been reported. Among these synthetic processes, one-pot synthesis of β-LAPA from 2-hydroxy-1,4-naphtoquinone (lawsone) recently published by Ferreira *et al*. has some problems with a lot of times, use of gas reagents and hazardous solvent. To overcome these difficulties, we have developed a highly regioselective, one-step synthesis of β-lapachone, no α-lapachone formed, from lawsone using allylic alcohol, Lewis acid and mineral acid. NMR, HPLC and deuterium-quenching works have been done to elucidate the mechanism of this one-step reaction



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Highly Efficient Synthesis of 1,3,4-Oxadiazoles and Its Evaluation as Electron Transporting Materials

이고은* 김유로* 유영민[1],* 김학원*

경희대학교 응용화학과 [1]이화여자대학교 화학신소재공학부

1,3,4-Oxadiazole derivatives are considered as important compounds due to their pharmaceutical, biological, corrosion inhibition and electron transporting properties. Especially, a variety of bis-1,3,4-oxadiazole compounds have found their utility for hole-blocking and electron-transporting layers in organic light-emitting devices (OLEDs).In this work, we prepared novel mono- and bis-1,3,4-oxadiazoles for applications in electron transporting materials, using our previously developed synthetic method. The method carries several advantages, as it permits a highly efficient, solvent-free, one pot synthesis of 1,3,4-oxadiazole from hydrazide through a *N*-acylhydrazone intermediate. To evaluate utility for electron-transporting materials, electrochemical measurements using cyclic voltammetry have been performed.

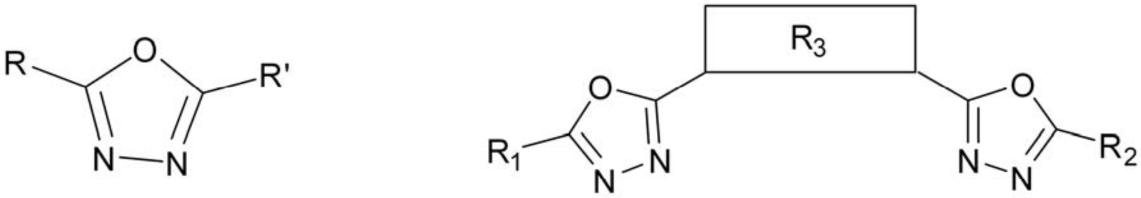

Figure 1. Various Mono- and Bis-1,3,4-Oxadiazoles

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Regioselective methylation of tetrazole by using methyl salicylate

<u>박찬용</u> 강영구 송창식 고영관[1] 이일영[1,*]

성균관대학교 화학과 [1]한국화학연구원 친환경신물질연구센터

N-methyl tetrazole moiety has known one of the biological component. In the known procedure for the synthesis of 2-methyl tetrazole, the ratio range of N2/N1-methyl phenyl tetrazole is form 1:1 to 4:1 by reaction with MeI or dimethyl sulfate in polar aprotic solvent under various basic conditions. Methyl salicylate is a mild methylation agent for the esterification of carboxylic acids by hydrogen bonds effect between the hydroxyl groups. When we applied methyl salicylate as a methylation reagent for a synthesis of 5-phenyl-2-methyl-2H-tetrazole with functional groups, the ratio of N2/N1-methyl phenyl tetrazole is more than 6:1. We will introduce reaction conditions and scope for a synthesis of 2-alkyl tetrazoles.

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A new red-emissive two-photon fluorescence dye for designing bioprobes

시호영 김환명*

아주대학교 에너지시스템학부

Two-photon microscopy (TPM) utilizes two photons of lower energy to obtain the excited state of a fluorophore, and thus has more advantageous features over OPM including less phototoxicity, better three dimensional spatial localization, deeper penetration depth and lower self-absorption. However, the progress in this field remains challenging, in large part due to the lack of useful TP scaffolds for designing various TP probes.Red emissive fluorescent probes are attractive for imaging in live cells and tissues, because they have better spectral separation from cellular absorption and auto fluorescence than probes that emit in the blue to yellow fluorescence range, thereby enhancing the contrast between the readout and background emission.1We have developed a red emissive fluorescence dye (BTDAN-ex) derived from 6-(benzo[d]thiazol-20-yl)-2-(N,N-dimethylamino)naphthalene(BTDAN). BTDAN-ex shows 40~80nm red-shifted spectra than BTDAN. The BTDAN-ex is expected to be applying in various ways, for example as a tracker for targeting specific organelles such as lysosome, mitochondria or as a fluorophore attached to receptor to detect specific metal ion.

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β-Galactosidase Selective Two-Photon Fluorescent Probefor Biomedical Applications

이효원 엄윤주 김환명*

아주대학교 에너지시스템학부

Human β-galactosidase (β-gal) is a lysosomal exoglycosidase that removes galactose residues from various substrates, such as gangliosides, glycoproteins, sphingolipids, and keratin sulfate.[1] Interestingly, abnormally accumulated β-gal activity has long been reported in diverse senescent cells and tissues, showing this senescence-associated β-gal (SA-β-gal) as an important biomarker for cellular senescence.[2] We report ratiometric two-photon fluorescent probe (SG1) for β-galactosidase and its application to quantitative detection of β-gal activity during cellular senescence in live cells and tissues. This probe shows a significant two-photon excited fluorescence, a marked blue-to-yellow emission color change (SG1 to 1, Scheme 1) in response to β-gal, easy loading into cells, insensitivity to pH and ROS, high photostability and low cytotoxicity. Moreover, we show that ratiometric two-photon microscopy (TPM) imaging using SG1 is suitable for quantitative detection of SA-β-gal. This probe will be an effective tool for biomedical research, including studies of cellular senescence.

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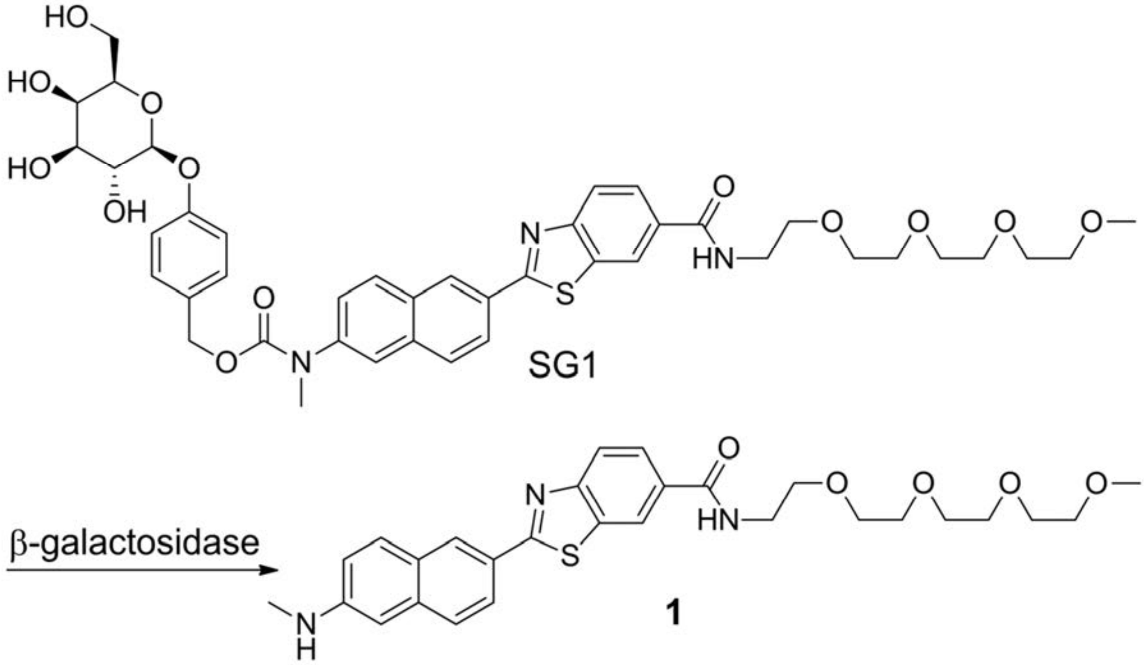
SG1
β-galactosidase
1

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Ratiometric Detection of Intracellular Calcium Ions using aTwo-photon Probe

이혜수 김환명[1,*]

아주대학교 에너지시스템학부 응용화학전공 [1]아주대학교 에너지시스템학부

The calcium ion (Ca^{2+}) is a universal intracellular messenger that mediating a diverse range of cellular processes, such as gene transcription, muscle contraction, ion transport and cell proliferation. In most mammalian cells, Ca^{2+} has a major signaling function when it is elevated in the cytosolic compartment.[1] The Ca^{2+} concentration inside in the resting cell reserved in very low concentration 100-200 nM, which was increased through transport protein, ATP hydrolysis or Na^{+}/Ca^{2+} ion exchange processes.[2]To date, several fluorescent probes for detecting intracellular Ca^{2+} using two-photon microscopy (TPM) are developed. However, there are few reliable methods for the quantitative measurement of the Ca^{2+} concentration in live tissues. Therefore, tools to quantitatively detect Ca^{2+} concentrations in living tissue would be useful.We anticipated that a two-photon (TP) turn-on probe linked to an internal reference through a spacer could be achieved this goal. In this study, we designed and synthesized TP probes for Ca^{2+} with internal reference (SCa1-IR and SCa1-IR_AM). These probes are derived from methoxy-benzochromene moiety as an internal reference unit and 6-(benzo[d]thiazol-2'-yl)-2-(methylamino)naphthalene as the TP fluorophore, with the piperazine moiety as the linker. The working of such system involves the change in the fluorescence intensity of one of the fluorophores that is directly linked to binding unit, keeping the fluorescence of other fluorophore unchanged. This probe shows a significant TP cross section, high selectivity for Ca^{2+} and can quantitatively monitor Ca^{2+} in subcellular level with minimum interference from the experimental effects such as probe distribution and incident laser power.

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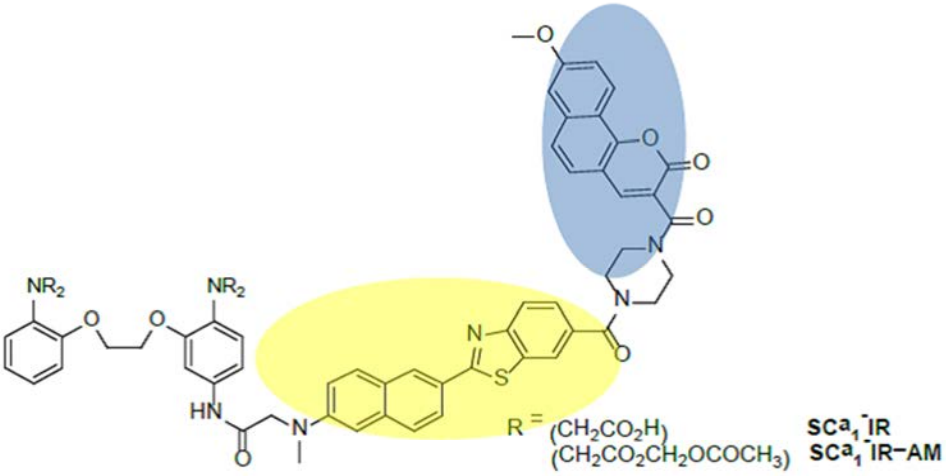

Figure 1. Structures of SCa1-IR and SCa1-IR_AM

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A Two-Photon Fluorescent Probe for Ratiometric Bioimaging of Cysteamine

Sarkar Avik Ranjan 박상준 **김환명***

아주대학교 에너지시스템학부

Cysteamine (CS) is the simplest stable aminothiole and a decarboxylate form of cysteine.1 CS is distributed in all living organisms due to the degradation of coenzyme A and plays a key role in several physiological processes such as amino acid transport,2 protein synthesis,3 reduction of disulfides4 and protection in oxidative damage.5 In medical application, CS has shown its potentiality in cystinosis treatment. Moreover, CS has shown unique biological function enhancing the chemotherapeutic effect through the autophagy modulation in cancer cells. To detect thiols in cells, a number of fluorescent probes have been developed using various thiol-reactive functional groups.6 Recently, probes bearing acrylates as the thiol-reactive unit have been widely used.7 To enhancing the selectivity to the different thiols have been based upon the alterations in the pKa values and the bulkiness of the target thiol. However, the selectivity of these thiols toward CS has yet to be reported. Herein, we report a ratiometric TP fluorescent probe (SCS1) for selectively and precisely monitoring CS in live cells and tissues. This probe shows blue-to-yellow emission color change in response to CS, high selectivity for CS over other thiols and biologically relevant species, and pH insensitivity and can be easily loaded into the cells. We assume SCS1 could play a vital role in understanding the biological and medicinal roles of CS in living systems.

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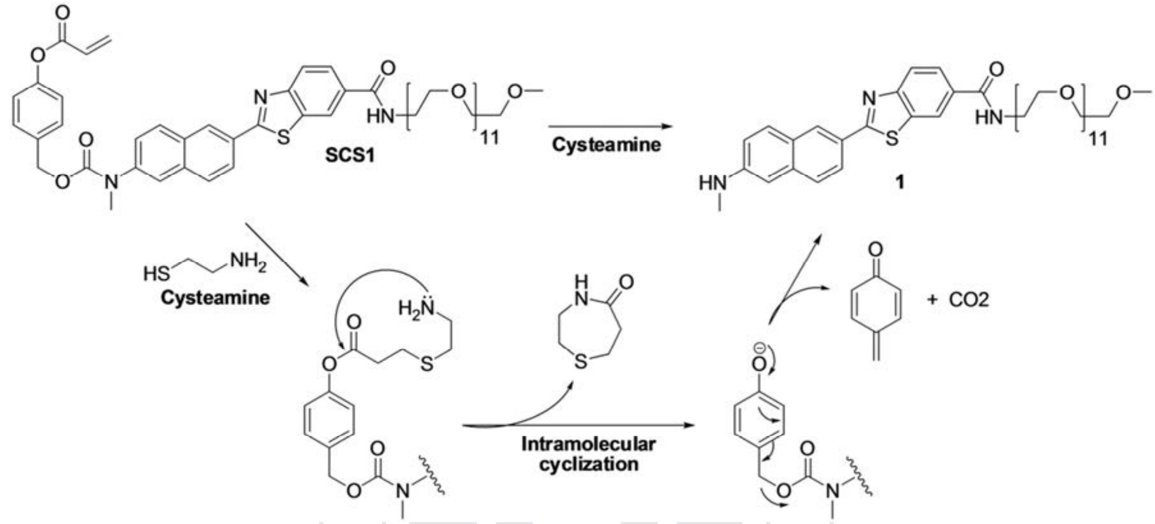

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Two-Photon Fluorescent Probe for Zinc Ions in Golgi Apparatus

Hardev Singh Virdi 이효원 김환명*

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Zinc ion plays crucial roles in the survival, growth, and metabolism of unicellular and multicellular organisms. So far, little is known about subcellular Zinc ion distribution. Especially, endoplasmic reticulum (ER) and Golgi apparatus sequester excess cytosolic Zn^{2+} indicating that organelles have the potential to play an important role in maintaining the intracellular $[Zn^{2+}]$ at physiological level.[1]To understand its role in physiology, it is crucial to visualize the distribution and transport of Zn^{2+} in live cells and intact tissues. For this purpose, we used two-photon microscopy (TPM), which utilizes two photons of lower energy for the excitation. TPM has the advantages of increased penetration depth (> 500 μm), localized excitation, and prolonged observation time. We therefore developed two-photon fluorescent (TPF) turn-on probe (SZn1-acid) for imaging of intracellular free zinc ion in Golgi apparatus. This probe shows high TPF enhancement in response to Zn^{2+}. The probe is highly selective towards Zn^{2+} ions over the other cations and also insensitive in the biologically relevant pH range. This novel probe can selectively detect Zn^{2+} in Golgi apparatus by using TPM.

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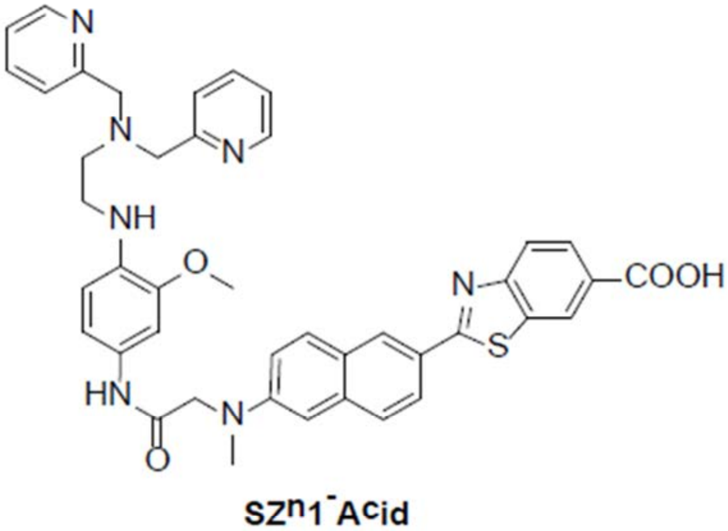

Scheme 1. Structures of SZn1-acid.

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Ratiometric Two-Photon Probes for Mitochondrial pH

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아주대학교 에너지시스템학부

Mitochondria are the double-membrane-bound subcellular organelles play a crucial role in cell metabolic processes.[1] The mitochondrial function depends on its pH. At alkaline pH (pH ~ 8.0) mitochondria shown its efficiency to operate its cellular process whereas alters in pH brake down its normal function and leads to generate reactive oxygen species and mitochondrial depolarization.[2] The mitochondrial depolarization is associated with cardiovascular diseases, neurodegenerative and Reye's syndrome.[3] To monitor the change in mitochondrial pH handful OP (one photon) probes have been reported.[4] To the best of our knowledge two-photon probe for monitoring the mitochondrial pH have yet to be reported.

Recently, two-photon microscopy (TPM) took a great attention due to its advantage over the OPM (one-photon microscopy) because it provides greater tissue penetration, localization of the excitation and longer observation.[5] Whereas the fluorophore with emission intensity at longer wavelength provide a better spectral separation from cellular absorption and auto fluorescence in compare with a fluorophore that have intensity in lower wavelength region. Take into consideration of the above mention facts. Here, we report two-photon probes for monitoring mitochondrial pH in live cells and living tissue. The probes are able to monitoring the mitochondrial pH value in a ratiometric manner.

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Development of related substances test method for CARDIOXANE Injection :Identification of degradation products through stress testing of Dexrazoxane and Tandem mass spectrometry

한남석* 김재민 이지혜

보령제약(주) 중앙연구소

의약품 개발에 있어서 제품의 품질 확보가 가장 큰 이슈이면서 지속적으로 논란이 되고 있다. 그 중 제품의 고품질 확보를 위해서는 유연물질에 대한 정확한 구조 확인과 정량에 대한 정확한 자료를 확보하는 것이 관건이다. 또한 최근 ICH 에서는 API 에 존재하는 모든 불순물에 대한 발생경로와 품질 관리에 대한 부분을 강조하고 있다. 일반적으로 최근에 개발된 의약품의 유연물질 표준품을 쉽게 확보할 수 없기 때문에 정확한 품질관리가 어렵다. 따라서 표준품이 없이 제품의 유연물질을 확인할 수 있는 방법을 탐색하기 위해 이 연구를 수행하였다. 주사용 심장보호제인 카디옥산 주사제 분석법 개발에 있어서 가혹 시험 (Stress testing)을 통한 분해산물을 생성시켜 이들의 구조를 확인하고, 특이성을 갖는 유연물질 분석법을 개발하여 Dexrazoxane 유연물질의 설정과 이에 대한 근거 자료를 확보하는 것이다.

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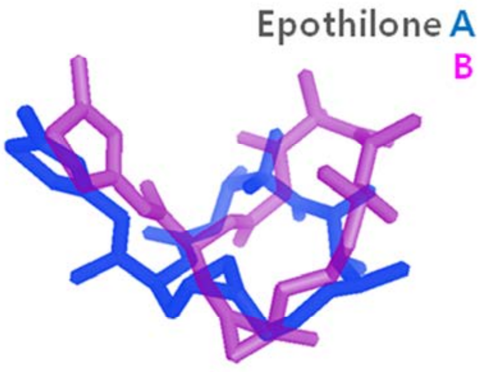
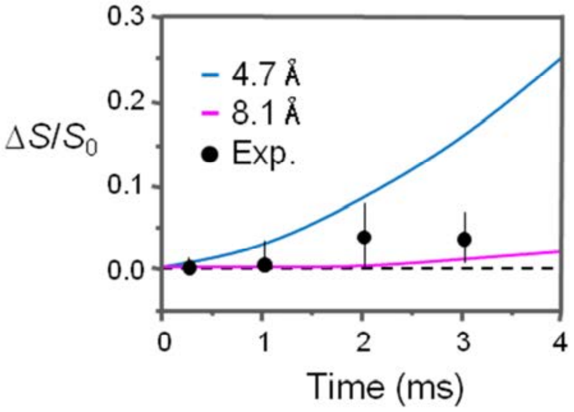
An NMR Study of Microtubule-bound Epothilone B

백윤기* 이효원[1]

한국기초과학지원연구원 대구센터 [1]충북대학교 화학과

Epothilones represent prominent antitumor agents to overcome multidrug resistance and limited supply of taxane derivatives for microtubule-targeting drugs. However, the fundamental question on the origin of the difference between the biological activities of epothilone A and B has remained unanswered. A deuterium and fluorine labeled analog of epothilone B was designed and synthesized, and its microtubule bound-conformation was investigated using solid-state REDOR NMR techniques. Our NMR resutls indicated that the macrolide conformation of epothilone B might be different from the one previously reported for tubulin-bound epothilone A in zinc-stabilized 2D sheets but, instead, be similar to the conformation found in the crystal structure of epothilone B-bound P450epoK complex. Docking calculations of epothilone B with tubulin dimer suggest that epothilone A and B possibly share in common the hydrogen bond interactions between the hydrophilic side of the ligands and the Thr274 residue of beta-tubulin, but their binding modes, especially the conformations of macrolides, may be different from each other in order to find optimal binding environments for their dissimilar expoxide moieties with beta-tubulin.





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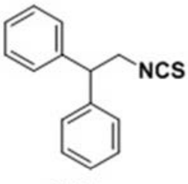
Biological evaluation of sulforaphane analogues as protective agents against cisplatin induced cytotoxicity in kidney cells

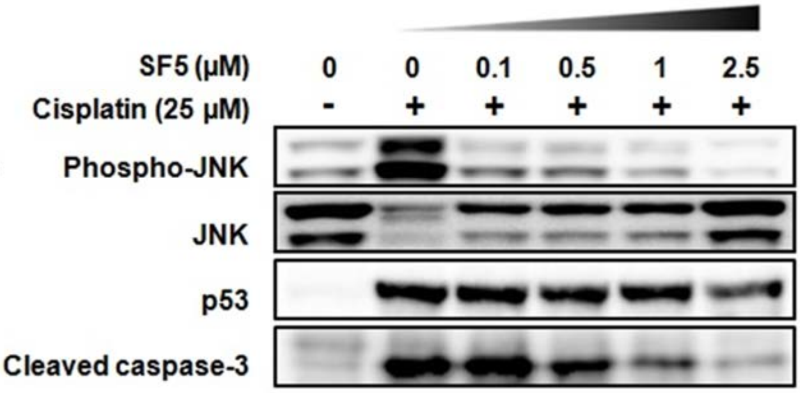
이재욱* 함정엽[1]

한국과학기술연구원(KIST) 천연의약센터 [1]한국과학기술연구원(KIST) 강릉분원

Sulforaphane analogues were prepared and evaluated for any renoprotective effects on cisplatin-treated cultured kidney cells (LLC-PK); two kinds of natural product analogues exhibited a potent renoprotective effect. In an additional study, we demonstrated that the blocking of MAPKs-p53-caspase-3 signaling cascade plays an important role in mediating the protective effect of these compounds against oxidative cytotoxicity in cultured LLC-PK1 cells.



SF5


SF5 (μM) 0 0 0.1 0.5 1 2.5
Cisplatin (25 μM) - + + + + +
Phospho-JNK
JNK
p53
Cleaved caspase-3

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Structure-Activity Relationship Study of Novel IM3829 Analogues as Potential Radiosensitizers

최현경* 남기엽[1,*] <u>김미정</u>

중원대학교 의약화학과 [1]서울아산병원 항암선도기술개발지원센터

Nine novel IM3829 derivatives were designed with diverse functional groups and were evaluated for the ability to inhibit Nrf2 and increase the cytotoxicity of lung cancer cells. We identified an effective IM3829 derivative by a structure-activity relationship study. Our results demonstrate that the treatment with compound 2g inhibits Nrf2 binding activity to ARE consensus sequences. It also inhibits mRNA and protein expression of Nrf2 and HO-1 more effectively than the mother compound. In addition, we observed the enhancement in IR-induced cell death in H1299 cells using compound 2g. These data suggested that combination of compound 2g and IR might be a useful radiosensitizing treatment, guiding the development of newly improved IM3289 derivatives through SAR models.

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Design, synthesis, and biological evaluation of new EGFR/HER2 dual inhibitors

Ahmed Elkamhawy 노은주[1,*]

과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]한국과학기술연구원(KIST) 화학키노믹스 연구센터

Overexpression of the epidermal growth factor receptor (EGFR or ErbB1) and human epidermal growth factor receptor 2 (HER2 or ErbB2) which are members of the ErbB family of receptor tyrosine kinases (RTKs) is frequently observed in various solid tumors. Both kinases have been validated as rational targets for cancer therapy. Herein, our team has designed and synthesized new eighteen analogues of 6-substituted 4-anilinoquinazolines to selectively inhibit EGFR/HER2 tyrosine kinases. The pharmacological results indicated that twelve compounds showed excellent inhibitory activities with nanomolar range of IC50 values on EGFR and/or HER2 kinases. Molecular docking study was carried out to predict the binding modes and affinity scores of all the final compounds at the ATP active site of both kinases.

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Design, synthesis, and biological evaluation of new EGFR/HER2 dual inhibitors

Ahmed Karam Mohamed 노은주[1,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

Coexpression of EGFR and HER2 has been found in many tumors such as breast, ovarian, colon and prostate cancers, with poor prognosis of the patients. Therefore, it is more effective to dual target EGFR/HER2 rather than just EGFR inhibition. Our team has designed and synthesized new eighteen analogues of 6-substituted 4-anilinoquinazolines to selectively inhibit EGFR/HER2 tyrosine kinases. A cell-based assay was performed to evaluate the antiproliferative activity of the new agents using the human breast carcinoma cell line (BT-474) which characterized by the overexpression of HER2. The ureido series (8a?8d) and ethyl ureas (9a?9d) that exhibited promising results on the enzyme assay, showed the best antiproliferative effects on the cellular level too. Respecting these two series, compounds with 3-fluorobenzyloxy (8c and 9c) and pyridyloxy moieties (9d and 9d) showed better antiproliferative activities than the other analogues containing phenoxy moieties (8a, 9a, and 9b). Molecular docking study was carried out to predict the possible binding mode of the most active compounds with the targeted kinases.

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Acuminolide A : Structure and Bioactive of a New Polyether Macrolide from Dinoflagellate *Dinophysis acuminata*

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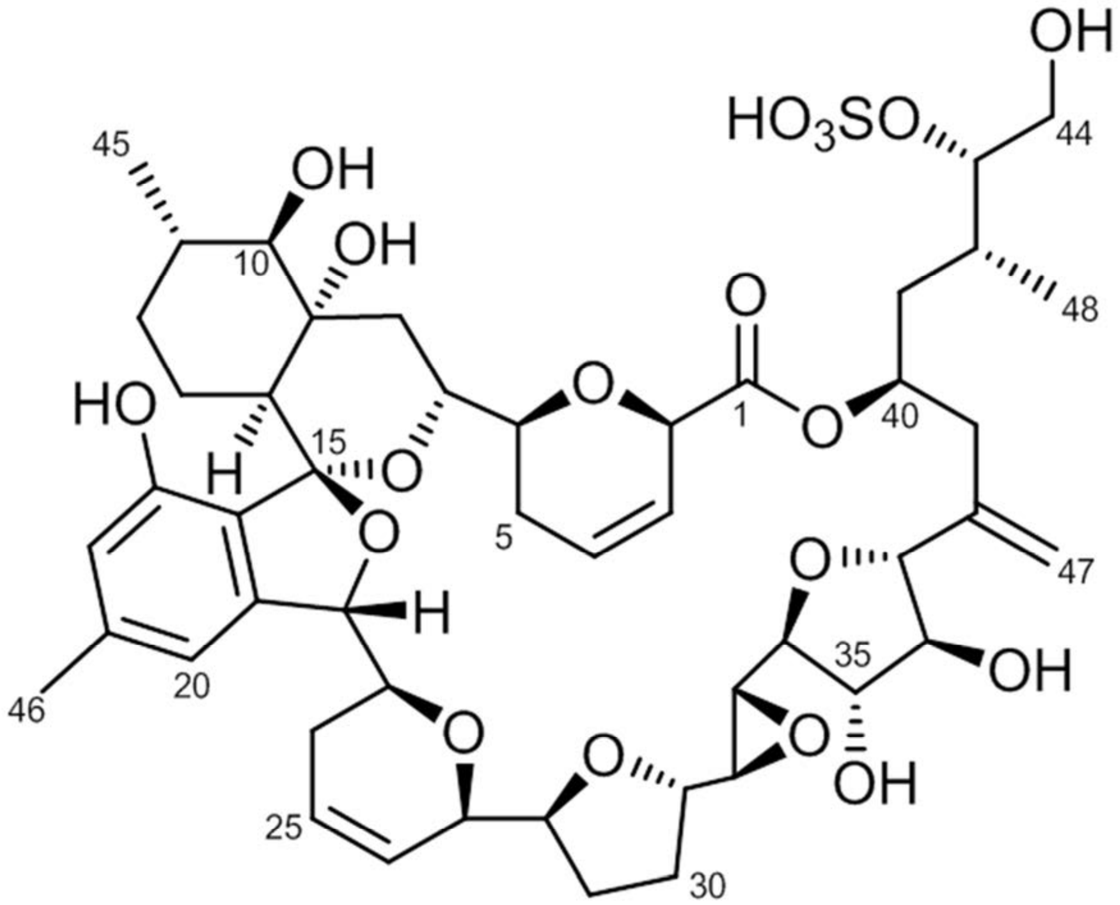
한국과학기술연구원(KIST) 천연물연구소 [1]강릉원주대학교 화학신소재학과

Several marine dinoflagellates are known to produce a variety of structureally compound biologically toxic secondary metabolites. The *Dinophysis* species is a well-known example of such harmful dinoflagellates because it is economically damaging to the bivalve culturing industry through diarrhetic shellfish poisoning (DSP). For a long time, in-depth study of this species was hampered due to the unavailability of laboratory strains. However, after the successful culturing of *D. acuminata* in 2006, much research has been now conducted on this species. In particular, well-known toxins were identified from the culture of *D. acuminata*, including pectenotoxin II (PTX-2) which is isolated primarily from the *Dinophysis* species. To this end, we successfully isolated 225 mg of PTX-2 from a 10000 L culture of *D. acuminata*. While separating other toxins, an interesting macrolide, acuminolide A (1), was isolated with the other known toxins, dinophysistoxin I (DTX-1), okadaic acid (OA), and 7-epi-PTX-2 seco acid. Acuminolide A (1) was purified with high performance liquid chromatography (HPLC), and also structure was completely elucidated by a combination of NMR and LC-MS/MS technique. In contrast to the other well-known toxins that were isolated, compound 1 showed no cytotoxicity against four cancer cell lines but caused potent stimulation of actomyosin ATPase activity.


OH
HO₃SO
44
45
OH
10
OH
48
O
HO
1
40
15
O
H
O
5
O
47
H
O
35
OH
46
20
O
O
O
OH
25
30

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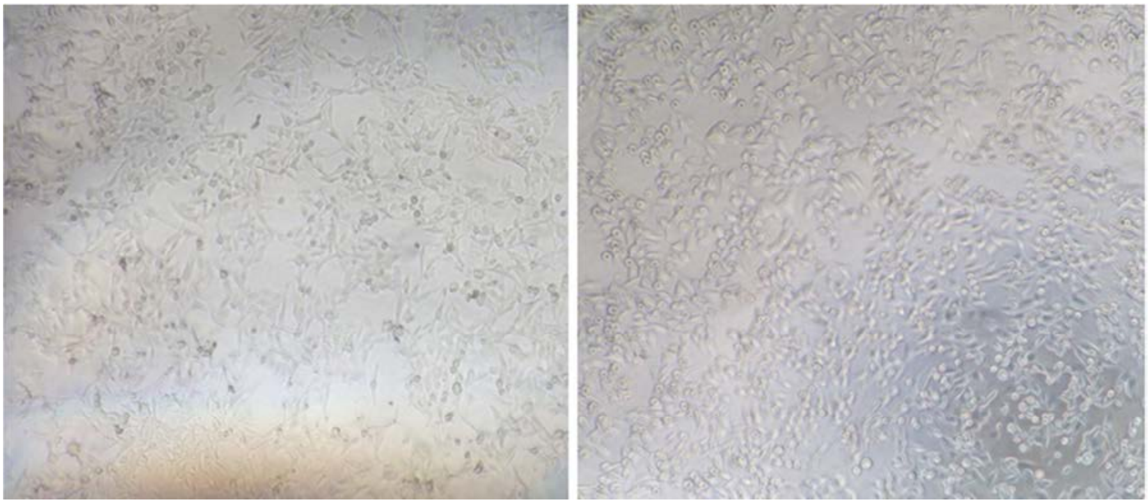
인삼의 신규가공법을 통한 유효성분 극대화 및 항암활성 연구

김관태 최필주 김규선[1] 함정엽[*]

한국과학기술연구원(KIST) 천연물연구소 [1]강릉원주대학교 해양자원육성학과

인삼은 다양한 질병의 예방과 치료, 건강증진을 위해 널리 사용되고 있는 한 약재이다. 특히 최근 들어 인삼 내 포함된 사포닌인 진세노사이드를 활용한 항산화, 항암, 항염증, 항바이러스, 기억력 개선, 면역증진, 신경조절, 간 보호, 혈당저하 및 지방흡수 조절작용 등의 연구결과가 보고되고 있는 것처럼 진세노사이드의 다양한 생리활성연구는 그 폭이 넓어지리라 판단된다. 한편, 가공인삼인 홍삼은 진세노사이드 Rg3, Rk1, Rg5 가 많이 포함되어 항암활성이 월등하고 혈관이완작용, 혈소판 응집억제 효과 등에서 가공하지 않은 인삼보다 좋은 효과가 알려져 왔고, 이로 인해 인삼의 새로운 가공방법 개발이 꾸준히 이루어지고 있다. 최근, 식생활변화 및 평균수명이 증가함에 따라 암으로 인한 사망률이 급격히 증가하는 추세이고 이는 사회적, 경제적으로 엄청난 비용이 발생됨으로써 국가적으로 문제가 되고 있는 상황이다. 하지만 항암치료 시 사용하는 합성의약품들은 종양세포뿐만 아니라 정상세포도 같이 파괴하는 부작용이 발생함으로 전통한약처방 및 소재를 활용한 천연물 유래의 항암제 개발은 매우 중요하다고 볼 수 있다.이에 본 연구자들은 약리작용이 뛰어난 인삼의 신규가공법을 개발하였고, 이로부터 인삼 유효성분인 진세노사이드 Rg3, Rk1, Rg5 의 함량을 극대화 함으로써 다양한 의약품, 기능성식품 및 향장소재의 원료가 되는 신개념의 인삼가공물을 소개하고 항암효과를 발표하고자 한다.



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Synthesis and characterization of covalent bonded chlorin derivatives on graphene oxide nanosheets for photodynamic theraphy

강은선 윤일[1] 심영기[2,*]

인제대학교 나노융합공학과 [1]인제대학교 PDT 연구소 [2]인제대학교 나노공학부

Graphene oxide nanosheets were prepared and characterized. Chlorin derivatives were synthesized and covalent bonded on the graphene oxide nanosheets, which was characterized by FT-IR, NMR, Raman, XPS, TGA, etc.

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A Medusa-Like β-cyclodextrin with Maleic Anhydride Derivatives, A Potential Carrier for pH-Sensitive Drug Release

강선영 이연*

서울대학교 화학부

We developed a new pH-sensitive drug delivery carrier based on β-cyclodextrin (β-CD) and 1-methyl-2-(2'-carboxyethyl) maleic anhydrides (MCM). To optimize pH-sensitivity for controlled drug release, we synthesized five maleic acid amide derivatives (maleic, citraconic, cis-aconitic, 2-(2'-carboxyethyl) maleic, MCM) maleic acid amide), and compared their degradabilities for the development of pH-sensitive biomaterials with tailored kinetics of the release of drugs. Based on these results, we selected MCM and the primary hydroxyl groups of β-CD were successfully attached to MCM residues to produce a medusa-like β-CD-MCM. The MCM residue was conjugated with cephradine (CP) with high efficiency (>90%). More importantly, β-CD-MCM-CP responded to the small pH drop from 7.4 to 5.5 and released greater than 80% of the drugs within 0.5 h at pH 5.5. In addition, the inclusion complex between β-CD-MCM-CP and the adamantane derivative was formed by simple mixing to show the possibility of introducing multifunctionality. Based on these results, β-CD-MCM can target weakly acidic tissues or organelles, such as tumours, inflammatory tissues, abscesses, or endosomes, and be easily modified with various functional moieties, such as ligands for cell binding or penetration, enabling more efficient and specific drug delivery.

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Development of Deoxoartemisinin-Glycolipid Hybrids as Anti-oral Cancer Agents

민동국 김민규[1] 정만길*

연세대학교 화학과 [1]연세대학교 화학과

In order to improve anticancer activity, treatment using hybrids drugs, an approach that incorporates two drugs into a single molecule, has been developed. The use of hybrid drugs can impact multiple targets simultaneously. Furthermore, no anti-oral cancer agent has been reported in the literature to date. In this study we report on the practical synthesis and the first potent in vitro anti-oral cancer activity of derivatives of artemisinins, glycolipids, and trioxane-glycolipid hybrids. Novel trioxaneglycolipid hybrids were directly synthesized from 12β(C-C)-type deoxoartemisinin and glycolipid by coupling reaction and exhibited exceptional in vitro anticancer activity, particularly against the oral carcinoma cancer cell lines, HSC-2 and Ca.9-22, respectively. The trioxane-glycolipid hybrids, with effective concentrations under 20 µM, demonstrated better anticancer activity than either artemisinin or glycolipid alone and showed five times more anti-oral cancer activity than either cisplatin or paclitaxel.

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Light-Induced pH-Responsive Degradation of Fumaramic Acid Derivatives

송영준 이연*

서울대학교 화학부

트랜스 형태의 Fumaramic 산 유도체는 UV light 조명 하에서 이성질체인 시스 형태 이성질체인 말레 산 유도체로 전환 될 수 있으며, 이러한 말레 산 유도체는 광이성화 후 산성 pH 에서 pH 응답 분해성을 보여준다. 이러한 fumaramic 산 유도체의 광이성화에 의한 pH 감응성 분해 속도는 이중결합의 치환체를 변화시킴으로써 제어 될 수 있다. Fumaramic 산 유도체의 광이성화 기반 pH 응답 분해성의 성질은 생물 의학 응용분야에서 다중 신호에 반응하는 스마트 재료의 개발을 위한 물질로써 잠재력을 가지고 있다.

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New PreQ1 Analogues as PreQ1 Riboswitch Regulators; Synthesis and NMR Study

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Riboswitches are primarily found in the 5′ untranslated regions (UTRs) of bacterial messenger RNAs and are cis-acting elements that control gene expression by directly binding specific small molecule metabolites. Riboswitches are different from other RNA drug targets because they have unique aptamers for binding specific metabolites, thereby acting as regulators of bacterial gene expression. Several compounds have been developed for targeting riboswitches. Nucleobase riboswitch classes have been characterized that respond to ligands such as guanine, adenine, 2’-deoxyguanosine, and preQ1. We are focusing on the preQ1 riboswitch, which has a unique aptamer structure; we have synthesized new preQ1 derivatives as preQ1 riboswitch regulators.The NMR study of compounds 15h, 15k, and 15l was performed by using 600 MHz NMR. The NMR spectra of compound 15h demonstrated the same conformation as did preQ1. However, the imino resonances of the two compounds 15k and 15l exhibited different spectra, compared with those obtained in previous results and relative to those of each other. We hypothesize that their side chains influenced formation of the secondary structure of the newly generated loop or P stems after binding to the riboswitches. These two compounds are currently being studied to determine their conformations. Furthermore, three compounds will also be evaluated biologically.

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Synthesis of a Novel N-five-membered-heterocycle-N',N"-disubstituted guanidine derivatives for S-nitrosoglutathione reductase inhibition

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S-Nitrosoglutathione reductase (GSNOR) is an alcohol dehydrogenase (ADH) involved in the regulation of intracellular levels of S-nitrosoglutatione (GSNO). GSNO is an endogenous bronchodilator that elicits many biological functions of NO, increases of which are associated with dilation of bronchi and bronchioles and the bronchial smooth muscle relaxant effects. In human asthma, there are lower GSNO concentrations in the lungs, likely attractable to up-regulated GSNOR. This has emerged as a potentially important target for the treatment of asthma, which has lowered levels of NO as a basis to their pathophysiology. These results implicate GSNO metabolism as a target for therapeutic intervention of asthma. Along these lines, we focus our effort to construct benzopyran derivatives which showed goal biological activity to inhibit S-nitroglutathione reductase. Now we are turn our interest to a synthesis of five-membered heterocycle derivatives having a N',N"-disubstituted guanidine as a novel small organic drug-like lead compound without side-effect of existing Asthma drugs.

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Solid-phase synthesis of 2-Amino/amido-1,3,4-Oxadiazole and 1,3,4-Thiadiazole Through Reagent-based Regioselective Cyclization Process of Thiosemicarbazide

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Solid-phase organic synthesis(SPOS) is now routinely used to prepare druglike, small organic molecules in medical chemistry programs. Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In this family, 1,3,4-oxadiazoles and 1,3,4-thiadiazoles have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as anti-inflammatory, anti-microbial, anti-convulsant, anti-cancer, and anti-hypertensive. In this reason, we had an interest to the synthesis of 1,3,4-oxadiazole and 1,3,4-thiadiazole analogues and then developed efficient solid-phase synthetic methodology. As a results, we constructed 2-amino/2-amido-1,3,4-oxadiazole and 1,3,4-thiadiazole library in a high yields and purities.

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Copper-mediated Synthesis of 1,3,5-Trisubstituted 1,2,4-Triazoles via Oxidative Intramolecular N-N Bond Coupling using Cerium Sulfate as oxidant

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For the synthesis of pharmaceutically important 1,2,4-triazoles, many synthetic methods utilized hydrazines and their derivatives having N-N bond. Instead of using the building blocks, we applied copper-mediated N-N bond coupling reaction to produce 1,3,5-trisubstituted 1,2,4-triazoles via imidoyl isothiourea prepared from amidines and isothiocyantes using cerium sulfate as oxidant. This new synthetic route can facilitate production of the range of the compounds because intermediates incorporating N-N bond that would be difficult to prepare could be avoided. In addition, the transformation does not require a leaving group on the nitrogen atom to create N-N bond, which makes it atom- and step-economical.

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A Novel 2-Arylethynyl-substituted Heterocyclic pyrazine Derivatives as a Human Trasnglutaminase 2 inhibitor

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동국대학교 화학과 [1]동국대학교 의약화학연구실

A transglutaminase is an enzyme that catalyzes the formation of an isopeptide bond between a free amine group. TGase 2 is associated with various diseases in particular it influences drug resistance in cancer cells. we have focused on the exploration of small novel molecules as a TGase 2 inhibitor as these kind of molecules have become good candidates to replace peptide based inhibitor drugs. After an initial screening of skeletal representative , ethynyl substituted pyrazine derivatives showed strong inhibition properties against TGase 2 activity. In order to discover better drug like compounds we have designed new core skeletons based on the bioisostere concept. We have tried to develop core skeleton by changing the quinoxaline ring. An unprecedented core skeleton that could improve the physiological properties and cell proliferation compared with quinoxaline compound in renal cancer cells.

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Design and Optimization of Inhibitors on AIMP2-DX2, oncogenic splicing variant

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Aminoacyl-tRNA synthestase-interacting multifunctional protein 2 (AIMP2) is a potent tumor suppressor inducing apoptosis upon various signals. AIMP2-DX2, an exon2-deleted splicing variant of AIMP2, is upregulated in lung cancer and competitively suppresses the pro-apoptotic activity of AIMP2 resulting in tumorigenesis. From high throughput screening, we found three chemical classes of compounds which selectively inhibited AIMP-DX2 without inhibition on AIMP2. Herein, we reported that 1) how new scaffolds were found and validated; 2) optimization process though syntheses and evaluation of derivatives; 3) structure-activity relationship (SAR) analysis of a series of compounds; 4) profiles of validated hits.

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Design and Optimization of Pyrrolopyrimidine-based MELK (maternal embryonic leucine zipper kinase) inhibitors

wadoodabdul 김성우[1,*] 이선경[2,*] 박철민[3,*] 송종환[4,*]

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Murine protein serin/theronin kinase 38 (MPK38), also known as maternal embryonic leucine zipper kinase (MELK), has been implicated in stem cell renewal, cell cycle progression, cytokines, mRNA-splicing and apoptosis. MELK is correlated with several human cancers and associated with poor prognosis in breast cancer and gliobalstoma patients. In this study, we are reporting the design, synthesis, and evaluation of new compounds as MELK inhibitors based on pyrrolopyrimidine scaffold. New compounds were designed and optimized based on the structure of hits from HTS and crystal structure of enzyme.

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First total synthesis of natural pulsatilla saponin D via highly stereospecific glycosylation

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연세대학교 화학과 [1]연세대학교 화학과

Oleanane-type saponins that extracted from roots of Pulsatilla koreana have been showed a good cytotoxic activity on several human cancer cell lines. Pulsatilla saponin D, one of the oleanane-type saponins has exhibited a great anti-lung cancer activity. The first total synthesis of pulsatilla saponin D was accomplished in eight steps from protected L-arabinopyranoside in high overall yield via a highly stereospecific glycosylation featuring an oxocarbenium mechanism between the trisaccharide derivative and aglycone as the key step

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Clicked Synthesis of Purpurinimide Derivatives for Photodynamic Therapy

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Photodynamic therapy (PDT) is based on the accumulation of a photosensitizer (PS) in tumors, for which given exposure of light at an appropriate wavelength generates reactive oxygen species (ROS, e.g.singlet oxygen) that results in tissue destruction. Photodynamic study for various functional groups (about shift of wavelength of maximum absorption and biological efficiency) will cause the more convenience about the prediction and control of the photodynamic properties of PS.In this study, purpurinimide methyl ester derivatives were synthesized using N-propargyl-purpurinimide methyl ester as starting material. The derivatives were synthesized by 1,3-dipolar cycloaddition of N-propargyl-purpurinimide methyl ester containing a terminal triple bond and azide derivatives containing various functional groups. The click reaction, which was carried out using 10 mol% of copper(I) iodide in dichloromethane with an addition of diisopropylethylamine (DIPEA). Each derivative was characterized by 1H-NMR and IR spectroscopies for structure determination, configurations and functional groups.For photodynamic effect of the derivatives, bioassays were investigated by MTT assay against A549 and HeLa cell lines, and shift of wavelength of maximum absorption assays was determined by UV-vis spectroscopy.And then, each photodynamic result was compared with previous studies for cationic chlorins.

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Comparision study of phoroactivity of MPPd-Oxime Derivative and HPPH(Photochlor)

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C3-ethynylated chlorophyll derivative was increases the maximum absorption wave length of the UV spectrum through the various substitutions.We are manufactures HPPd- oxime derivative with similar the structure of HPPH generally known, and compare maximum absorption wavelength.

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종양 진단과 치료를 위한 다기능 나노복합물질 (^{198}Au@Si-folate)의 합성 및 생물학적 평가

이준영 김상욱*

동국대학교 신소재화학과

나노복합물질은 센서, 이미징, 약물전달을 목적으로 연구가 활발히 진행 중인 가운데 실리카로 코팅된 금 나노복합물질에 화학물질로서 엽산을 결합하여 엽산 수용체를 타겟으로 다양한 암 종에 대한 진단 및 치료제로서 역할을 수행할 수 있다. Active targeting 을 위한 표적지향형 나노복합체로서 코어로서 사용된 금 나노입자를 원자로에서 ^{197}Au(n, r)^{198}Au 핵반응을 통해 방사화하여 방사성의약품으로서 기능 할 수 있을 것으로 보여 지며, 합성된 나노 복합물질은 분광학적 분석 장비인 ^{1}H-NMR, UV-Vis, SEM, TEM-EDS, Solid state ^{13}C-NMR 등을 통해 분석하였다. 엽산과 암세포에 과발현된 엽산 수용체와의 결합을 통해서 표적된 암세포에 ^{198}Au 에서 나오는 베타선으로 암 치료제로서 치료용 방사성의약품의 기능을 수행할 수 있다. In vitro, 합성된 나노복합물질로 마우스 대장암 세포인 CT-26 과 유방암 세포인 SK-BR-3 를 대상으로 세포 섭취도 실험을 진행한 결과, 15, 30, 60, 120 분에서 각각 CT-26 세포는 35%, 39%, 41%, 49%이며, SK-BR-3 에서는 32%, 38%, 40%, 48%로 시간이 지남에 따라 약물에 대한 세포 섭취도가 증가함을 확인 하였다. In vivo, 엽산 수용체가 과발현 되어 있는 CT-26 세포주가 이식된 balb/c 마우스로 나노복합물질의 생체내분포도를 측정한 결과 혈액대비 종양이 시간이 증가함에 따라 분포도가 120 분에서 약 2 배 이상 증가 하였다. 또한, 합성된 나노복합물질에 형광을 도입하여 암세포에 uptake 된 형광 이미지를 측정하였다. 이러한 연구 결과를 토대로, ^{198}Au-나노복합물질은 방출되는 베타선으로 암 치료제로서 방사성의약품으로 사용 할 수 있을 것으로 보여 진다.Keywords: 나노복합체, 금-198, 엽산 수용체, 방사성의약품

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[발표취소] Development and Optimization of TR-FRET Assay for Identification of NF-κB Inducing Kinase (NIK) Inhibitors

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양전자방출핵종 ^{68}Ga을 이용한 DOTA-capsaicin 표지 및 생물학적 평가

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Capsaicin 은 다양한 암 세포에서 peroxisome 활성이 증가되면서 apoptosis 가 유발되어 신생혈관억제 및 변형세포, 불멸화 악성세포 성장을 억제한다는 선행 연구가 보고된바 있다. MCF-7 (human breast cancer) 유방암 세포주에 과발현 되어 있는 Estrogen 수용체와 선택적으로 결합하는 효과가 있다. 본 연구에서는, capsaicin 에 양전자방출핵종인 ^{68}Ga 을 도입하기 위해 양기능성킬레이트제인 NOTA(1,4,7-triazacyclononane-1,4,7-triacetic acid)를 사용하였다. [^{69}Ga]NOTA-capsaicin 은, 분광학적분석장비인 UV-Vis, ^{1}H, ^{13}C-NMR, LC-MS 으로 구조분석과 ICP-MS 로 ^{69}Ga 원소분석을 진행하였다. 양전자방출핵종인 ^{68}Ga 은 0.1N-HCl 을 용출액으로 ^{68}Ge/^{68}Ga 발생기에서 추출한 74 MBq 의 $^{68}GaCl_3^+$ 를 NOTA-Capsaicin 에 표지하여 Radio-TLC 및 역상크로마토그래피법(RP-HPLC)을 통하여 표지여부를 확인하였다. 방사화학적수율(RCY%)은 >90% 이였으며, 방사화학적순도(RCP%)는 >99% 이였다. 지용성평가는 1-Octanol 과 PBS 에 [^{68}Ga]NOTA-Capsaicin 18.5 MBq 을 교반하여 측정한 결과, logP 는 -2.31 값으로 수용성임을 나타냈다. 사람 혈청에 대한 화합물 안정성평가는 [^{68}Ga]NOTA-Capsaicin 37 MBq 도입하여 15, 30, 60, 120 분 동안 진행한 결과 90% 이상의 안정성을 보였다. 세포섭취도 평가는 MCF-7, HepG2 (river cancer), CT-26 (coloractal cancer) 암 세포주를 대상으로 15, 30, 60, 120 분 동안 측정 한 결과, 60 분에서 Estrogen 수용체가 발현되어있는 MCF-7 유방암 세포주에서 섭취도가 높은 것을 확인하였으며, 이 후에 시간이 지남에 따라 clearence 가 일어나는 것을 확인 하였다. [^{68}Ga]NOTA-Capsaicin 화합물은 암 진단을 위한 양전자 방출 단층 촬영기(Positron Emission Tomography)의 이미징 시약으로 사용가능할 것으로 전망된다.

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Mode of Inhibition of Serum and Glucocorticoid-Inducible Kinases (SGKs) by a Pyrrolopyridine Derivative

김정은 **HONG VICTOR SUKBONG***

계명대학교 화학과

Serum and glucocorticoid-inducible kinases (SGKs) that are a subfamily of serine/threonine kinases have been implicated in the regulation of inflammation, cell growth, survival and proliferation. Therefore, SGKs are considered potential therapeutic targets for the treatment of several diseases such as cancer, diabetes, and stroke. Modulation of SGK activity by selective small molecule inhibitors would be effective for patients who are suffering from those diseases. GSK650394 is a pyrrolopyridine compound, which is a known SGK inhibitor. Here, we report on the inhibitory mechanism of GSK650394 inhibitor of SGKs by using an immobilized metal ion affinity-based fluorescence polarization (IMAP) method which was already optimized in our laboratory. Lineweaver-Burk double-reciprocal plots and nonlinear regression revealed that GSK650394 is an ATP-competitive inhibitor with the apparent Ki values of 4.57±0.60 nM, 19.42±1.85 nM, and 1.91±0.28 uM for SGK1, SGK2, and SGK3, respectively.

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BGB324 (R428) Is a Highly Potent and Selective ATP-Competitive Inhibitor of the AXL Receptor Tyrosine kinase

김송이 **HONG VICTOR SUKBONG***

계명대학교 화학과

AXL kinase which belongs to a family of TAM(Tyro-3, AXL, cMER) receptor tyrosine plays important roles in tumor progression, invasion, metastasis and chemoresistance. Overexpression of AXL has been shown to be directly proportional to non-small cell lung cancer(NSCLC), metastatic breast cancer and other many solid cancers. Thus AXL has been widely studied as a potential target for cancer therapy. BGB324, which is formerly known as R428, is a heteroaryl substituted triazole compound, and is reported to be a highly selective and potent AXL preclinical candidate. In the present study, we have examined the mode of inhibition of AXL kinase as well as cMET, cMER, ROS1, and TYRO3 by BGB324. We report that BGB324 is an ATP-competitive inhibitor of AXL kinase with the apparent Ki value of 4.8±0.53 nM, BGB324 is also found to be an ATP-competitive inhibitor of the related receptor tyrosine kinases cMET, cMER, ROS1, and TYRO3, but exhibited >64-fold selectivity for AXL kinase.

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Folate receptor가 발현된 암세포의 PET 진단을 위한 ^{44}Sc, ^{68}Ga-HBED-CC-EDBE-Folate PET 진단용 방사성의약품 합성 및 연구

최평석 김상욱*

동국대학교 신소재화학과

Sc-44 는 양전자 방출 핵종으로서 최근 ^{44}Ti/^{44}Sc 제네레이터에서 쉽게 생산이 가능하고 기존에 양전자 방출 핵종으로 연구 되었던 Ga-68 보다 반감기가 길어 PET 측정시간을 연장시킬 수 있다는 장점이 있다. 또한 Sc^{3+}양이온은 Ga^{3+} 양이온과 비슷한 굳은 산 성질의 금속이온으로 킬레이트와 쉽게 착화합물을 형성한다. 이에 선행 연구에서 DOTA, NOTA 와 같은 거대고리킬레이트 보다 온화한 조건에서 빠르게 표지가 가능하고 표지 후 구조적 안정성이 높은 것으로 알려진 양기능성 킬레이트제 HBED-CC 에 Sc-44 를 표지 시키고 생리활성물질을 부착하여 표적지향적 약물전달체로 PET 진단용 방사성의약품로서의 가능성을 확인하고자 하였다. 유방암, 난소암, 직장암과 같은 Folate receptor 가 발현된 암세포를 목표로 하기 위해 Folate receptor 에 특이적으로 결합하는 Folic acid 를 HBED-CC 말단 Carboxyl 기에 coupling 시켰으며 약물의 친수성을 높이기 위해 linker 로 hydrophilic 한 EDBE (2,2'(Ethylenedioy)bis(ethylamine)를 선택 하였다. 먼저 기준물질로 안정동위원소 Sc-45 와 Ga-69 을 HBED-CC-EDBE-Folate 에 표지시켜 표지율, 안정성, 지용성 평가를 실시하였다. 추후에 Sc-44 와 Ga-68 을 표지시킨 후 In vitro 와 In vivo 실험을 통해 세포 섭취율과 표적세포와의 결합성을 테스트하고 생체 내 분포도를 측정하여 체내 동태 및 정상장기와 표적 암세포와의 섭취율, 마우스 모델 PET 영상을 확보하여 ^{68}Ga-HBED-CC-EDBE-Folate, ^{44}Sc-HBED-CC-EDBE-Folate 착화합물의 PET 진단용 방사성의약품으로서 활용 가능성이 있음을 확인 할 예정이다.

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화합물분야 국가 연구성과물 기탁제

황순희 이현연 이현규*

한국화학연구원 한국화합물은행

국가는 연구성과의 활용성 증대를 위해 9 대 연구성과물 전담기관을 지정・운영하고 있다. 한국화합물은행은 2003 년 (구)과학기술부 특정연구개발사업 연구성과물 기탁 및 등록제 화합물분야 중심기관으로 선정, 2008 년 연구성과 관리.유통 전담기관 고시, 2012 년 그 범위가 '국가연구개발사업'으로 확대되었고, 「국가연구개발사업의 관리 등에 관한 규정」 제 25 조제 13 항에 따라 연구성과중 화합물분야 관리・유통 전담기관으로 지정, 2014 년 화합물분야 관리・유통 전담기관으로 지정되어 국가연구개발사업 수행을 통해 창출된 연구성과중 화합물 및 관련 정보의 관리・유통체계 구축・운영의 업무를 수행하고 있다. 한국화합물은행(www.chembank.org)에서는 국가연구개발사업을 통해 창출된 국내고유 양질의 합성 화합물들이 기탁되고 있으며, 기탁된 화합물에 대해 기탁필증을 발급하고 있다.기탁된 화합물들은 다양한 focused 라이브러리(Clinical collection, Kinase, Fragment 등)를 구축하여 연 평균 40 여건 다양한 질병 타겟의 고효율약효검색(HTS)에 활용되고 있으며, 기탁 화합물 및 약효시험결과를 매개로한 산・학・연 공동연구 추진하고 있으며 신약후보물질 발굴에 기여하고 있다.

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Synthesis and antitubercular activity of PA-824 analogs containing 2-methyl-2H-tetrazol at the C-7 position

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Tuberculosis (TB) is an infectious disease that remains a major health problem worldwide. Among the TB, multidrug resistant TB (MDR-TB) needed development of new antibacterial agent. In the course of continuing efforts to sturdy for development new TB drug, recently we selected PA-824 as a promising new class. The PA-824 ((6S)-2-nitro-6-{[4-(trifluoromethoxy)benzyl]oxy}-6,7-dihydro-5H-imidazo[2,1-b][1,3] oxazine) containing nitroimidazooxazine has entered phase II clinical trials as novel TB therapeutics. OPC-67683 has already done clinical trials. Although many side chain analogue containing heterocycle at C-6 position, we try to extend carbon at C-7 position nitroimidazooxazine analogs with 2-methyl-2H-tetrazol to improve potency for antituberculosis than conventional nitroimidazooxazine compound.

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Resioselective bromination of 3-acetyl thiophene and synthetic application to bicyclic thiophene

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Generally, well-known process for the bromination to the 2- and 5-positions of 3-acetyl thiophene. However the yield of regioselectivitie bromination at the 5-position of 3-acetyl thiophene is too low. The best yield of known procedures for the synthesis of 5-bromo-3-acetyl thiophene is 33% by Br_2/AcOH. As another pathway, 5-bromo-3-acetyl tyhiophene was prepared from 2,5-dibromo-3-acetyl thiophene by selective reduction with zinc in AcOH and water. So we studied to obtain 2-bromo-4-acetyl thiophene from 3-acetyl thiophene. In the several reaction conditions, $Br_2/AlCl_3/CH_2Cl_2$ showed in 94% yield. In addition we tried to get bicyclic thiophene from 2-bromo-3-acetyl thiophene as synthetic application.

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Synthesis of Benzoisoxazole Derivatives and Evaluation of choline esterase inhibitory activity

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Even though cholinesterase (ChE) inhibitors and N-Methyl-D-aspartate (NMDA) receptor antagonist are clinically approved to treat Alzheimer's disease (AD) patients, new therapeutic compounds are still needed to be developed. Therefore, many new targets and novel anti-Alzheimer’s disease (AD) drugs have been developed. Since inhibition of cholinesterase (ChE) is still considered to be one of the most effective targets to treat AD patients, many new classes of ChE inhibitors have been synthesized. In an effort of identifying new type of cholinergic drug, the benzoisoxazole moiety of risperidone, which has been reported to possess a wide range of biological activities and mainly used as the anti-psychotic drug to treat schizophrenia, was coupled with the natural antioxidants. Since benzoisoxazole derivatives selectively inhibited butyrylcholinesterase (BuChE) over acetylcholinesterase, they can be a new type inhibitor for BuChE and can be applied to be a novel natural compound derivative drug to treat AD patients. The IC_{50} value of compound 17 was IC_{50} = 0.72 ± 0.11 ?M against butyrylcholinesterase. It is about 13 times more effective butyrylcholinesterase inhibitor compared to Galantamine (IC_{50} = 9.49 ± 2.5 ?M).

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Design and synthesis of novel 2,4-dimaminopyrimidine analogs bearing 2-(isopropylsulfonyl)aniline and benzoazepine moieties for anaplastic lymphoma kinase (ALK) inhibitor

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Anaplastic lymphoma kinase (ALK) belongs to the insulin receptor superfamily of tyrosine kinase. ALK-fused genes such as NPM-ALK, EML4-ALK, KIF5-ALK are putative oncogenes and responsible for many cancers including anaplastic large-cell lymphomas (ALCL), inflammatory myofibroblastic tumors (IMT), diffuse large B cell lymphoma (DLBCL) and a variety of solid tumor types. Crizotinib (Xalkori, Pfizer) is the first approved drug by FDA in 2011 for the treatment of ALK-positive lung cancer patients. Recently, Ceritinib (LDK378, Zykadia, Novatis) was approved in 2014 for the treatment of ALK-positive cancer following treatment with crizotinib. LDK378 retains potency towards L1196M, G1269A, and S1206Y, but loses potency towards G1202R and 1151Tins. In our effort to discovery of potent ALK inhibitor we designed novel 2,4-diaminopyrimidine analogs (KRCAs) which have 2-(isopropylsulfonyl)aniline and benzoazepine moieties. Here we report the synthesis of KRCAs and their anti-ALK activities in biochemical and cellular assay. In addition, PK and in vivo xenograft data of the selected compound will be discussed.

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Mesoporous Silica Nnanoparticle in Macroparge Cell by Endocytosis Based Pretargeting PET Imaging using Bio-orthogonal Strain-Promoted Cycloaddition Reaction

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인하대학교 화학과

An aza-dibenzocyclooctyne-functionalized PEGylated mesoporous silica nanoparticles (ADIBO-PEG-MSN) cell tracer in macrophage cell based pretargeting by bio-orthogonal strain-promoted alkyne azide cycloaddition (SPAAC) using mesoporous silica nanoparticles (MSNs) as precursors with 18F-azide synthon of PEG to develop positron emission tomography (PET) imaging probe through endocytosis for tumor targeting. Here in, ADIBO-PEG-MSN was prepared, which was treated to rADSC and RAW264.7. The pretargeting of particle in RAW264.7 by endocytosis was injected into a living body of U87MG-bearing mice. After 1h, flouring-18 labeled azide-PEG radiotracer was post-injected to the U87MG-bearing mice. We have obtained a PET image of tumor uptake by phagocytosis of macrophage cell through the SPAAC conjugation reaction in the pretargeting mice. The nanoparticles were potentially used safety cell tracking using radioisotope without gene manipulation such as reporter gene.

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Synthesis and biological property of 7,9-dideaza-7-oxa-adenosine

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(2S,3R,4S,5R)-2-(4-aminofuro[3,2-d]pyrimidin-7-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol as a 7,9-dideaza-7-oxa-adenosine was prepared from ribose in 10 steps. The key steps involve the LDA-promoted cyclization of cyano ether(3-amino-4-((2S,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)furan-2-carbonitrile) with furan C-nucleoside. In this key step, this compound is not the mixture of α and β anomer, only one β form compound. Also we tried to prepare new branched purine C-nucleosides from 3-amino-4-((2S,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)furan-2-carbonitrile and (2S,3R,4S,5R)-2-(4-aminofuro[3,2-d]pyrimidin-7-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol. We will introduce biological property of these compounds.

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Activator protein(AP-1)

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인하대학교 화학과

Abstract: Activator protein 1(AP-1)is a transcription factor which is a heterodimeric proteins belonging to the c-Fos, c-Jun, ATF and JDP families. AP-1 regulates a wide range cellular processes, including cell proliferation, death, survival and differentiation. Transactivation is required for tumor promoter-induced transformation in mouse epidermal JB6 cells and for progression in mouse and human keratinocytes. By using mouse and cells lacking AP-1 components, the target-genes and molecular mechanisms mediating these processes were recently identified. The growth-promoting activity of c-June is mediated by repression of tumor suppressors, as well as upregulation of positive cell cycle regulators. JunB has the converse effect. We conclude that transactivation of a subset of AP-1 dependent genes is required for tumor promotion and may be targeted for cancer prevention.

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Structure-Activity Relationships of Anaplastic Lymphoma Kinase (ALK) Inhibitors derived from LDK378

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As ALK-fusion genes have been found in various cancer patients, discovery of ALK inhibitors have been pursued in the field of cancer drug development. As the first ALK inhibitor, crizotinib developed by Pfizer was approved by the US FDA. Since then crizotinib-resistant mutants were clinically isolated and various efforts to overcome resistance issues have been performed. In this regard, LDK378 developed by Novartis was approved for ALK-positive non-small cell lung cancer patients. As our ongoing search for discovery of novel ALK inhibitors, a series of new chemical entities derived from LDK378 were designed and synthesized. Biological assay results of these compounds against ALK wild type as well as mutants were investigated. The design, synthesis, and structure-activity relationship of these compounds will be described.

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Novel 2,5-disubstituted quinolines: Design, synthesis, in-vitro antiproliferative activity and kinase profile

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Three novel series of 2,5-disubstituted quinolines have been designed and synthesized as anticancer sorafenib analogues. Two series (amides & ureas) were designed to possess a spacer between the terminal aryl and 2-aminoquinoline scaffold, whereas the other series (C) lack the spacer while conserving the oxypicolinamide moiety at 5-position. All the target compounds were preliminary evaluated for their antiproliferative effect against three cancer cell lines (MCF7, HCT116 and SKBR3) by MTT assay and exhibited promising antitumor activity. Therefore, 24 compounds were selected to be tested over a panel of 60 cancer cell lines at a single dose concentration of 10 uM at NCI to broadly screen their antiproliferative activity. Six compounds have showed promising mean growth inhibitions and thus were further tested at five-dose testing mode to determine their GI50, TGI and LC50 over the 60 cell lines.

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Development of selective mGluR5 negative allosteric modulators for treatment of neuropathic pain

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Glutamate is the major excitatory neurotransmitter of mammalian in central nervous system and peripheral nervous system. Glutamate receptors regulate glutamate for post-synaptic excitation in neural cell, involved in pathologies of many brain diseases. There are two types of receptors depending on the mechanism of activation: ionotropic glutamate receptors (iGluRs) and metabotropic glutamate receptors (mGluRs). Metabotropic glutamate receptors are one of the type C classes of GPCR (G protein coupled receptors) and they are divided into three groups with eight subtypes on the basis of their sequence hormonology, pharmacology, and signal transduction mechanism. Group I consists of the mGluR1 and mGluR5, which are predominantly identified in post-synapses in the brain region, including the hippocampus, cerebellum, thalamic nuclei, and spinal cord. Recently studies showed that selective mGluR5 antagonists may play a role in the treatment of neuropathic pain and other brain diseases.In efforts to identify selective mGluR5 negative modulators for clinical use, we have synthesized and evaluated several lead compounds on the basis of arylethynylpyridines. Due to their poor pharmacokinetics and solubility, however, they could not proceed to further optimization. In this poster, we will present the design and synthesis of novel heteroarylcarboxamides as mGluR5 negative allosteric modulators (NAMs). Additionally, the results of their antagonistic activity against mGluR5 will be addressed.

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Synthesis of heat shock protein 90 inhibitors and their anti-proliferative ecffects on cancer cells

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Heat shock protein (Hsp90) is an ubiquitous molecular chaperone protein, which accounts for 1-2% of the cytosolic protein under non-stressed conditions. Hsp90 plays an important role in regulating maturation and stabilization of many oncogenic proteins in ten essential hallmarks of cancer. Its client proteins include EGFR, Her2, Met, Akt, Raf, HIF-1, and MMP2. Hsp90 is overexpressed in tumor cell more than normal cell. Hsp90 inhibitor can lead to the degradation of a large collection of oncogenic proteins. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways.Non-small cell lung cancer (NSCLC) is the most common type of lung cancer and that is responsible for 85% of lung cancer patients. Despite several EGER inhibitors have been developed in the treatment of NSCLC, the clinical efficacy of EGFR inhibitors in NSCLC is limited by the development of drug-resistance through the mutation of EGFR and the overexpression of Met. Considering both EGFR and Met are client proteins of Hsp90, blocking Hsp90 folding machinery may be best suited to overcome the resistance form EGFR mutation and Met amplification.In this study, we designed and synthesized a number of inhibitors and they disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer (H1975). The result suggested that these compounds could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

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Targeting Hsp90 chaperone machinery with small molecule inhibitors

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Over the past two decades, several targeted drugs have been discovered to eradicate cancers in specific ways and reduce the harmful nonspecific side effects of conventional chemotherapeutics. However, not all the diseases are amenable to this one disease-one target approach. Also, these drugs are not effective for the treatment of complex diseases, such as cancer. Recent evidence has shown that most single-target drug encounters the emergence of drug-resistance in long-term use. The tumor cells outsmart single-target drugs to escape from their destiny by mutating targeted proteins, down-regulating death signals, or up-regulating survival pathways. Heat shock protein90 (Hsp90) is a molecular chaperone that maintains function of numerous intracellular signaling nodes, utilized by cancer cells for proliferation and survival. Hsp90 is documented to interact with more than 200 different “client” protein involved in signal transduction, receptor maturation and protein trafficking. Most of Hsp90 clients are oncoproteins, including MET, Akt, Raf-1 MMP-2 and HIF-1α. Accordingly, the inhibition of Hsp90 function promotes ubiquitin-dependent proteasomal degradation of its client proteins, which can eventually lead to cell death. For this reason, Hsp90 has emerged as attractive therapeutic target in cancer research and some of them are currently tested clinical trials. As part of our ongoing efforts to discover small molecules targeting N-terminal ATP-binding pocket of Hsp90, we had performed a structure-based drug design (SBDD) of small molecule inhibitors against Hsp90. Designed inhibitors were synthesized and their anti-cancerous activities were evaluated. Here, we report our effort to develop therapeutic agents against Hsp90 in cancer

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Structure-Based Drug Design of Hsp90 Inhibitors and Their Biological Evalution

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Heat shock protein 90 (Hsp90) is a molecular chaperone that is required for the folding, activation and stabilization of numerous client proteins. Many Hsp90 client proteins play significant roles in six essential hallmarks of cancer cell, including Akt, Raf-1, mutant p53, Cdk4, VGEF, MET and HIF-a. The therapeutic potential of targeting Hsp90 may be best appreciated by simultaneously attacking the six hallmarks of cancer cells. Accordingly, the inhibition of Hsp90 function promotes ubiquitin-dependent proteasomal degradation of its client proteins, which can eventually lead to cell death.In this study, we had performed a structure-based drug design (SBDD) of small molecule inhibitiors against Hsp90. Designed inhibitors were synthesized and their antitumor activities were evaluated. Consequently we discoverd potent compounds with nanomolar efficacy. Our data indicates that the compound can serve as a novel clinical candidate for the cancer treatment.

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Development of a ^{68}Ga labeled water dispersible Fe_3O_4 NPs for dual modality of PET and MRI

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동국대학교 화학과

Dual modality imaging is powerful tools to obtain valuable information on function in biomedicine. Isotope-magnetic NPs for dual modality PET/MRI imaging provide an opportunity to combine the power of MRI and PET, which has better anatomical resolution with the sensitivity. In this present work, nano-bio composites were designed and successfully synthesized using Fe_3O_4 nanoparticles (NPs) and ^{68}Ga radioisotope dual applications of diagnostic imaging agent in Positron Emission Tomography (PET) and Magnetic Resonance Imaging (MRI). The ^{68}Ga-SCN-NOTA-Hydrazine-Fe_3O_4 NPs (^{68}Ga NHFCNP) as targeted compound were synthesized via surface modified Fe_3O_4 NPs and NOTA as bi-functional chelating agent with ^{68}Ga radioisotope from an in-house generator. Thus ^{68}Ga NHFCNP could exhibit synergic property such as the magnetic behavior and radio activity.

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Synthesis and Biological Evaluation of Analogues of KTH-13 Isolated from Cordyceps Bassiana

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광운대학교 화학과

KTH-13 [4-Isopropyl-2,6-bis(1-phenylethyl)phenol] was isolated from artificially cultivated fruit bodies of Cordyceps bassiana, which is one of the most important species in traditional herbal medicine in Korea. In order to explore its anti-cancer activity, we synthesized KTH-13 started from 4-isopropylphenol and 1-phenylethanol through the electrophilic aromatic substitution reaction. In this presentation, the detail synthesis of a series of KTH-13 derivatives and their anti-cancer activity will be discussed.

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Synthesis and Biological Evaluation of Cu-64 DOTA-aptamer Conjugates as Theranostic Agent for Lymphoma

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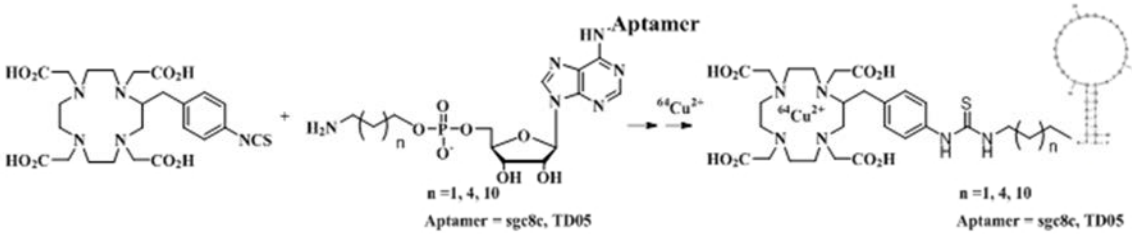
Purpose: Aptamers, composed of many nucleic acids like DNA or RNA, are well- known as targeting molecule for Burkitt's lymphoma or acute lymphoblastic leukemia one of the most progressive cancers in human.[1] To dignosis and therapy for lymphoma, we designed and synthesized six kinds of aptamer analogues, conjugated with bifunctioanl chelator (DOTA) and one adenosine located at the end of aptamer sge8c and TD05.[2]Methods: Six kinds of aptamer analogues were prepared by SPPS (Solid-Phase Peptide Synthesis) method at IDT (Integrated DNA Technologies, U.S.A). At the end of aptamer anologues, the adenosine was exchanged from 5'-hydroxy group to 5'-amino alkyl group, increasing alkyl chain (n = C3, C6, C12) between amino group and sugar ring. To label a metallic radioisotope, six aptamer analogues were conjugated with bifunctional chelator, DOTA. After labeling of Cu-64, [Cu-64]DOTA-aptamer conjugates were evaluated as serum stability, LogP values, cell uptake and in vivo PET imaging.Result: The radiochemical yield and purity of [Cu-64]DOTA-aptamer conjugates was showed over 95% at 80oC for 5 mins. They was very stable as the radiochemical purity of over 95% for 24 hrs. Biodistribution results of each derivatives were showed higher tumor uptake after 24h.Conclusion: We introduced six types of [Cu-64]DOTA-aptamer conjugates and confirm their high serum stability, the binding affinity in tumor cell and good imaging with their potential PET radiotracer for lymphoma.Acknowledgements: This research was supported from National Reaserch foundation of Korea(NRF) grant funded by the Korean government(MEST)(2011-0030161 and 2011-0030162).References: [1] Zhiwen Tang, et al (2007) Analytical Chemistry, 79, 4900-4907.[2] Kwame Sefah. et al (2010) Nature protocols, vol 5, 1169-1185.


HN-Aptamer
HO₂C
CO₂H
N
NCS
+
H₂N
O-P-O
OH
n =1, 4, 10
Aptamer = sgc8c, TD05
64Cu2+
S
N H
n =1, 4, 10
Aptamer = sgc8c, TD05

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Zebrafish Toxicity Screening and in-silico Structure Analysis of Korea Chemical Bank Library

이주연* 이현규

한국화학연구원 한국화합물은행

Korea Chemical Bank (KCB) is the infrastructure division of the discovery of biologically active substance in drug discovery and biotechnology areas by open access with synergy through the cooperation between chemistry and biology. We have established a compound management system and cheminformatics database for bioactive chemical entities. KCB contains over 320,000 chemical libraries since 2000 and we have created a new set of diversity libraries which consist of 8,400 structural diverse in the last year. Among them, we had studied toxicity screening with zebrafish model for selected 1,000 compounds and we analyzed the result to find out the factor that causes toxicity from a structural perspective using cheminformatics and modeling tools.

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Synthesis of Ga-68 labeled chromene derivative

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The chromene ring is widely found in a number of natural products such as flavonoids. These natural products have demonstrated numerous biological activities such as antiviral, antiinflammatory, antiallergic, antimutagenic and anticarcinogenic activities. In this study, a Ga-68 labeled chromene derivative was synthesized for investigation as a potent imaging agent for breast cancer. The reference compound was synthesized starting from 2-hydroxy-5-nitroacetophenone via six steps, and confirmed through ^{1}H NMR spectroscopy and mass spectrometry. The radiolabeling reaction was monitored using a radio-TLC and the radiochemical and purified by HPLC.

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Chemiverse: Total service of Drug Discovery

강경태 김한조 서영주 정우성 장병하 윤정혁[1,*]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

Previously the medicinal chemists have depended on random screening or high-throughput screening(HTS) in drug discovery research, but currently the researchers use chemical filtering or simulation techniques using computing resources and cheminfomatics before actual experiment. The typical examples of these techniques are chemical filtering by molecular descriptors or prediction values using QSAR model and virtual screening. Chemical filtering and Virtual screening is an essential technique in current medicinal chemistry field to search new drug. It does not require the real chemicals and proteins, because of using computer simulation and then carries out actual experiment by the obtained result. And this technique demands less cost and time than the conventional high-throughput screening(HTS). For this reason, the virtual screening is widely used in drug discovery field. Furthermore, previously this technique is in the region of the experts, but currently the user is increasing due to release of simple and easy tools. In spite of many strong points, chemical filtering tools that is based on molecular descriptors, QSAR prediction tools or virtual screening tools are present, but the integrated solution or services for above-mentioned functions is not exist. Here we present the integrated service include chemical database to chemical purchase for actual experiment. The integrated service is a step by step progression. First, search chemical from database using specific condition, second, carry out virtual screening for finding druggable chemical structure. Finally, order the chemical and then do actual in vitro/in vivo test of chemical. This service can provide convenience and quickness in the medicinal chemistry field.

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PharosQSAR: Generalization of Descriptors

서영주 김한조 정우성 강경태 장병하 윤정혁[1,*]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

The QSAR(Quantitative Structure-Activity Relationship) technique is for analyzing quantitative relationship between the structure of chemicals and the efficacy or characteristic of them. The difference of QSAR with SAR, a routine technique of medicinal chemists, is that it expresses the quantitative relationship in mathematical expressions which can capture more complex, sometimes non-linear relations. Since the QSAR research began in early 1960s, it has been developed in mainly two directions; new molecular descriptors and novel statistical methods. In recent years, the exponential increase of computing resources and available data opens the era of big data and QSAR is one of the very first successful applications of big data technique in chemistry field. In spite of this importance, the molecular descriptors(called descriptor), are essential to the QSAR study, are not generalized yet. Many tools for calculating the descriptors compute the same values, but these values are expressed in different way for each tools such as the descriptor that means total “number of atoms” is expressed “nAtom” in PaDEL-Descriptor, “No_Total_atoms in Topomol or “nAT” in Dragon6. These differences in expression are restricted to the employment of QSAR models that is exponential increasing by available data and cause to waste of cost purchased by variety of tools. Here we present a generalized descriptor table include descriptor from the number of tools and generalized descriptor code such as “number of atoms” integrate to “N00000001”. The generalized descriptors table to calculate the values from the tool the researcher has is to eliminated barriers to employ the developed QSAR study which helps many researchers applying QSAR in a variety of fields other than medicinal chemistry.

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Drug repositioning based on the water network analysis for the discovery of IRAK4 inhibitors

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Drug repositioning is the application of known drugs and compounds to new therapeutic indications. However, to identify multiple targets for a drug is a complex and challenging task. We developed the new computational method to identify the novel drug targets based on the analysis of the water network similarity between the binding sites of proteins. We have applied the method to kinase target space, and effectively find a new inhibitor for IRAK4 among different kinases. The computational prediction is confirmed by *in vitro* biological assays. Herein we report our strategy to aid the rapid identification of the novel IRAK4 inhibitor.

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Synthesis and Application of Molybdenum Dioxide Formed from the Thermal Reactions of MoS_2 with LiF in Air

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단국대학교 자연과학대학 화학과

In the presence of LiF, MoS_2 reacts with oxygen gases in air to generate Li_2MoO_4 and MoO_2 depending on the amount of LiF. The thermal reactions of MoS_2 with LiF (MoS_2: LiF = 1: 2) in air give α-MoO_3 by 600 ^{0}C and new phase over 600 ^{0}C is observed until 900 ^{0}C and identified as MoO_2. No impurity peaks are noticeable. The products are characterized by X-ray powder diffraction (XRD) and scanning electron microscope (SEM). For the application of this synthetic method, coating of MoO_2 to the surface of CNT are investigated.

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Synthesis and Characterization of $Ag_2Mo_2O_7$ and Ag_2MoO_4 Prepared by Thermal Reaction of MoS_2 with Ag in Air

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In the presence of Ag particles, the thermal reactions of MoS_2 at 400~900 ^{0}C are monitored by X-ray powder diffraction (XRD). At 400 ^{0}C, most of MoS_2 converted to MoO_3 and silver particles became smaller, evidencing peaks broadening of silver particles. Amorphous phases were observed at 500 ^{0}C ~600 ^{0}C and new phase of $Ag_2Mo_2O_7$ was observed at 700 ^{0}C. All the diffraction peaks at 700 ^{0}C can be indexed as the cubic phase of $Ag_2Mo_2O_7$ (JCPDS Card No. 75-1505). No characteristic peaks belonging to other impurities were detected, indicating the synthesis of pure product. At 900 ^{0}C, new major peaks are appeared and can be indexed as the cubic phase of Ag_2MoO_4 (JCPDS Card No. 75-250). This reaction can be described as follows: $Ag_2Mo_2O_7 \rightarrow Ag_2MoO_4 + MoO_3$

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Synthesis of Chemical Vapor Deposition (CVD) grown Monolayer MoS2, CVD grown graphene and their hybrid

홍광택 김성진[1,*]

이화여자대학교 나노과학부 [1]이화여자대학교 화학과

For post silicon device technology, the layered chalcogenides (MX2, M = Mo,W X = S,Se, Te) materials are potential alternatives for Si. The MoS2 is one of the most relevant material in this series. It shows the direct band transition when it transfer from bulk nature to monolayer form. The optical band gap is about 1.8 eV and it shows some intrinsic physical and chemical properties. We synthesized monolayer MoS2 by Chemical Vapor Deposition and characterized their structural and electrical properties by various method. After characterizing monolayer MoS2 by various method, we will also characterized MoS2 and graphene hybrid structure. If it modifies their proper properties, it shows the synergetic electrical effects and applicable uses in opto-electric devices.

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Hollow silica micelle: superhydrophobic, efficient and recyclable carrier for ultra-high loading of GOD enzyme

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Hollow silica micelles (HSMs); polymer assisted superhydrophobic (CA = 163^o on glass surface) carrier with ultra-high loading efficiency of glucose oxidase (GOD) were synthesized by sonochemical method. HSMs possess hydrophilic core consist of silica-PAH network and hydrophobic shell where, long-chain hydrocarbon N-octadecyltrimethoxysilane (OTMS) was grafted covalently. Due to their mesoporous hollow structured, HSMs were served as excellent hosts for GOD immobilization. After loading of GOD in sodium acetate buffer, BET surface area was decreased to 43.7 m^2/g compare to the blank (154.78 m^2/g). Also, pore size was reduced from 11.2 to 3.3 nm and estimated loading capacity was 0.473 mg/mg of HSMs. High sensitivity (>98%) of the immobilized GOD was evaluated by the Fenton's standard assay observing the rate of iron oxidation and the catalytic oxidation of glucose to D-gluconic acid and hydrogen peroxide by GOD. More importantly, the HSMs showed very strong mechanical stability exhibiting low desorption rate (~6%) of GOD even after 12 hours stirring in buffer solution. Also, it exhibited great reusability for the glucose oxidation (up to 8 cycles). We believe the HSMs could be novel carriers for ultra-high loading of enzymes or drugs with excellent bioactivities, high sensitivity and low leaching rate leading to faster kinetic response.

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UV-block effect of 2,4-dihydroxy benzophenone with acrylate materials

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Recently, many eye disease associated with ultraviolet radiation were reported. In this study, the UV-block hydrophilic lens using 2,4-dihydroxy benzophenone were manufactured and the optical properties of copolymerized materials were measured. The basic hydrophilic lens material with addition of MMA(methyl methacrylate), BMA(butyl methacrylate) and HEA(2-Hydroxyethyl acrylate) respectively were polymerized and the hydrophilic ophthalmic lens was manufactured by cast mould method. The hydrophilic lenses were stored in a 0.9% NaCl normal saline for 24 hrs. In the measurement of MMA(methyl methacrylate) sample, the optical transmittance measurement showed the UV-B transmittance of 8.0%, UV-A transmittance of 26.0% and visible transmittance 92.0%. And also, in the case of BMA(butyl methacrylate) sample, the optical transmittance of UV-B, UV-A and visible transmittance was 7.0%, 25.0% and 92.0%, respectively. Also, in the case of HEA(2-hydroxyethyl acrylate) sample, the optical transmittance of UV-B, UV-A and visible transmittance was 24.0%, 44.0% and 92.0%, respectively.

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Facet-dependent antibacterial activities of Ag3PO4 and Cu2O microcrystals

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Cubic and rhombic dodecahedral Ag3PO4 microcrystals were prepared for examination of the facet-dependent antibacterial activities against E. coli {100} facets in the cube exhibited much higher antibacterial activity than {110} facets in the rhombic dodecahedral Ag3PO4 microcrystals against E. coli. Various morphologies from octahedral through truncated octahedral and truncated rhombic dodecahedral and finally rhombic dodecahedral Cu2O microcrystals were also obtained by using a solvothermal method. The antibacterial activities of rhombic dodecahedral Cu2O crystals against E. coli were superior to those obtained from octahedral Cu2O crystals. The antibacterial activity against E. coli strongly depended on the Ag3PO4 and Cu2O crystal facets.

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Optical transmittance and oxygen permeability of hydrogel ophthalmic lens containing UV absorbent

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Recently, the functional hydrogel ophthalmic lens with UV-Blocking and high oxygen permeability is getting very popular. In this study, the functional hydrogel ophthalmic lens containing aniline group (3-iodo, 3-chloro and 4-fluoroaniline) were manufactured. Also, the physical properties such as refractive index, water content, spectral transmittance and oxygen permeability of copolymerized ophthalmic lens were measured. The results of the sample with addition 3-iodo, 3-chloro and 4-fluoroaniline showed that the DK value was 15.33~18.94, 16.14~19.28 and 16.52~21.72×10-11(cm2/sec)(mlO2/ml×mmHg) respectively. The optical transmittance of opthalmic lens containg 3-iodoaniline was the 2.0 ~ 15.2% of UV-B, 40.6 ~ 67.8% of UV-A and 89.4 ~ 90.8% of visible light respectively. Also, in the case of 3-chloroaniline, the UV-B(5.0 ~ 22.2%), UV-A(57.6 ~ 73.8%) and visible transmittance(89.8 ~ 90.6%) was measured respectively. Based on the results, aniline group are considered to satisfy the basic requirements of hydrogel ophthalmic lenses and can be used effectively as additives for functional ophthalmic lenses.

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Synthesis of topological insulator $Ag_2Se_{1-x}Te_x$ nanostructure

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A topological insulator is a material that is an insulator in its interior but a conductor on its surface. Electrons flow only along the surface and the moving electrons are not hindered by other obstacles. Because of this interesting property, the topological insulator has a possibility to be applied for spintronics devices and quantum computing. The properties of this material are studied on with its peak interest. Metal chalcogenides, such as bismuth selenide (Bi_2Se_3), bismuth telluride (Bi_2Te_3), antimony telluride (Sb_2Te_3), silver telluride (Ag_2Te) and silver selenide (Ag_2Se), are known as a topological insulator. Since both Ag_2Te and Ag_2Se are topological insulator, it is worth exploring the silver selenide telluride ($Ag_2Se_{1-x}Te_x$) in order to assess whether phase competition and subsequent complexity can improve topological property. Here we report $Ag_2Se_{1-x}Te_x$ nanostructure as a new topological insulator. The synthesized $Ag_2Se_{1-x}Te_x$ nanostructure were characterized by using X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy dispersive X-ray spectroscope (EDS) attached to the TEM and the electromagnetic properties were also studied.

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Injectable hydrogels derived from phosphorylated alginic acid calcium complexes

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Phosphorylation of sodium alginate salt (NaAlg) was carried out using $H_3PO_4/P_2O_5/Et_3PO_4$ followed by acid-base reaction with $Ca(OAc)_2$ to give phosphorylated alginic acid calcium complexes (CaPAlg), as a water dispersible alginic acid derivative. The modified alginate derivatives including phosphorylated alginic acid (PAlg) and CaPAlg were characterized by nuclear magnetic resonance spectroscopy for ^{1}H, and ^{31}P nuclei, high resolution inductively coupled plasma optical emission spectroscopy, fourier transform infrared spectroscopy, and thermogravimetric analysis. CaPAlg hydrogels were prepared simply by mixing CaPAlg solution (2 w/v%) with NaAlg solution (2 w/v%) in various ratios (2:8, 4:6, 6:4, 8:2) of volume. No additional calcium salts such as $CaSO_4$ or $CaCl_2$ were added externally. The gelation was completed within about 3-40 minutes indicating a high potential of hydrogel delivery by injection in vivo. Their mechanical properties were tested to be $\leq$6.7 kPa for compressive strength at break and about 8.4 kPa/mm for elastic modulus. SEM analysis of the CaPAlg hydrogels showed highly porous morphology with interconnected pores of width in the range of 100-800 μm. Cell culture results showed that the injectable hydrogels exhibited comparable properties to the pure alginate hydrogel in terms of cytotoxicity and 3D encapsulation of cells for short time period. The developed injectable hydrogels showed suitable physicochemical and mechanical properties for injection in vivo, and could therefore be beneficial for the field of soft tissue engineering.

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Production of CNT-taxol-embedded PCL microspheres using an ammonium-based room temperature ionic liquid: As a sustained drug delivery system

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We describe a one-pot method for the mass production of polymeric microspheres containing water-soluble carbon-nanotube (w-CNT)-taxol complexes using an ammonium-based room temperature ionic liquid. Polycaprolactone (PCL), trioctylmethylammonium chloride (TOMAC; liquid state from -20 to 240℃) and taxol were used, respectively, as a model polymer, room temperature ionic liquid, and drug. Large quantities of white colored PCL powder without w-CNT-taxol complexes and gray colored PCL powders containing w-CNT-taxol (1:1 or 1:2 wt/wt) complexes were produced by phase separation between the hydrophilic TOMAC and the hydrophobic PCL. Both microsphere types had a uniform, spherical structure of average diameter 3?5 lm. The amount of taxol embedded in PCL microspheres was determined by HPLC and 1H NMR to be 8?12 lg per 1.0 mg of PCL (loading capacity (LC): 0.8?1.2%; entrapment efficiency (EE): 16?24%). An in vitro HPLC release assay showed sustain release of taxol without an initial burst over 60 days at an average rate of 0.003?0.0073 mg per day. The viability patterns of human breast cancer cells (MCF-7) for PCTx-1 and -2 showed dose-dependent inhibitory effects. In the presence of PCTx-1 and -2, the MCF-7 cells showed high viability in the concentration level of, respectably,

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Ionic liquid-doped and p-NIPAAm-based copolymer (p-NIBIm): extraordinary drug-entrapping and -releasing behaviors at 38~42 °C

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Ionic liquid (IL)-doping of the temperature responsive p-NIPAAm was achieved by radical copolymerization of N-isopropyl acryl amide (NIPAAm; 90 mol%) and 1-butyl-3-vinylimidazolium bromide ([BVIm]Br; 10 mol%) to give a new temperature responsive copolymer (p-NIBIm). The as-prepared p-NIBIm copolymer showed a highly increased zeta potential value and optimal LCST (lower critical solution temperatures) value, respectively, +9.8 mV at pH = 7 and 38.2 °C, compared to those (+0.3 mV at pH = 7 and 32.1 °C) of p-NIPAAm. The temperature-dependent size change of the p-NIBIm micelles was determined in the range from 25 to 45 °C by SEM under dry conditions and by a zeta sizer under wet conditions, showing a certain size contraction from 253 ± 12.1 to 90.5 ± 7.8 nm in diameter (about 95.4% of volume contraction). The thermo-sensitive behavior to entrap BSA protein at body temperature (37 °C) and to release the protein between 38~42 °C (near the LCST) were also tested by sizing of the complexes of p-NIBIm/BSA using a zeta sizer and also by a colorimetric assay (Bio-Rad DC Protein Assay), resulting in a maximum entrapment of 1.02 mg BSA for 1.0 mg of the polymer at body temperature (37 °C) and in a maximum release of 0.73 mg BSA for 1.0 mg of the polymer (about 73% release of the entrapped amount) in the temperature range of 38~42 °C. Toxicity of the p-NIBIm micelles (in the range of $^{-1}$) without drug for human embryonic kidney (HEK 293) cells was minimal in vitro. These results revealed that the IL-doped and temperature responsive co-polymeric systems have a very high applicability as a novel delivery system for charged (or polar) molecules as a natural (or synthetic) drug and DNA.

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Surface-Selective Deposition of a Reusable Gold Catalyst on a Thin Film of Metal Hydroxide Nanocrystals

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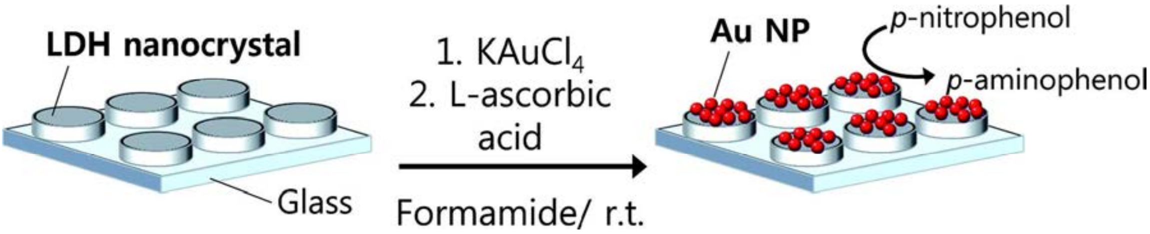
가톨릭대학교 화학 [1]가톨릭대학교 화학과

We have developed a simple and facile method to fabricate gold nanoparticles (Au NPs) deposited on thin films of layered double hydroxide (LDH) nanocrystals. The oriented thin film of LDH nanocrystals was employed for the preferential deposition of Au NPs by in situ growth of Au NPs on the monolayer thin film of LDH nanocrystals, which effectively provided a large and uniform active hydroxide surface for deposition of a dense monolayer of Au NPs. The reactive hydroxide groups and the positive potential of the LDH surfaces play an important role in the uniform growth of the Au NPs and in their stabilization against agglomeration. This LDH-supported Au NP catalyst exhibits superior catalytic efficiency and reusability without significant loss in conversion efficiency for the reduction of p-nitrophenol with $NaBH_4$, maintaining more than 96% catalytic conversion efficiency.



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High-Performance, Low-Voltage Pentacene-based OFETs using Organic-Inorganic Hybrid Gate Dielectrics

오정도 김대규 최종호*

고려대학교 화학과

High-performance low-voltage pentacene-based organic field-effect transistors (OFETs) were prepared using using a neutral cluster beam deposition (NCBD) method. We report the fabrication and systematic comparative analysis of the low-voltage pentacene-based OFETs using bare HfO_x and cross-linked HfO_x/1,6-bis(trimethoxysily)hexane blend (CLHB) gate dielectrics. Simplified solution-processed sol-gel chemistry was employed to deposit the dielectrics. The optimized CLHB films ($HfCl_4$: BTMH = 1 : 0.5) exhibit excellent dielectric properties (leakage current ~2 x 10^{-7} at 2 MV/cm and high capacitance ~137 nF/cm^2) and smooth surfaces. The OFETs fabricated with pentacene using CLHB gate dielectric operated at low operating voltage (<-4V) and exhibited high mobilities of 1.6 cm^2/Vs and current on/off ratio of 2 x 10^5.

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Organic Light-Emitting Field-Effect Transistors based upon Pentacene and DCM Doped Alq_3 Prepared by The Neutral Cluster Beam Deposition Method

김대규 오정도 최종호*

고려대학교 화학과

Since the recent fabrication of unipolar light-emitting transistors based on tetracene thin films, the combination of both electrical switching and luminescence functionalities in a single organic device has attracted much attention and become a new class of optoelectronic devices known as organic light-emitting field-effect transistors (OLEFETs). We present our application of the neutral cluster beam deposition method to fabricate bilayer heterojunction-based OLEFETs by superimposing two layers of pentacene and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) doped into tris(8-hydroxyquinoline) aluminum (Alq_3) as p-type and emissive layers, respectively. The OLEFETs with asymmetric electrodes (source: Au and drain: Li:Al or Li:F/Al) demonstrate efficient charge injection of holes and electrons, good field-effect characteristics and electroluminescence (EL) under ambient conditions. We observed the EL enhancement with DCM. The operating EL mechanisms are analyzed with the aid of light-emission images obtained using CCD camera.

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Sb-SnO_2@SiO_2 복합 재료 합성 및 전기적/광학적 특성 규명

고하니 이석우*

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본 연구에서는 SiO_2 기반 ATO(antimony doped tin oxide) 코어-쉘 복합 재료를 합성하였으며, 전도성을 갖는 회색 안료로써의 응용성에 대하여 살펴보았다. 코어 물질인 구형 실리카 입자는 염기성 조건에서 TEOS(tetraethylorthosilicate) 전구체의 가수분해로 SiO_2 핵을 생성한 후, TEOS 의 반복적인 가수 분해/축합 과정을 통하여 평균 1 ㎛ 크기의 입자로 합성되었다. Ethylene glycol 과 citrate 이온 및 코어 입자가 포함된 혼합물에 $SbCl_3$/$SnCl_4$ 혼합 용액을 첨가한 후, 환류시켜 코어-쉘 복합 재료 전구체를 형성하였으며, 800℃에서 소성하여 SiO_2 코어에 ATO 쉘을 형성하였다. XRF 를 이용하여 화학 조성을 측정하였으며, FE-SEM 과 PXRD 분석으로 각각 형태, 크기 및 구조를 관찰하였고, TGA/DSC 분석으로 열에 의한 화학 반응을 규명하였다. 복합 재료의 전기적 성질과 반사율에 미치는 ATO 입자의 형태, ATO 입자의 화학 조성 및 코어-쉘 구조의 영향을 규명하였다.

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Poly(MAA-co-EGDMA) 중합체를 주형으로 이용한 구형 Hollow TiO_2 합성 및 광반사 특성 규명

유민지 고하니 이석우*

공주대학교 화학과

본 연구에서는 poly(MAA-co-EGDMA) 중합체를 주형으로 사용하여 구형 poly(MAA-co-EGDMA)@TiO_2 복합 재료를 합성하였으며, 소성에 의해 주형을 제거하여 속이 빈 산화 타이타늄을 합성하였다. 형성된 복합 재료의 열에 의한 화학 반응은 TGA/DSC 를 이용하여 구명하였으며, 복합체, 속이 빈 산화 타이타늄의 형태는 FE-SEM 에 의해 규명하였으며, 복합 재료의 소성 과정에서 일어나는 무정형-anatase-rutile 의 구조 변화는 XRD 를 이용하여 규명하였다. 산화 타이타늄의 껍질의 두께 및 입자 크기에 따른 광반사 특성은 DRS-UV/Vis/NIR 를 이용하여 분석하여 구조-특성 상관관계를 규명하였다.

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Effect of Co incorporation of Sn-based intermetallic material on electrochemical reaction for Li-ion battery

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Ordered mesoporous CoSn intermetallic (Co_xSn_y) materials with various Co/Sn atomic ratios are are successfully synthesized for the first time through nano-replication technique as stable and high high-power anode materials for Li-ion battery. The electrochemical results show that reversible capacity, Coulombic efficiency and cycle stability of mesoporous Co_xSn_y materials are dependent on their structure and composition. Especially, the ordered mesoporous $Co_{0.3}Sn_{0.7}$ material shows exhibits 83% capacity retention after 50th cycle, which means that mesoporosity as well as Co atoms incorporation effectively accommodate the volume strain during lithiation?delithiation processes. Rate performance of mesoporous $Co_{0.3}Sn_{0.7}$ anode is also significantly improved, which was is deeply probably related to the kinetic behaviors such as low polarization resistance and large diffusion coefficient. Electron microscopy and small angle X-ray scattering investigations have proved our understating of the sustainable pore system and the effectivity of mesostructure.

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Forward Osmosis Desalination by Lower Critical Solution Temperature Phase Transition Materials

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Water crisis is the serious global challenge. To obtain fresh water from seawater, recently a forward osmosis (FO) process has been developed as an attractive alternative to distillation and reverse osmosis. FO uses a 'draw solution' to osmotically pump water molecules out from feed solutions through a semipermeable membrane. Solutes in this draw solution are separated to produce usable water. However, the FO method for practical desalination remains problematic given its drawing system, low drawing power, energy costs, complicated separation, and difficult recovery of the draw solutes. In this study, we present an innovative method based on draw solutes with lower critical solution temperature (LCST) phase separation from water to induce the abrupt change of effective concentrations and osmotic pressure.Thermosensitive materials show temperature-driven hydrophilic to hydrophobic transition in aqueous condition. Therefore, corresponding abrupt changes of effective concentration in the solution containing those materials could induce conversion of osmotic flows. Derived from the structure of LCST polymer, we synthesized N-acylated tris(2-aminoethyl)amine (nBu-TAEA). It has low MW (356g/mol) and shows LCST-type phase separation above ~27 Celsius. nBu-TAEA aqueous solution showed clear conversion of osmotic pressure upon low and high temperature. The nBu-TAEA solution could draw fresh water from a seawater (0.6 M NaCl) at the temperature below the phase separation point, and release the drawn fresh water into low-salt water at higher temperatures. In conclusion, a new desalination system was produced via circulation of the draw solutions between low and high temperature sets allowing direct seawaterdrawing, transfer and release of water, and separation and recovery of draw solutes in a simultaneous and continuous manner with high energy efficiency.

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Preparation of Alumina-graphene composites (AGC's) from partially nitrided alumina powder

정주희 정우식*

영남대학교 화학공학부

Alumina(Al_2O_3)-graphene composites (AGC's) was were prepared by the reaction between partially nitrided alumina (PNA) powder and carbon monoxide (CO). The former powder was obtained by the carbothermal reduction and nitridation of a mixture of Al_2O_3 and carbon powders under a flow of N_2. The AGC powders were characterized by powder X-ray diffraction, micro-Raman and X-ray photoelectron spectroscopy, and scanning electron microscopy high-resolution transmission electron microscopy. The graphene sheets, which wrapped alumina particles, were formed by the reduction of CO and their characteristics depended on the species of Al_2O_3, calcination temperature, and duration. The AGC powders are expected to be used as a thermal conductive filler.

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Luminescence spectra of Ce^{3+}-doped greenish blue phosphors using the reaction system of CeF_3-$CaCO_3$-Al_2O_3-Li_2CO_3

최연희 이민호 정우식*

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Ce^{3+}-doped greenish blue phosphors were prepared by calcining a mixture of CeF_3, $CaCO_3$, Li_2CO_3 and Al_2O_3 powders under a flow of inert gas. Li^+ ions were used to compensate for the charge imbalance caused by the substitution of Ce^{3+} ions for Ca^{2+} ions. The phosphors were characterized by X-ray diffraction, infrared and luminescence spectroscopy, and scanning electron microscopy. The emission peaks were observed at 475 (greenish blue) and 550 nm (yellow). The emission intensity depended on calcination temperature and amount of CeF_3.

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Synthesis of $LaAl_{12}O_{18}N$ and Eu(II)- and Ce(III)-doped $LaAl_{12}O_{18}N$ by the carbothermal reduction and nitridation

이민호 최연희 정우식*

영남대학교 화학공학부

$LaAl_{12}O_{18}N$ powder was prepared by the carbothermal reduction and nitridation of a mixture of La_2O_3, Al_2O_3 and carbon powders under a flow of N_2 and characterized by powder X-ray diffraction, infrared and X-ray photoelectron spectroscopy, and field-emission scanning electron microscopy. The luminescence spectra of Eu(II)- and Ce(III)-doped $LaAl_{12}O_{18}N$ showed that the peaks assigned to 5d → 4f transition of Eu(II) and Ce(III) appeared at 445 (blue) and 350 nm (UV), respectively. The intensity of the peaks depended on concentration of doped ions and the dependence was discussed.

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Enhance the low-temperature water-gas shift activity of $Cu_xCo_{3-x}O_4$/ mesoporous CeO_2 catalyst

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성균관대학교 화학과 [1]성균관대학교 자연과학대/화학과 [2]성균관대학교 화학과

In this work, we report on the low water-gas shift (WGS, CO + H2O →H2 + CO2) activity of CuxCo3-xO4 supported on highly ordered mesoporous ceria oxide with high surface area and a large pore volume. The preparation method was via a nano-replication method using a KIT-6 template to get highly ordered mesoporous CeO2 support, then loading CuxCo3-xO4 on the meso-CeO2 by an incipient wetness impregnation. The structure of the catalysts and the WGS reaction intermediate were characterized using powder X-ray diffraction (XRD), nitrogen sorption & adsorption isotherms, scanning electron microscopy (SEM), temperature programmed surface experiments. XRD showed the existence of CuxCo3-xO4 phase on the surface of meso-CeO2. A 20 wt% CuxCo3-xO4/meso-CeO2 catalyst displayed the highest catalytic activity among all the prepared catalysts. Beside high activity, the 20 wt% CuxCo3-xO4/meso-CeO2 catalyst also exhibited the stability under WGS conditions compared to 20 wt% CuxCo3-xO4. The loading of CuxCo3-xO4 on the ceria oxide favored the formation of O vacancies that facilitated the dissociation of water, preventing the dissociation of CO and the formation of methane. Because of the special chemical properties the more methane was product with the more CuxCo3-xO4 loading.

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Fabrication of TiO_2 Incorporated Frameworks of Ordered Mesoporous Carbon and Their Application for Lithium-Sulfur Battery Cathode

오세민 김지만* 최윤석 **JINXING**

성균관대학교 화학과

Porous carbon material with sulfur embedded has been designed to mitigate the shuttle effect in lithium-sulfur battery so far. However, porous carbon is not fully capable to capture polysulfide intermediate due to weak physisorption. Recently, other candidates such as metal, metal oxides, metal sulfides are emerging. Herein, X wt% TiO_2-Ordered Mesoporous Carbon (OMC) materials were synthesized by nano-replication via mesoporous silica KIT-6 as a hard template with $TiCl_4$ and sucrose aqueous solution as TiO_2 and carbon precursors, respectively. The prepared materials were characterized by small angle X-ray scattering (SAXS), powder X-ray diffraction, N_2 adsorption-desorption, scanning electron microscopy (SEM), transmission electron microscopy (TEM), raman spectroscopy and thermo-gravimetric analysis (TGA). And Electrochemical performance was investigated. It showed superior cycling performance to pure carbon material due to strong chemisorption with polysulfide from TiO_2 which is located in the carbon frame.

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High-Performance Flexible Transparent Conductive Film Based on Graphene/AgNW/Graphene Sandwich Structure

이동화 이형진 이윤구[*]

대구경북과학기술원(DGIST) 에너지시스템공학전공

Transparent conductive films (TCFs) based on vacuum-deposited indium tin oxide (ITO) have been widely used in various electronic application such as organic light-emitting diodes (OLEDs), touch screen panels (TSPs) and organic solar cells (OSCs). However, it has several drawbacks such as brittleness, high refractive index, and high processing temperature. Accordingly, the application of ITO is not suitable in flexible devices. Recently, chemical vapor deposition (CVD)-grown graphene showed the excellent optical and mechanical performance. However, it is still required to decrease the sheet resistance without a significant loss of mechanical flexibility and optical transparency for achieving the large area. In this work, we fabricated a sandwich-structure TCF in which the AgNW layer embedded by CVD graphene layers. The graphene/AgNW/graphene TCF exhibited high optical transmittance (88.6% at 550 nm) and low sheet resistance (19.9 ± 1.2 ohm/sq). Moreover, the reliability and long-term stability of the graphene/AgNW/graphene TCF were greatly enhanced because of the superior gas-barrier property of the graphene as the encapsulation layer.

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High Performance Silver Nanowire-Based Phosphorescent Organic Light-Emitting Diodes

이형진 이동화 이윤구*

대구경북과학기술원(DGIST) 에너지시스템공학전공

Silver nanowires (AgNWs) transparent conducting electrode (TCE) has been considered as one of the most promising candidates to replace conventional Indium tin oxide (ITO) TCE for flexible optoelectronic devices such as organic light-emitting diodes (OLEDs), touch screen panels (TSPs), and solar cells thanks to its excellent electrical, optical, and mechanical properties. However, the inherent surface roughness and low work function value of AgNWs TCE are considered as drawbacks against fabrication of reliable and high performance OLEDs. Since AgNWs TCE is based on a random network of AgNWs with 20~100 nm in diameter, the overlapping AgNWs might lead to protrusions or spikes causing electrical shorts in OLEDs. In addition, compared to ITO, AgNWs TCE possesses low work function value, which is not closely matched with conventional amine-type hole injection layer (HIL) materials, leading to high hole injection barriers.Here, we report a combination system of AgNWs TCE and n-type HIL for extremely flexible and high-performance phosphorescent OLEDs (PHOLEDs). We demonstrate a new approach to obtain a smooth surface morphology and decrease hole injection barrier by employing the thick n-type HIL between AgNWs TCE and hole transporting layer (HTL). The fabricated PHOLEDs without light outcoupling structures exhibited excellent device characteristics such as extremely low turn-on voltage (3.6 V) and high current and power efficiencies (44.5 cdA^{-1} and 35.8 lmW^{-1}). The flexible PHOLED with AgNWs TCE was successfully fabricated onto a plastic substrate. It showed remarkable mechanical flexibility as well as device performance.

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Removal of Aromatic Sulfur Compounds using the Oxidative Desulfurization Process Catalyzed by WO_3/KIT-6 catalysts

홍경희 LIZHENGHUA[1] LICHENGBIN[2] 김지만[2,*]

성균관대학교 자연과학대/화학과 [1]성균관대학교 화학과 [2]성균관대학교 화학과

Oxidative desulfurization with various S-containing compounds (benzothiophene (BT), dibenzothiophene (DBT), and 4,6-dimethyldibenzothiophene (4,6-DMDBT)) has been carried out using mesoporous WO3/KIT-6 as catalyst. In this work, mesoporous KIT-6 supported WO_3 catalysts (with various WO_3 loadings of 5, 10, 15and 20wt%) were synthesized by incipient impregnation method using $(NH_4)_6H_2W_{12}O_{40}\cdot xH_2O$ as a tungsten precursor. The synthesized samples were calcined at 400°C and characterized using various physicochemical characterization techniques, such as X-ray diffraction (XRD), N_2-adsorption, Scanning electron microscope (SEM), Raman spectroscopy etc. Oxidative desulfurization of a model oil with H_2O_2 as the oxidant was carried out at 50°C under atmospheric pressure in order to analyze the catalytic activity. And the results show that the WO_3/KIT-6 catalyst with a WO_3 content up to 10wt% exhibit the best catalytic activity which due to the well dispersed on the support of mesoporous KIT-6 support, and from 15wt%, crystalline WO_3 was generated. The effects of reaction temperature, catalyst amount, and H_2O_2/S ratio on the desulfurization of DBT over 10wt% WO_3/KIT-6 were studied in detail. And when the temperature increased to 70°C, treatment of BT, DBT, 4,6-DMDBT with 10wt% WO_3/KIT-6 showed 100% removal of sulfur compounds in 2h. In addition, the catalyst could be recycled several times with only a slight reduction in catalytic activity after regenerated by calcination.

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Effect of iron precursor on the chemical properties and catalytic activity of Fe,N doped ordered mesoporous carbon

<u>JINXING</u> 이창현 황윤경 원종구 LICHENGBIN 김지만*

성균관대학교 화학과

Polymer electrolyte membrane fuel cells (PEMFC) are appealing for transportation, stationary and portable applications due to their high conversion efficiency (up to 60%) and their zero pollutant and greenhouse gas emissions.[1-3] Electrocatalytic oxygen reduction, the reaction at fuel cell cathodes, has been the focus of attention because of cathode catalyst layer used of expensive and less earth-abundant noble metals such as platinum and the oxygen reduction reaction (ORR) which typically occurs with overpotentials more higher than hydrogen oxidation reaction (HOR) on the anode side of fuel cells.[4] Since Jasinski's[5] discovery that cobalt phthalovyanie exhibits catalytic activity for the ORR, research on metal-N4 macrocycles as a class of non-precious cathode catalysts has received considerable attention. In recent years, iron (cobalt)-nitrogen doped carbon (Fe(Co)-N-Cabon) nanomaterials have been proposed as promising non-precious metal catalysts for ORR because of their superior electrocatalytic activity, low cost, long durability and high tolerance to methanol.[6]As continuation of our previous studies, herein, we report the facile synthesis of Fe-N-OMC catalysts. Catalysts were prepared by nanocasting method 1,10-phenanthroline as the nitrogen-rich ligand to form the Fe-1,10-phenanthroline (ferroin) complex precursor, sulfuric acid as the catalysts and rod-type SBA-15 as template, through a solid-state reaction, which was then pyrolyzed to from a carbon supported ORR catalyst. And the effect of iron precursor on Fe, N doped ordered mesoporous carbon for ORR.REFERENCES (1) Crabtree, G. W.; Dresselhaus, M. S. MRS Bulletin 2008, 33, 421.(2) Nørskov, J. K.; Rossmeisl, J.; Logadottir, A.; Lindqvist, L.; Kitchin, J. R.; Bligaard, T.; J?nsson, H. The Journal of Physical Chemistry B 2004, 108, 17886.(3) Wu, G.; More, K. L.; Johnston, C. M.; Zelenay, P. Science 2011, 332, 443.(4) Silva, R.; Voiry, D.; Chhowalla, M.; Asefa, T. Journal of the American Chemical Society 2013, 135, 7823.(5) Dorjgotov, A.; Ok, J.; Jeon, Y.; Yoon, S.-H.; Shul, Y. G. Journal of Solid State Electrochemistry 2013, 17, 2567.(6) Cheon, J. Y.; Kim, T.; Choi, Y.;

Jeong, H. Y.; Kim, M. G.; Sa, Y. J.; Kim, J.; Lee, Z.; Yang, T. H.; Kwon, K.; Terasaki, O.; Park, G. G.; Adzic, R. R.; Joo, S. H. Scientific reports 2013, 3, 2715.

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Chemical Bath Deposition of Ag_3PO_4 Thin Films with Fine-Control of Crystal Facet

Gunjakar Jayavant Laxman 이장미[1] 황성주*

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Facet-controlled Ag_3PO_4 thin films highly efficient for visible light-induced degradation of toxic organic compounds are synthesized via a facile, economic, and reproducible chemical bath deposition (CBD) method. The control of preparative parameters like bath temperature, precursor type and concentration, complexation agent, substrate, and solution pH is fairly effective in tailoring the crystal shape of deposited Ag_3PO_4 nanocrystals from cubic to rhombic dodecahedron. The shape-controlled Ag_3PO_4 thin films show improved visible light photocatalytic activity for the degradation of organic molecules. The present finding clearly demonstrates that the present CBD method provides useful method to explore efficient photocatalyst thin films with controlled crystal facets.

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Control of the Photocatalytic Activity of TiO_2-based Nanocomposite via the Tuning of Band Position

JINXIAOYAN 황성주*

이화여자대학교 화학·나노과학과

The electronic coupling and photocatalytic activity of Ag_2CO_3-TiO_2 nanocomposite can be optimized by the fine-tuning of the band position of titanium oxide via N-doping. The Ag_2CO_3-TiO_2 nanocomposite suffers from the mismatch of the band positions of the component semiconductors, which frustrates an efficient electronic coupling between them. To circumvent the mismatch of electronic structures, we try to tune the valence band positon of TiO_2 through the doping of nitrogen. The resulting higher VB energy of N-doped TiO_2 is supposed to allow an efficient hole transfer from Ag_2CO_3 to TiO_2, resulting in the spatial separation of photogenerated electrons and holes. As a result, the N-doped TiO_2-Ag_2CO_3 nanocomposite shows higher photocatalytic activity than does the undoped one. The present study clearly demonstrates the importance of the fine-tuning of band position in determining the photocatalytic activity of composite photocatalysts.

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New Polyindenopyrazine Derivatives Electroluminescent Property for OLEDs

김승호 이재현 박종욱*

가톨릭대학교 화학과

New indenopyrazine derivative of 6,6,12,12-tetrahexyl-2,8-di-thiophen-2-yl-6,12-dihydro-diindeno [1,2-b;1',2'-e]pyrazine (m-thio-HPY) and new indenopyrazine polymer of poly (6,6,12,12-tetrahexyl-2,8-di-thiophen-2-yl-6,12-dihydro-diindeno [1,2-b;1',2'-e]pyrazine) (poly(m-thio-HPY)) were synthesized based on suzuki coupling reaction and Yamamoto polymerization. Optical and electronic properties were examined by UV-Vis. absorption spectrum, PL spectrum, and cyclic voltammetry. PL maximum values of synthesized compounds are 524 and 590 nm (m-thio-HPY) and 529 and 563 nm (Poly(m-thio-HPY)) in film state. Poly(m-thio-HPY) as an emitting material was tested in organic light emitting diodes (OLEDs). The device showed 0.38cd/A of luminance efficiency and CIE value of (0.39, 0.59).

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Fine-tuning of liposome composition for high tumor uptake

이웅희 안광일[1] 유정수*

경북대학교 의과대학 분자의학교실 [1]한국원자력의학원 방사성의약품 개발실

In our previous work, we developed a facile method for preparation of a tri-modal tumor imaging agent using liposome platform. By development of a radiotracer that emits strong Cerenkov luminescence light, optical and nuclear images were obtained from the single imaging component. Tumors were detected by all optical, nuclear and magnetic resonance imaging modalities. The liposome-carried radiotracer showed longer retention in tumor but cleared quickly from reticuloendothelial organs. However, we need to optimize uptake of liposome-carried radiotracer into tumor at various conditions. Herein, we focused on optimization of liposome compositon, difference of tumor uptake based on liposome size (30 - 100 nm) and concentration, tumor size, effect of tumor positon, sex of mice and housing condition. Finally, we compared tumor uptake of liposome-carried radiotracer in several type of xenograft tumor models. A reduction in cholesterol showed decreasing tumor uptake, whereas an increase in lipids and polyethyleneglycol (PEG) showed enhanced tumor uptake. So, we could optimize the ratio of liposome composition. Existing size of liposome (100 nm) was more effective than smaller size of liposome and the effect of concentration was marginal. Tumor position, sex of mice and housing condition was not significant in tumor uptake, while smaller tumor size led to higher tumor uptake. Among several type of tumor models, tumor uptake of liposome was best in murine colon carcinoma (CT26) tumor model. Consequently, we could get vivid tumor imaging repeatedly with minimum background. We could optimize liposome-carried radiotracer into tumor uptake at these various conditions and select best condition.

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Magnesiothermic Synthesis of Porous Silicon 2D Plates with Promising Electrode Performance for Lithium Ion Batteries

<u>AdpakpangKanyaporn</u> 황성주*

이화여자대학교 화학·나노과학과

Porous 2D nanoplates of elemental silicon can be synthesized via the magnesiothermic reduction of silicate clay nanosheets. The precursor nanosheets are prepared by the exfoliation of laponite clay, which is followed by the restacking of the obtained anionic clay nanosheets with Mg^{2+} cations. The magnesiothermic reaction induces the transformation of exfoliated laponite nanosheets into elemental silicon 2D nanoplates. The porous stacking structure of the precursor laponite remains intact during the magnesiothermic process. The resulting porous nanoplates of silicon element show outstanding electrode performance with the huge discharge capacity and excellent rate characteristics. This result is mainly attributable to the minimization of volume change during the electrochemical cycling and the enhanced diffusion of lithium ions caused by the porous 2D plate-shaped morphology of silicon electrode. This work highlights the effectiveness of laponite clay as economic precursor for high performance silicon electrode with controlled morphology.

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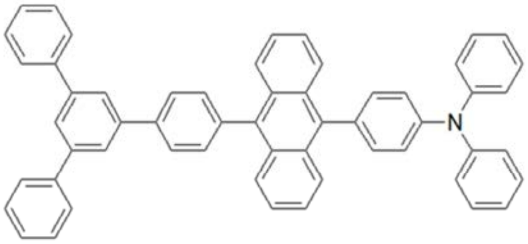
A New Blue Emitting Material for Solution Process OLEDs

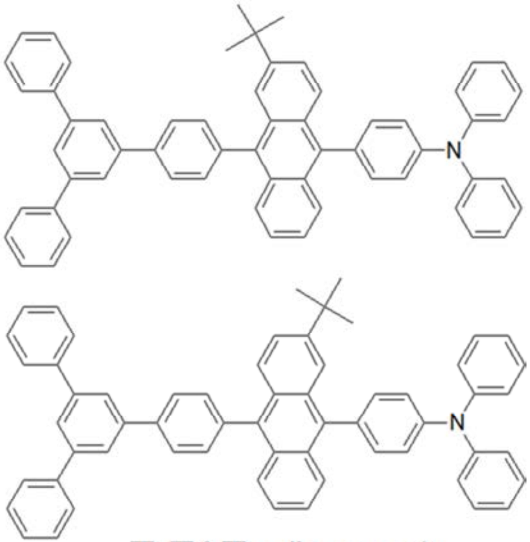
이재현 김승호 박종욱*

가톨릭대학교 화학과

Organic light-emitting diodes (OLEDs) are optoelectronic devices based on the photoluminescent properties of π-conjugated organic materials, and are useful for lighting applications and next-generation flat panel displays. Especially, OLED TV technology has been focused very much in recent. In this work, we synthesized a new anthracene derivative by using substituted t-butyl group. The OLED device of a new anthracene derivative containing t-butyl group is fabricated by solution process and we investigated its physical properties such as optical, electrochemical, and electroluminescent properties. The luminance efficiency of the synthesized compounds at 20mA/cm2 was measured 0.85cd/A for TATa, 1.49cd/A for T-TATa, respectively.



TATa



T-TATa (isomer)

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-999**
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Synthesis and Electroluminescent Properties of Highly Efficient Multi-Core Chromophores for OLEDs

이수지 이하윤 정효철 이재현 박종욱*

가톨릭대학교 화학과

Our research team have synthesized a novel blue emission materials based on a type of dual core concept(TP-AP-TP).Here in, We synthesized new blue emission materials based on this dual core system added to another chromophores.These materials were synthesized through boronylation and Suzuki coupling reactions.DSF-AP exhibited an PLmax value of 443nm and DCP-AP exhibited an PLmax value of 446nm.The dual core chromophore materials had narrow PL and EL spectra.The thermal properities of these materials were caracterized with TGA/DSC. The electro-optical properties of these materials were characterized with cyclic voltammetry (CV), and UV-visible and photoluminescence (PL) spectroscopy. Moreover, multilayered EL devices were fabricated using these materials.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A green process for oxidative desulfurization of dibenzothiophene by mesoporous WO_x catalyst with aqueous H_2O_2

LIZHENGHUA LICHENGBIN[1] 홍경희[2] 김지만[1,*]

성균관대학교 화학과 [1]성균관대학교 화학과 [2]성균관대학교 자연과학대/화학과

In this work, highly ordered mesoporous tungsten oxide was synthesized by using nano-replication method via mesoporous silica KIT-6 as a hard template with different calcination temperatures. The synthesized mesoporous tungsten oxides were well-characterized with various techniques. The characterization results showed that the calcination temperature of W-KIT-6 composites (before removal of the silica template) was essential to the crystalline structure evolution. Combination of XRD and SEM techniques showed that the highly ordered mesoporous structure was formed at least 400oC. The catalytic performance of prepared mesoporous tungsten oxides which were calcinated at different temperatures for the oxidative desulfurization of dibenzothiophene (DBT) with H2O2 as the oxidant in model oil were also investigated under atmospheric pressure at 50oC. The results showed that the catalytic activity was increased in the order: WOx(400oC) ≥ WOx(500oC) ≥ WOx(600oC) > WOx(300oC) > WOx(200oC), and the catalytic activity decreases in the order of DBT > BT for the various sulfur-containing compounds (benzothiophene (BT), dibenzothiophene (DBT)). The catalytic activity decreases in the order of DBT > BT for the various sulfur-containing compounds (benzothiophene (BT), dibenzothiophene (DBT)). Mesoporous WO3 was also investigated to be used for catalytic oxidation of sulfur-containing molecules in model oil under different reaction conditions (including different desulfurization systems, H2O2/S molar ratio and different solvent), and the activity was maintained during 5 times recycle-test without any regeneration process. The high catalytic activity and durability is mainly attributed to well-defined mesopores and high surface area of mesoporous WO3 catalyst.

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Large-scale one pot synthesis of metal oxide nanoparticles by decomposition of bulk metal carbonate

김병윤 이광렬*

고려대학교 화학과

In the most representative technological applications, oxides are used in the fabrication of microelectronic circuits, sensors, piezoelectric devices, fuel cells, coatings for the passivation of surfaces against corrosion, and catalysts. The properties of nanoparticles highly depend on their limited size and shape. Uniformly controlling surface/volume ratio and density of corner or edge surface sites have been the essence of manufacturing nanoparticles. To materialize the meaning of metal oxide nanoparticles as industrial materials, manufacturing methods which can produce in large quantity with low cost and also uniformly manipulate size and shape are demanded. The most well-known method on the large-scale synthesis of metal oxide nanoparticles is called co-precipitation method based on water soluble metal salt precursors. Despite the good flexibility of synthesis scale, the method gives a disadvantage in controlling morphology of nanoparticles. Thermal decomposition of a molecular metal precursor with surfactants and organic solvents gives well-controlled metal oxide nanoparticles. However, conventional thermal decomposition methods demand preparation steps of molecular metal precursors such as metal carbonyls, acetylacetonates, carboxylates and organometallic compounds that incur additional cost. Here, instead of preparing the molecular metal precursors, we carried out thermal decomposition of bulk metal carbonate in organic solvent to give metal oxide nanoparticles. The size and shape of nanoparticles could be controlled with surfactants while conducting large-scale one pot synthesis.

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발표분야: 재료화학
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Immobilization of Silver Phosphate on Exfoliated RuO_2 Nanosheet for Improving Visible Light Photocatalytic Activity

목은경 황성주*

이화여자대학교 화학·나노과학과

The hybridization of semiconductor with metal nanoparticle is one of the most effective ways to improve its photocatalytic activity due to the role of metal species as an electron reservoir. The high electric conductivity of RuO_2 nanosheet renders this material a promising candidate for efficient cocatalysts. In this study, we synthesize novel RuO_2-Ag_3PO_4nanocomposite via the immobilization of silver phosphate on layered RuO_2 nanosheets. The hybridization with the highly conductive RuO_2 nanosheet induces an efficient depression of photoluminescence signal, indicating the depression of electron-hole recombination. The RuO_2-Ag_3PO_4 nanocomposite shows higher photocatalytic activity than does unhybridized silver phosphate. The observed improvement of photocatalytic activity upon the hybridization with the RuO_2 nanosheet is attributable to the increase of the lifetime of electrons and holes, and also to the expansion of surface area. The present result clearly demonstrates the beneficial role of the RuO_2 nanosheet as a cocatalyst in exploring new efficient photocatalysts.

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발표코드: **MAT.P-1003**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ordered Mesoporous Mixed Mn-Ni System as High Performance Anode Material in Lithium Ion Battery

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성균관대학교 화학과 [1]성균관대학교 에너지과학과

Manganese oxide is one of the most promising anode materials for lithium ion battery since it is naturally abundant, low cost, eco-friendly, and high theoretical capacity (1000 mAh/g). However, manganese oxide shows low initial Coulombic efficiency originated by poor decomposition of Li_2O at the first charge. Nickel oxide introduction within transition metal oxide frameworks is the breakthrough to overcome the present problem due to the high catalytic activity of Li_2O decomposition of nickel oxide. Also, the initial coulombic efficiency of transition metal oxide would be enhanced. In this study, nickel oxide was introduced into the mesoporous manganese oxide frameworks by the nano-casting method using mesoporous silica template (KIT-6). Therefore, ordered mesoporous mixed Mn-Ni system was successfully prepared and analyzed. Synthesized material has a specific BET surface area of 140 m^2/g and pore diameters of 3 nm and 10-20 nm. As-prepared product was evaluated as the anode material for lithium ion battery. It exhibits high reversible capacity (1437 mAh/g), and higher initial Coulombic efficiency (71%) than mesoporous manganese oxide at the first cycle.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Excellent Photo-Degradation and Thermal Stability of Mesoporous TiO_2 by Heat Treatment Conditions

박수빈 **LIZHENGHUA**[1] 김지만*

성균관대학교 화학과 [1]성균관대학교 화학과

In environmental pollutions, pollutants cause the contamination of water and air. TiO_2 is one of the best semiconductors for photocatalysis due to its differentiated advantages from the others: high band gap energy, high stability and catalytic activity, and non-toxicity. For high photocatalytic activity, photocatalysts should have high specific area and crystallinity. However, nanopores could be collapsed at high temperature which is the condition to form high crystallinity. Here, we reported that thermally stable disordered nanoporous TiO_2 was synthesized by in-situ hydrolysis of titanium glycolate at various heat treatment conditions. As the heat treatment temperature increases, BET surface area tends to decrease and grains of nanoporous TiO_2 grows. Upto 500 °C, nanoporous structure of synthesized material is thermally stable with relatively high BET surface area (50 $m^2?g^{-1}$) and high anatase crystallinity.Photocatalytic activity of synthesized products was evaluated with methylene blue solution under UV 254 nm lamp. Among the samples, heat treated at 500 °C sample exhibits the highest photocatalytic activity due to its relatively higher surface area and crystallinity.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Seed-mediated synthesis of copper nanowires and their application to transparent conducting electrode

김현홍 최성현[1] 황의탁 박종남[2,*]

울산과학기술대학교(UNIST) 화학공학과 [1]울산과학기술대학교(UNIST) 에너지 및 화학공학부 [2]울산과학기술대학교(UNIST) 친환경에너지공학부

최근 Indium tin oxide (ITO)를 대체하기위한 유연 투명 전극 소재가 많은 관심을 받고 있으며, 활발한 연구가 진행되고 있다. 그래핀, 탄소나노튜브, 전도성 폴리머, 금속 박막, 금속 메쉬, 금속 나노선 등 다양한 유연 투명 전극소재들이 연구되고 있으며, 이 가운데 금속 나노선을 이용한 유연소재는 다양한 물질과의 복합체를 형성할 수 있으며, 대량 생산 및 용액 공정에 있어 장점을 보이고 있다. 본 연구에서는 기존의 값비싼 은 나노선 대비 저렴한 구리 나노선을 새로운 방법으로 합성하여, 투명 전극으로의 응용 가능성을 살펴보았다. 기존의 구리 나노선은 수계 반응에서의 환원법이나, 촉매를 이용한 제조 방법이 모색되었으나, 본 연구에서는 유기계 용매에서 구리 나노 입자를 제조하고, 이를 seed 로 이용하여 용액 안에서 나노선을 성장시켰다. 합성된 구리 나노선의 구조 분석 (XRD, SEM and TEM)을 통해 순수하고 높은 결정성의 구리 나노선임을 확인하였으며, 또한 TEM 과 UV spectra 분석을 통해 성장 mechanism 을 제안하였다. 합성된 구리 나노선을 이용하여 투명 전극을 만든 결과, 투과도 87%, 면저항 146 ohm/sq 의 박막을 제조할 수 있었다.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of First Transition Metal Oxides with Ordered Nanoporous Structure and their Application for Lithium Sulfur Battery Cathode

최윤석 오세민 김지만*

성균관대학교 화학과

Lithium-sulfur batteries are up-and-coming electrochemical devices due to its advantages such as high specific capacity and energy density compared to conventional LIBs. Despite its superiority, practical use of Li-S battery is impeded because of its obstacles; insulating characteristic of sulfur and dissolution of polysulfide Intermediates during charge/discharge process. To overcome these problems, majority of studies in this field have focused on porous carbon materials not only to impart sulfur conductivity but also to capture polysulfide by physisorption, capillary force. In this work, we present new possibility of porous metal oxides (MO_x) for Li-S battery cathode as host material to embed sulfur. We expect that the ordered mesoporous MO_x cathode can effectively trap polysulfide by chemisorption and retard the dissolution of it. Consequently, it results in better cycling performance of battery. Ordered mesoporous MO_x in the first row transition metal (TiO_2,MnO,NiO) were synthesized by a nano-replication method via ordered mesoporous silica template (KIT-6). The materials were characterized by X-ray diffraction (XRD), N_2 adsorption/desorption, scanning electron microscopy (SEM). And electrochemical investigation was performed.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of carbonization temperature on electrochemical performance of Ordered Mesoporous Carbon in Supercapacitors

원종구 이창현 황윤경 JINXING 김지만*

성균관대학교 화학과

The electrochemical supercapacitors are energy storage devices which can be categorized into electrochemical double layer capacitors(EDLC) or pseudo-capacitors. They can have higher power and transport higher energy compared to batteries. When high power or their applications are required, they can be used as an auxiliary energy device for batteries or fuel cells to enhance power. There are two properties to increase electrochemical performance in electrodes of supercapacitors : 1) high-capacitance materials that have high surface area or pseudo-active species is needed to ensure high energy density. 2) high electrical conductivity materials is a key factor to ensure a high rate capability. One of the most promising electrode materials is ordered mesoporous carbon because of its huge specific surface area, electrical conductivity, chemical stability, controllable porosity and pseudo-active sites for a variety of redox reactions. However, ordered mesoporous carbons have relatively low electrical conductivity due to amorphous phase. To improve electrical conductivity, we control carbonization temperature to increase electrical conductivity of ordered mesoporous carbon. In our study, ordered mesoporous carbons(CMK3) were synthesized by hard template method through impregnation the carbon precursor into the template(SBA-15) then carbonization at 900℃, 1200℃, 1350℃, and 1450℃. The as-synthesized ordered mesoporous carbons were characterized by X-ray diffraction (XRD), N2-sorption isotherm, Raman, and scanning electron microscope (SEM).

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발표분야: 재료화학
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Heteroatom Doped Ordered Mesoporous Carbon as Cathode materials for Na/SO2 Batteries

이창현 원종구 황윤경 **JINXING** 김지만*

성균관대학교 화학과

Despite superior electrochemical properties of lithium ion batteries such as high energy density, long life cycle, the limitations of the lithium reserves limit large-scale applications for the electric devices. Sodium based batteries are one possible alternative to the lithium ion batteries due to the low cost and comparatively higher natural abundance of sodium. We suggest that Na/SO2 batteries are made up of an inorganic electrolyte, sodium as the anode and carbon materials as the cathode. The ordered mesoporous carbon (OMC) known as one of the most promising cathode material has a remarkable characteristic such as a high specific surface areas, large pore volumes, chemical inertness, and controllable porosity. Particularly, the modification of ordered mesoporous carbon by substituting some atoms with heteroatoms, such as nitrogen (N), oxygen (O), sulfur (S) and phosphorus (P) is an effective way to tailor the electrical and chemical performance of their surface. In this study, we were synthesized by hard template method through using a variety of carbon precursor (e.g. phenanthrene, 1,10-phenanthroline, sucrose, p-toluenesulfonic acid (p-TSA), 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide (DOPO)) and then the difference in their surface chemistry was confirmed through an electrochemical analysis.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Modification of Ordered Mesoporous Metal Oxide with Hexamethyldisilazane and their Electrochemical Characteristic for Lithium Ion Battereis

이현아 박귀옥[1] 김경호 김지만[*]

성균관대학교 화학과 [1]성균관대학교 에너지과학과

Transition metal oxides have been investigated as alternative anodes for lithium ion battery. It shows a specific capacity of 2-3 folds to that of commercially adopted graphite (372 mAh g^{-1}) because it undergoes a conversion reaction yielding pure metal and Li_2O. Among them, Cobalt monoxide (CoO) has high capacity (715 mAh g^{-1}) due to conversion reaction. ($CoO + 2Li^+ + 2e^- \rightarrow Co + Li_2O$). However, it occurs extreme volume changes (in case of metal oxides: >100%) during lithiation and de-lithiation leading to material cracking and degradation, which would result in a major problem for electrochemical performance such as the loss of electrical conductivity and a rapid capacity fading in the cycling. Ordered mesoporous CoO were previously synthesized since each mesopore acts as a buffer for volume changes. But it tends to show drastic capacity fading. So, in addition to this method, we distinctively suggested useful surface modification to enhance cycle capacity retention as the CoO surface attached functional groups are expected to act important role in electrochemical performance. Here, we report simple and effective strategy for lithium ion battery through surface modification in ordered mesoporous CoO by silylation with Hexamethyldisilazane (HMDS). Silyl groups attached on CoO surface make its surface hydrophobic. Furthermore, we applied gas treatment procedures under air, N_2, and H_2 atmospheres, which allow to modify metal oxides surface parameters, especially. The surface chemistry of ordered mesoporous CoO expects to efficiently work during lithiation and de-lithiation and improve cycle capacity retention due to introduction of silane-containing surface on ordered mesoporous CoO.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of surface chemistry of ordered mesoporous carbon on Na/SO_2 battery

황윤경 원종구 이창현 **JINXING** 김지만*

성균관대학교 화학과

Recently, sodium secondary batteries are receiving much attention in energy storage system(ESS) because of their high abundance and low cost of sodium. However, it has some disadvantage like lack of battery performance and safety in the practical applications. Hence, we have suggested that Na/SO_2 batteries could use with SO_2-based inorganic molten complex electrolyte and operate at room temperature also. Therefore, we introduce ordered mesoporous carbon (OMC) as cathode material. Due to high surface area and pore volume, which is reduce the migrating distance of Na ions, facilitating the sodium ion exchange across the interfaces and tolerating the large volume change of the electrodes during the Na ions insertion/extraction. Hence, the ordered mesoporous carbon(OMC) greatly enhance the Na ion storage kinetics and structural stability. In our study, we have synthesized ordered mesorporous carbon (CMK3) by hard template method throughout impregnation the carbon precursor into the template (SBA-15) followed by carbonization at 900℃. And then functionalizeordered mesoporous carbon surface to see the effect of chemical properties of the surface. The synthesized material was identified by high angle X-ray diffraction (XRD), N_2 adsorption-desorption isotherms, scanning electron microscope (SEM), and electrochemical properties were analyzed by charge-discharge profile and cycle performance.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution Synthesis of Superionic Copper Selenideand Their Thermoelectric Properties

JINYINGSHI 한미경[1] 김성진[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학부 [2]이화여자대학교 화학과

Thermoelectric (TE) effects and related technologies have attached considerable attentions due to their abilities of converting heat into electricity and vice versa. It has a potential impact on efficient world?wide energy harvesting. TE energy conversion efficiency is dominated by the dimensionless TE figure of merit ZT ($ZT = S2\sigma T/\kappa$). The parameters described ZT values are interdependent. Therefore it is challenging task to optimize thermoelectric efficiency. Among the TE materials, transition-metal chalcogenides have exhibited good TE properties, because of their complicated crystal structures and variable compositions. Especially, copper selenide Cu2Se has been studied as a representative. Copper selenide Cu2-xSe ($0 \leq x \leq 1$) with a significant deficiency of Cu occurs phase transition from low symmetry α-phase to high symmetry β-phase at temperatures above 400K. In this work, we synthesized surfactant-free copper selenide nanowires and nanoplates. The morphology of the copper selenide can be easily controlled by choosing appropriate reaction time and solvent concentration. We prepared Cu2-xSe ingot from the nanostructured copper selenide using spark plasma sintering (SPS) and evaluated their thermoelectric properties.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Label-Free Colorimetric Detection of Zinc(Ⅱ) Based on Electrostatic Attraction Using Silver Nanoparticles

이수진 남윤식[1] 이강봉[1,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 특성분석센터

A simple label-free detection method had been developed using borohydride-coated AgNPs as a colorimetric probe. This method exploits the electrostatic attraction between AgNPs and Zn2+ ion in solution and allows for the rapid detection of Zn2+ ions. The concentration of Zn2+ ion in aqueous solution can be monitored using a colorimetric assay, whose readout can be visualized with the naked eye, and UV-vis spectroscopy at room temperature. NaDDBS enhanced the reaction rate 2-fold of Zn2+ and AgNPs to be aggregated and Zn2+ AgNPs stabilized with NaDDBS show a higher selectivity and sensitivity to Zn2+ ions over other metal ions. The use of borohydride-coated AgNPs in the absence of conjugation to any other chemical could offer a new approach for the determination of Zn2+ ion levels in aqueous environmental and human blood samples.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The preparation and properties of covalently cross-linked High sulfonation degree SPEEK/Cellulose sulfate composite membranes for water electrolysis

윤영요 정장훈[1,*]

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Covalently cross-linked high sulfonation degree SPEEK/Cellulose sulfate (sulfonated poly ether ether ketone) composite membrane was prepared for the polymer electrolyte membrane water electrolysis. Cellulose sulfate is the derivative of Cellulose in hydroxy group substituted by suflate group in partially. Cellulose can extracted by natural wood and regenerated. so it cheap and environmentally friendly. Cellulose has abundant hydroxy group, it is believed that intermolecular hydrogen bond provide high chemical durability. In this study, reinforced chemical durability due to hydroxy group and increased proton conductivity by sulate group of Cellulose.

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Preparation and characterization of covalently cross-linked medium sulfonation degree SPEEK/Cs-MoPA/CeO2 composite membrane for water electrolysis

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Covalently cross-linked medium sulfonation degree SPEEK/Cs-MoPA/CeO2 (SPEEK: sulfonated polyether ether ketone) composite membrane was prepared for the polymer electrolyte membrane of water electrolysis. Phosphomolybdic acid substituted with a cesium (Cs-MoPA) was added to SPEEK to increase proton conductivity. CeO2 was used to scavenge free radicals which attack the membrane in the water electrolysis and to improve the durability of the membrane. The composite membrane featured the electrochemical properties, such as 0.128 S/cm of proton conductivity at 80 ℃, and 1160 h of oxidative durability. This composite membrane was used as an electrolyte to prepare the membrane electrode assembly (MEA), Pt-Pd/PEM/Pd, and Pt/PEM/Pt by means of non-equilibrium impregnation-reduction method.

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Multilayer films comprising a carbon dioxide responsive polymer

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This study describes the layer-by-layer (LBL) self- assembly of a carbon dioxide responsive living polymer, poly(dimethylaminoethyl methacrylate) (PDMAEMA) with poly(acrylic acid) (PAA) as a function of solution pH and carbon dioxide. The PDMAEMA carries positively charged ammonium group in carbon dioxide atmosphere, which can interact electrostatically with the negatively charged PAA. The behavior of the carbon dioxide-, pH- and temperature-sensitive polymer was studied in aqueous solution by measuring the lower critical solution temperature (LCST) by UV/vis spectroscopy.

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Conjugated Small Molecules bearing Diketopyrrolopyrrole Moiety for Studying Charge Transport Phenomena

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Diketopyrrolopyrrole (DPP) is a promising building block for use in constructing molecules on account of its high optical density and electron affinity. Also, because of oxygen atom in unit, formation of hydrogen bonds can strengthen coplanarity of the molecules, which results in strong intermolecular π-π stacking. Therefore, DPP-derivatives were found to exhibit high charge carrier mobility in organic thin film transistor devices. In this work, we designed and synthesized small molecules bearing DPP unit. Thermal analysis, cyclic voltammetry, absorption spectroscopy and photoluminescence spectroscopy were employed to investigate their physical properties. Eventually, we characterized the properties of thin film transitors.

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Catalyst and Hydroxyl ion effect on Formation of $5Mg(OH)_2.MgSO_4.3H_2O$ Whiskers and Their Ceramic Coating

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Whisker types magnesium hydroxide sulfate hydrate ($5Mg(OH)_2.MgSO_4.3H_2O$, abbreviated 513 MHSH) was used in filler and flame-retardant composites due to their hydrate phase in strctures and ability to undergo endothermic dehydration in fire conditions, respectively. In geneal, length of whisher and structure of hydrate form were determined various synthetic condition in hydrothermal reaction with high temperature(~180 °C). However, it is difficult to produce high quality MHSH because plate-like $Mg(OH)_2$ impurities were formed in high concentrations of OH^- and interaction between Mg^{2+} and OH^-. In this work, we synthesized high purity 513 MHSH by controlling of OH^- ion content in ambient conditions without high pressure. Also, we adopted ceramic coating approachs for improving mechanical and thermal stability of MHSH whisker. Their morphologies and structures were determined by powder X-ray diffraction (XRD) scanning electron microscopy (SEM) and thermo-gravimetric analyzer (TGA).

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Fabrication of 2D-circular silver nanorings by using hollow silica template in solution phase

송유경 장희정 박성호*

성균관대학교 화학과

In this work, we fabricated silver nanorings by using hollow silica nanoring in solution phase. Hollow silica nanoring with Pt support plays a major role as a template. Silver grows along Pt support and remains their nanoring structure in hollow silica template. We selected Pt@Au nanorings as a starting material for hollow silica ring structure. Silica was coated on the Pt@Au nanorings by two-step method and then etching of gold proceeded by using potassium iodide as an etchant, resulting in the formation of hollow silica template. After adding the silver ions and reducing agent subsequently, silver nanorings were synthesized at inner space of hollow silica template. Additionally, we studied optical properties of silver nanorings. In the nanoring with a diameter of about 100 nm, Ag nanoring has quadrupole in-plane mode. We also characterized all of the metal nanoring by using scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-vis-near IR spectroscopy.

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Pt-Coated Pd Nanospring Arrays : Fabrication and their High Electrocatalytic Activity in Methanol Oxidation

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성균관대학교 화학과 [1]성균관대학교 에너지과학과

Pt-coated Pd nanospring arrays (Pd@Pt NSs) were fabricated by coating with Pt on Pd nanospring arrays used as templates. The Pd nanospring arrays obtained by adding two steps, pore widening of anodic aluminum oxide (AAO) templates and slow etching of copper during the previous synthesis process of Pd nanosprings. Pd@Pt NSs maintained the spring shape depending on the total quantity of electric charge of Pt in electrochemical deposition. Due to a large surface area, vacant site of spring pitch and roughness surface, these Pd@Pt NSs exhibited significantly enhanced electrocatalytic activity toward the electrooxidation of methanol in comparison with Pd@Pt nanorod arrays.

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Synthesis of Pt@Au Nanorod Frame in solution phase and observing optical property

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Nanoframe has been interested in that it has large surface area and unique optical properties which could be applied to biosensor and drug delivery. Herein, Pt@Au Nanorod Frame is synthesized simply in solution phase. From pentagonal gold nanorod, Pt is selectively reduced on the edges of nanorod, having high surface energy, like island growth mode. By etching interior gold part, Pt nanorod frame could be obtained easily. Lastly after reduction gold ions onto Pt nanorod frame, I synthesized Pt@Au nanorod frame. Morphology and composition of nanorod are analyzed by Scanning electron microscopy and Transmission electron microscopy. Additionally we observed optical properties of nanorod frame in each step with UV-vis-NIR spectrum.

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Improved External Quantum Efficiency from Solution-Processed (CH3NH3)PbI3 Perovskite/PC71BM Planar Heterojunction for High Efficiency Hybrid Solar Cells

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Over the past few years, organometal halide perovskite solar cells have received considerable attention in the scientific community due to their promising breakthrough of over 15% power conversion efficiency (PCE) and readily available using efficient solution-processed techniques. the (CH3NH3)PbX3 (MAPbX3) perovskite stuctures effectively performed as superior photosensitizers and hole conductor as well as electron conductors. Very recently, the notable photovoltaic performances from planar heterojuction (PHJ) solar cell comprising of MAPbI3/PC61BM bilayer configuration were reported by several research groups. However, the additional functional layers such as Bis-C60 surfactant, bathocuproine, or LiF buffer were required to acheive the high PCEs. Thusly inspired, we have attempted to improve the performances of PHJ hybrid solar cells using MAPbI3 perovskite layer and PC71BM layer, which often exhibited a better performance than PC61BM due to a better spectral response in the visible region, and used the Ag eletrode as electron collecting material due to better practical in all solution-processed system than Al electrode. In this work, we wish to report the high-performance PHJ hybrid solar cells comprising of MAPbI3 (DMSO/GBL-Tol) perovskite and PC71BM PHJ films, exhibiting high PCEs of 12.2%. These outstanding performances were achieved from PHJ hybrid devices configuration of ITO/PEDOT:PSS/MAPbI3 (DMSO/GBL-Tol)/PC71BM/Ag without insertion of Bis-C60 surfactant, bathocuproine, or LiF buffer layers between PCBM film and metal electrode, which were compared with the PHJ hybrid solar cells fabricated with various counterparts such as MAPbI3 (DMF) and MAPbI3 (GBL) perovskite films or PC61BM layer.

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Nanostructured 3D Silicon Anode electrode for Lithium-ion battery

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성균관대학교 에너지과학과 [1]성균관대학교 화학과

Silicon is one of the most promising alloy-type anode materials in lithium ion battery because it has the highest theoretical capacity. However, due to its large volume change associated with the insertion and extraction of lithium ion, silicon leads to loss of electrical contact and fade capacity. To overcome this issue, three dimensional (3D) nanostructures can be used to reduce volume change while improving Li-ion diffusion and electron transport compared with two dimensional (2D) nanostructures. Here, we synthesized 3D silicon electrode coated on Cu nanorods array as current collector by using electrodeposition method and anodic aluminum oxide (AAO) as templates. Si/SiOx-C electrode as final product was formed after heat treatment. The 3D Si/SiOx-C electrode coated on Cu nanorods gives the possibility to have higher capacity over 2000 mAh g-1 and improve stability until 200 cycles compared with 2D Si/SiOx-C electrode films. The capacity of Si/SiOx-C electrode films (2D) is reduced as increasing the number of insertion and extraction of lithium ion. On the other hand, 3D Si/SiOx-C electrode had excellent reversible capacity, more stable cycle life and better rate capability. Heat treatment with electrode improved interfacial contact and conductivity between current collector and active electrode. The composition of carbon material which was made by heat treatment assisted the active material to enhance electrochemical performance.

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Tuning the optical property of Au-Fe-Au multiblock nanorods under the external magnetic field

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성균관대학교 화학과

Localized surface plasmon resonance (LSPR) of noble metal nanostructures has been investigated for a various range of applications. The oscillation of electrons is affected by the size, shape, and composition. There are many efforts to tuning the SPR, but still instant and reversible tuning of the plasmonic property remains a challenge. Here, we report magnetic manipulation of electrochemically synthesized Au nanorods with Fe segments. External magnetic field enables instant and reversible excitation of the plasmon modes of multiblock nanorods. It results multiblock NRs tend to align along the external magnetic field. Also we could observe the behaviors of nanorods as a function of the length as well as the quantity of Fe segments.

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Amino Acids Derived Nitrogen-Doped Carbon Materials for Electrochemical Capacitive Energy Storage

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Carbon materials has received a great deal of attention in scinetific applications, for example, as electrode materials in the fields of energy conversion and storage owing to their large surface area, high electrical conductivity, and exellent chemical stability. Over the past decades, considerable efforts have been made to develop porous carbon materials by using versatile activation methods or various templates from versatile carbon sources such as biomass or oil origins. Biomass is one of the most abundant and low-cost renewable resource, and hence, it has been widely used to synthesis of porous carbon materials via simply thermolysis or hydrothermal reaction. However, most of biomass resources are composed of macromolecules such as lignin and cellulose. Thusly inspired, we have attemped to develop the biomass inspired carbon precursors. In this work, we wish to report that natural amino acids, which are one of small molecular biomass, could be used as attractive carbon precursors. They are cheap and abundant biomass supplied continuously in living organism, and also environmentally benign as opposed to macromolecular biomass resources. Among amino acids, especially histidine-derived nitrogen-doped carbon materials (His-NCMs) were readily synthesized from polycondensation reaction and subsequent carbonization via the stepwise thermolysis process with high yields of ~40% even at a high temperature of 1000 °C and the nitrogen-atom contents of around 5 wt%. These materials possessed rolled planar structures as well as thick 2D-like planar structures with specific surface area of 455 m2/g, exhibiting a notable specific capacitance of 58 F/g at current densities of 100 mA/g and superior stability without deterioration of performance values up to 2000 times.

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Synthesis of 2-D porous MnO_2 nanoplate and searching for its potential applications in energy storage devices

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고려대학교 화학과

In the field of energy storage and conversion devices, manganese-based oxide is one of the hot spots that have shown versatile applications for active materials in batteries and supercapacitors. Besides the excellent electrochemical performance, its low price, high natural abundance and environmental friendliness also make Mn-based oxides as attractive future energy materials. However, the electrochemical performance of Mn-based oxides highly depend on their size, morphology and dimensionality. Previous researches on MnO_2 showed that nanosized MnO_2 outperforms its bulky structure due to high surface to volume ratio and the specific facets which are more exposed in nanosized MnO_2. In addition, dimensionality affects the rate of electron transport and that of ionic diffusion inside the active materials that it is obvious for 1-D and 2-D structure to have shorter ionic diffusion path and more direct electron transport compared to 3-D structure. In this study, we have devised a synthetic route to form 2-D porous MnO_2 nanoplate, which has both advantages of surface to volume ratio and dimensionality. We expect that further optimization of this nanomaterial will lead to a new application for lithium ion battery electrode material and other energy storage devices as well.

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Use of Pyrolyzed Amino Acids as Versatile Dopants for Synthesis of Heteroatoms-Doped Graphenes

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Heteroatoms-doped graphene has received a great deal of attention due to attractive electronic and catalytic properties for promising applications in the fields of electronics, sensors, and electrocatalysis. Heteroatoms substitution in the graphitic framework also induces unique electronic surfaces or active catalytic sites in graphene due to the difference in electronegativity and atomic size between carbon and heteroatoms. Recently, extending the concept of doped graphenes, there have been significant research attempts to harness synergistic effects in the catalytic activity of graphene by developing multiple doping in graphene structures. This includes dual and triple doping of heteroatoms by incorporating nitrogen and other elements such as phosphorus, boron or sulfur. However, these methods uses chemicals with high toxicity and usually results in the low doped heteroatom contents. Thus, there have been extended investigations on more environmentally friendly and efficient synthesis approaches on the heteroatom-doped graphene materials. In this regard, we have inversitigated natural amino acids as efficient and versitile heteroatom precursors to generate heteroatoms-doped carbon materials. In this work, we have successfully demonstrated synthesis and characterization of heteroatoms doped graphene from pyrolyzed natural amino acids, which contain nitrogen or sulfur atoms in side chain motifs. We proved that the pyrolyzed amino acids are excellent precursors for nitrogen doping in graphene, and the doping nitrogen atoms were originated from both amino unit and side chain of amino acids. Moreover, the amino acids such as Cys or Met could be potential candidates as the multielemental dopants such as nitrogen and sulfur.

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Synthesis of Copper sulfide hexagonal nanoplate and their photothermal effect

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고려대학교 화학과

We developed a facile scalable synthetic methodology for copper sulfide nanocrystals with high monodispersity. Copper sulfide nanocrystals have low optical bandgap covering visible and IR ranges. Their photothermal effect was investigated by photothermal optical coherence reflectometer (PT OCR). Copper sulfide hexagonal nanoplates show good photothermal effect depending on the concentration.

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Mechanochemically Iodinated Activated Charcoal as Metal-Free Electrocatalyst with High Activity and Stability for Oxygen Reduction Reaction

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Iodinated activated charcoal (IAcC) was mechanochemically prepared as a cheap, but efficient metal-free electrocatalyst for oxygen reduction reaction (ORR). A large quantity of IAcC could be produced by simple ball-milling with activated charcoal (AcC) in the presence of iodine (I2). After ball-milling, the morphology of the starting AcC was changed from amorphous carbonaceous powder to flake sheet for resulting IAcC, but the BET surface area of IAcC was increased approximately 14 % with larger pore volume. The iodine content in IAcC was 0.59 at.% (5.8 wt.%) and metallic impurities in the starting AcC was substantially reduced, indicating that the mechanochemical reaction through ball-milling induced not only functionalization but purification at the same time. Additionally, IAcC was readily dispersible in various polar solvents, allowing the fabrication of electrode as well as the efficient utilization via solution processing. The IAcC electrode as metal-free electrocatalysts for oxygen reduction reaction (ORR) exhibited outstanding electrocatalytic activities with higher selectivity, longer-term stability and better tolerance to methanol crossover/CO poisoning effects compared with the starting AcC and commercial Pt/C catalysts.

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Detection of pLDH by sandwich assay of aptamer-target-antibody using Au nanoparticles on a Au nanoplate

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Aptamers are the DNAs or RNAs that bind strongly to target molecules and they have lots of advantages like strong affinity and selectivity to target molecules, high thermal stability, small size, and ease of chemical synthesis and modification. Here, we report a sensitive detection way of pLDH(Plasmodium lactate dehydrogenase) which is one of the biomarkers for Malaria using gold nanoplates. We confirmed whether detection of pLDH is available by aptamer-aptamer sandwich structure by gold nanoparticle-gold nanoplate SERS platform and SNOF(single nanowire on film). The gold nanoparticles, gold nanoplates, and gold nanowires are surface-modified by pLDH aptamers. Also, we detected pLDH by aptamer-target-antibody sandwich structure using gold nanoparticle-on-gold nanoplate SERS platform. The gold nanoparticles or the gold nanoplates are surface-modified by anti-pLDH or pLDH aptamer. The gold nanoplates we used are synthesized by chemical vapor transport method and have very clean and smooth surface so that anti-pLDH can be uniformly immobilized on the surface of them. This helps to increase the reproducibility and sensitivity of SERS signals.

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Room Temperature Synthesis of Platinum nanoparticles dispersed on Multi-walled carbon nanotubes

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Carbon nanotube (CNT) is currently attracting much attention due to its unique physical and chemical properties. These exceptional properties make CNT an attractive support for metal nanoparticles. Carbon nanotube (CNT)-based hybrids have many potential applications ranging from advanced sensors to highly efficient fuel cells. Pt-based nanoparticles are widely used as a catalyst for application in fuel cells, where they are homogeneously dispersed on various types of carbon supports. In this study, a new synthesis route to decorate multi-walled carbon nanotubes (MWCNT) with platinum nanoparticles is presented via a simple proton beam irradiation process at room temperature. The characterization of the Pt nanoparticles and MWCNT-Pt composites has been done by using UV-Vis absorption spectroscopy, TEM and EDS analysis.

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An Effective Route for Size- and Morphology-controlled Synthesis of Pt nanomaterials

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We present a facile one-pot synthetic route for the production of platinum nanomaterials via a simple proton beam irradiation process at room temperature. Hexadecyltrimethylammonium bromide (CTAB) was used as a stabilizing reagent for the preparation of Pt nanomaterials. Hydrogen hexachloroplatinate(Ⅳ) solution and sodium hexachloroplatinate(Ⅳ) hexahydrate were used as metal precursors. Size- and shape-controlled Pt nanomaterials were prepared in an aqueous phase-based solution without the addition of any harsh reductants. We observed that the size and morphology of the Pt nanoparticles were easily varied by changing the proton beam current and duration time. It was also observed that the addition of isopropyl alcohol to the reaction mixture played a vital role for the morphology-controlled synthesis of Pt nanomaterials. The characterization was done by using UV-Vis absorption spectroscopy, TEM, and EDS analyses.

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Double-layered black electrochromic device with a single electrode

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This presentation describes a new electrochromic device (ECD) designed to achieve improved black color. We achieved these improvements by fabricating a double-layered nanostructure of two different electrochromic materials stacked in layers on a single electrode. The fabricated ECD maintains 90% of the light transmittance of the colored state even after 1 h if powered off in the colored state. To achieve an improved black, green and blue viologens were successively immobilized in the bottom and top layers of materials on an electrode. The green viologens are initially colored at low voltage, and the purple viologens become colored when the voltage increases. This is because the reduction potential of the green viologens is less than that of purple viologens. Finally, an improved black color is obtained through a mixture of the two colors.

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Relationship between the interlayer anion and the photoluminescence of Activator-Doped Layered Gadolinium Hydroxides

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The large field of applications of layered rare earth hydroxides (LRHs) are based on their abundant attractive optical properties arising from the 4f electronic shells of the rare earths in two-dimensionally stacked layers. However, the understanding of interrelationship between the photoluminescence of (RE $^{3+}$ doped-) LRH and host matrix, activator ion, and interlayer anion still remains limited to the only some particular example pairs of activator and interlayer organic anion. Because the improvement of luminescence efficiency can be quite different depending on the activator and interlayer anion in the starting host matrix, a systematic investigation for overall host/activator, host/interlayer anion, activator/interlayer anion, and host/activator/interlayer anion combinations is indispensably required to provide a guide to researches in need of a means to optimize the PL of LRHs for various applications. In this study, the change in luminescence properties of rare earth doped-layered gadolinium hydroxynitrates (LGdH:REs-NO_3) have been closely investigated by replacing NO_3^- interlayer anions with various organic or inorganic anions such as terephthalate, 2-naphthoate, F^-, Cl^-, I^-, S^{2-}, OH^-, CO_3^{2-}, SO_4^{2-} and ClO_3^-. As a luminescent center, Eu^{3+} , Tb^{3+}, and Ce^{3+} ions were doped into the LGdH matrix for red, green, and blue emissions, respectively. As expected, the exchange reaction of NO_3^- with other anions was accompanied with a significant change in photoluminescence behavior and, despite the same interlayer anion, the luminescence efficiency varied considerably with dependence on the activator ion (RE^{3+}).

Here, we demonstrate that the interlayer anions in the galleries of LGdH can act as just a spacer or a filter or harvester of UV energy for the excitation of LRHs and their roles are decided by the nature of activators.

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Fluorescent Sensor for Simple Detection of Cr(VI) based on Inner Filter Effect

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Hexavalent chromium Cr(VI) is seriously considered as hazardous substance due to its mutagenicity and carcinogenicity to living organisms, and its high solubility in neutral water allows it both mobility and bio-accessibility. Because the maximum allowed limit of Cr(VI) is strictly regulated for many water sources around the world, the development of techniques for simple and fast detection is necessarily required to monitor and maintain Cr(VI) concentrations in environmental waters at lower than limited levels. In this study, we have demonstrated Tb-doped layered yttrium hydroxychloride (LYH:Tb) as a sensor for the detection of Cr(VI) based on the inner filter effect (IFE), caused by absorption of excitation and/or emission light for fluorescent adsorbents by adsorbates. An inner filter effect system was constructed by the effective overlap between the excitation bands of LYH:Tb and absorption bands of Cr(VI) (both $HCrO_4^-$ and CrO_4^{2-} forms existing as a relative ratio according to the pH in dilute aqueous solution). This IFE system enables LYH:Tb adsorbents to be potentially applicable as a new fluorescent sensor for Cr(VI) in aqueous solution. The effective shielding of excitation light for LYH:Tb by adsorbed Cr(VI) could achieve a feasible IFE-based detection sensitivity. The striking contrast in brightness of green emission before and after adsorption of Cr(VI), which is distinguishable even with the naked eye, would enable LYH:Tb powder to be exploited as a portable kit for field detection of Cr(VI). This LYH:Tb sensor provides a simple, convenient, rapid, and sensitive method for the detection of Cr(VI) in environmental and industrial applications. Besides simplicity and convenience, the buffering capability of LYH:Tb provides the advantage of significant fluorescence quenching in both acidic and basic solutions at room temperature.

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Synthesis and microwave absorption properties of $Ni_{0.5}Zn_{0.5}Fe_2O_4$@PANI composite

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강릉원주대학교 화학과

전기,전자 산업의 급속한 발전과 함께 통신 장치들은 기기 내외에서 발생하는 전자기 문제를 해결하기 위해서 전자 차폐에 대한 필요성이 커지고 있다. 전자파 차폐중에서도 근래에는 주로 전자파 흡수제 개발에 집중하고 있는데 본 연구에서는 전도성 고분자 Polyaniline(PANI)와 $Ni_{0.5}Zn_{0.5}Fe_2O_4$ 페라이트계 나노입자를 사용하여 전자파 차폐제로서 $Ni_{0.5}Zn_{0.5}Fe_2O_4$@PANI 복합제를 Core/Shell 형태로 합성하였고 SEM, TEM, XRD, EDS, VSM, Network Analyzer 를 사용하여 형상과 특성 분석을 하였다.

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Highly enhanced photoluminescence of Eu-doped layered gadolinium hydroxide by sequential addition of organic anions and Meta-Vanadate

박성진 정희진 변송호*

경희대학교 응용화학과

Despite Eu^{3+}-doped Gd compounds are recognized as a family of excellent red phosphors, the layered rare earth hydroxide (LRH) matrix doped with Eu^{3+} does not yield high quantum efficiency because a lot of hydroxyl groups in the layer greatly increases the probability of non-radiative transition. For this reason, the photoluminescence (PL) property of layered europium hydroxide (LEuH) or Eu^{3+}-doped LRHs is dominated by the weak spin-forbidden $^7F_0 \rightarrow {}^5L_6$ intra $4f^6$ excitation of Eu^{3+} at ~396 nm. In this work, we demonstrate that the PL of LRH matrix can be drastically increased by the appropriate intercalation of organic anions followed by the adsorption of meta-vanadate antenna. Here, we explored a new hybrid system between meta-vanadate (VO_3^-) and organic carboxylates of different lengths to enhance the red emission of LGdH:Eu. The meta-vanadate ions were effectively adsorbed on the surface of LGdH:Eu-sensitizer nanosheets in aqueous solutions. After adsorption reaction of meta-vanadate, the structure of organic molecule intercalated matrix (LGdH:Eu-Org) was maintained. Interestingly, the red emission of VO_3^--adsorbed LGdH:Eu-Org was significantly enhanced in comparison with those of VO_3^- -adsorbed LGdH:Eu without organic or LGdH:Eu-Org before meta-vanadate adsorptions. This phenomenon suggests that the interlayer space of LGdH:Eu expanded by organic anions with long-chains can provide the pathway through which meta-vanadate ions readily access to the interlayer surface sites of the LGdH:Eu matrix. As a representative example, the LGdH:Eu-stearate showed the bright red emission after adsorption of meta-vanadate in aqueous solution of below 5 ppm, which is distinguishable even with the naked eyes.

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Organic spacer-assisted highly selective detector for Meta-Vanadate Ions

정희진 변송호*

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Although vanadium compounds were prescribed as therapeutic agents for anaemia, chlorosis, tuberculosis and diabetes in the past, they are regarded as the potential toxic due to their negative effects on the respiratory, circulatory and central nervous systems, the digestive organs, kidney, and skin. In general, the vanadium compounds mainly exists as oxo-anion forms (vanadates) in dilute aqueous solutions, and the toxicity increases with the oxidation states. In this work, we have developed Eu-doped layered gadolinium hydroxide (LGdH:Eu) modified through the intercalation of long-chain alkyl carboxylate anions (stearate, $C_{17}H_{35}CO_2^-$) as a novel fluorescent sensor for selective detection of meta-vanadate in aqueous solutions. It is interesting that the significantly enhanced sensitivity for meta-vanadate could be obtained by the simple exchange reaction with non-conjugated alkyl groups, where no energy transfer process can be occurred. When meta-vanadate ions were adsorbed on the organic anion exchanged LGdH:Eu, the strong red emission induced by the efficient metal-to-ligand charge transfer (MLCT) of meta-vanadate on LGdH:Eu matrix was observed. Furthermore, the luminescence improvement of this organic spacer-assisted LGdH:Eu by different oxoanions such as tungstate, molybdate, chromate, etc. was not comparable with that by meta-vanadate ion. Thus, the organic spacer-assisted LGdH:Eu sensor exhibited simple, fast, ultrasensitive performances applicable for the detection of meta-vanadate. The luminescent colloid of meta-vanadate adsorbed matrix showed in-turn potential utility as a new class of multimodal probe for biomedical applications.

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Thermal Decomposition of Layered Samarium Hydroxychlorides and Their Memory Effect in Aqueous Solutions

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The thermal decomposition and recovery behavior of layered samarium hydroxychloride ($Sm_2(OH)_5Cl{\cdot}nH_2O$, LSmH) has been closely studied on the basis of temperature dependent XRD and FT-IR patterns. Although the heat treatment of LSmH at 700 ˚C completely collapsed typical layered structure, the calcined LSmH(c-LSmH) recovered its layered characteristics and consequently its ability to intercalate anions into the interlayer galleries by rehydroxylation and rehydration in aqueous solutions containing organic(i.e. hexanesulfonate, $C_6H_{13}SO_3^-$) or inorganic anions(i.e. NaCl and $NaNO_3$). The addition of the organic or inorganic salt greatly facilitates the recovery reaction of c-LSmH. This phenomenon conceptually is similar to the memory effect frequently observed in classical layered double hydroxides (LDHs), where LDHs calcined into a mixture of metal oxides can recover their layered structures in aqueous solutions. In contrast, the recovery reaction of c-LSmH in water without any counter anions was unsuccessful and instead resulted in the formation of $Sm(OH)_3$. Such a difference was construed on the basis of the salt effect on $Sm_2(OH)_5Cl{\cdot}nH_2O{\cdot}Sm(OH)_3$ phase equilibria in water. The salt effect is supported by the highly increased stability of hydroxychloride form in $Sm_2(OH)_5Cl{\cdot}nH_2O{\cdot}Sm(OH)_3$ phase equilibria in NaCl solution, compared with that in pure water. Ultimately, the reconstructed layer structure endowed c-LSmH with the intercalation ability to form $Sm_2(OH)_5(C_6H_{13}SO_3){\cdot}nH_2O$, where $C_6H_{13}SO_3^-$ anions are inserted into the interlayer galleries of LSmH.

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Oligo(ethylene glycol)-incorporated hybrid linear alkyl side chains for n-channel polymer semiconductors and their effect on the thin-film crystalline structure

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경상대학교 화학과 [1]경상대학교 그린에너지융합연구소

A high-performance naphthalene diimide (NDI)-based conjugated polymers for use as the active layer of n-channel organic field-effect transistors (OFETs) were reported. Oligo(ethylene glycol)-incorporated hybrid linear side chains were designed and synthesized with n-channel NDI based copolymers (PNDI-OR and PNDI-RO). PNDI-OR and PNDI-RO were synthesized by the Stille coupling reaction. The structure of the monomers and polymers was confirmed by ^{1}H NMR and FT-IR. The optical, electrochemical and thermal properties have been investigated. The microstructural ordering of the resulting polymers was altered according to the attached side chains, without disrupting the rigidity of the polymer main chain. Unipolar n-channel charge-transport behavior was observed for the resulting copolymers. In particular, PNDI-RO showed a high electron mobility of up to 1.64 cm^2 V^{-1} s^{-1} with a high on?off current ratio of 10^5. These results demonstrate that hybrid side chains using oligo(ethylene glycol) are promising new solubilizing groups for high-performance organic semiconductor materials.

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Preparation and Characteristics of W/Mg co-doped VO_2(M) thermochromic films

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부경대학교 화학과 [1](주)마프로 기술연구소

Monoclinic vanadium dioxide(VO_2) undergoes phase transition from IR-transparent semiconductor to IR-reflective metal about 68℃. Due to this property, VO_2(M) is a promising material for smart windows. But in order to apply this material to real life, transition temperature, visible transmittance and NIR switching efficiency should be considered. By adding dopants, we can control transition temperature and optical properties. Tungsten is known as most efficient dopant that reduce transition temperature to room temperature. Also as magnesium are doped into VO_2, thermochromic properties are enhanced. In this study, we have synthesized W/Mg co-doped VO_2 by hydrothermal and post heat treatment from V_2O_5 precursor. The thin film of W/Mg co-doped VO_2(M) was also prepared by wet-coating method. We have investigated the morphologies, transition temperature, optical and electrical properties of W/Mg codoped VO_2(M) and its thin film by controlling the amounts of W and Mg.

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Quasi-one-dimensional Multiblock Nanorods for Magnetic Modulation of Localized Surface Plasmon Resonance

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Localized surface plasmon resonance (LSPR) has been studied for the fields of biosensors since it is sensitive to the size, shape and the surrounding environment such as dielectric constant. It is of great interest to control LSPR in an instant and selective way, for achieving tunable plasmonic property. Herein, we described the tuning of surface plasmon coupling of Au/Ni/Au multiblocks synthesized via electrochemical deposition method under an external magnetic field. Simple introduction of the nickel segments into Au nanorods can enable to achieve not only optical properties but also magnetic tuning of alignment, leading to the change of plasmonic response. We systematically investigated this important nanorod feature by comparing optical responses depending on the number of Ni segments forming penta- and heptablock nanorods with different aspect ratios of Ni, which facilitates either magnetic enhancement or cancellation.

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Layer-by-Layer Assembly of Layered Double Hydroxide /Graphene Oxide Hybrid Multilayer nanocomposite Films

김명신 남혜진 정덕영*

성균관대학교 화학과

Layer-by-layer stacked layered double hydroxide ($[Mg_2Al(OH)_6]CO_3 \cdot nH_2O$)and graphene oxide (GO) nanocomposites were prepared on Si substrate by layer-by-layer assembly method. We synthesized well-crystallized Mg_2Al-LDH, which has a diameter of from 200 to 400 nanometers and a thickness of about 100nm, using the co-precipitation and hydrothermal treatment method. For the preparation of the monolayer LDH on Si, the plasma treated Si substrates were dipped in the Mg_2Al-LDH colloidal solution and sonicated for 10min. Monolayer LDH nanosheets that covered 80% of substrate area was deposited. LDH substrates were immersed in water-dispersed graphene oxide solution to wrap GO sheet onto LDH monolayer by electrostatic interaction. These composite films with aligned graphene oxide and LDHs are expected to find potential applications in the electrical and magnetic fields. Morphology and structure of LDHs/GO nanocomposites are characterized by scanning electron microscopy (SEM), X-ray diffraction pattern (XRD) and Raman spectroscopy.

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Multifunctional Polydopamine-Layered Double Hydroxide Nanocomposites Induced by Intercalative Polymerization

남혜진 박은비 정덕영*

성균관대학교 화학과

A new mulutifunctional nanocomposite was prepared by an intercalative polymerization of polydopamine (PDA) on layered double hydroxide (LDH) nanoparticles. Spontaneous self-polymerization of dopamine (DA) in basic buffer solution was applied to layered double hydroxide, which provides a synthetic pathway to make the nanostructured PDA/LDH composites without the presence of nanosized polymer agglomerates. The decrease of the interlayer spacing in XRD data provided an evidence for the effective intercalation of the PDA into the interlayer space of the LDH nanoparticles. The catalytic efficiency of the nanocomposites was evaluated by the reduction of 4-nitrophenol in the presence of $NaBH_4$, in which the PDA exhibited the stabilizing and protecting effects in the PDA/LDH nanocomposites for the reduction of cobalt ion. The strong adhesion ability of the PDA and the effective control for the polymerization of DA enabled to prepare the multifunctional nanocomposites.

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Synthesis of $CuInS_2$ Colloidal Nanoparticles by using Metal Hydroxide Precursor

정선호 차지현 정덕영*

성균관대학교 화학과

We present synthesis of $CuInS_2$ colloidal nanoparticles via a facile solution-processed method, using $CuIn(OH)_5$ precursor. Cu?In metal hydroxide precursor was prepared by chemical co-precipitate method in aqueous solution; an aqueous NaOH solution reacted with the metal hydroxide solution containing Cu^{2+}, In^{3+} at room temperature. Then, it was dispersed in oleic acid (OA) and bis(trimethyldisilyl)sulfide was used to provide sulfur source for fabrication of $CuInS_2$ nanocrystals. The zinc blende-type $CuInS_2$ colloidal nanoparticles were confirmed by XRD measurement. TEM image shows $CuInS_2$ nanoparticles have an average size of 6.5 nm. Organic surfactants were removed to increase electrical conductivity by using $(NH_4)_2S$ solution, observed by FT-IR. The Cu-In-S composition ratios (%) were 1:1:2, measured by EDS, EPMA, and ICP.

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Direct growth of Co-Al layered double hydroxide nanoplates on Ni substrate for pseudocapacitor application

박은비 남혜진 차지현 정덕영*

성균관대학교 화학과

Cobalt aluminum layered double hydroxide (Co-Al LDH) nanoplates were synthesized on Ni substrate by direct growth method. The nickel substrate (foam, 1 cm x 3 cm) were immersed into aqueous solution containing $CoCl_2 \cdot 6H_2O$, $AlCl_3 \cdot 6H_2O$, NH_4F and urea. When ammonia was released by decomposition of urea at 95 °C, Co-Al LDH nanoplates were vertically grown on Ni substrate. X-ray powder diffraction patterns indicated that the interlayer spacing of hexagonal structure Co-Al LDH was 22.78 Å when carbonate anion was intercalated. The loading mass and thickness of Co-Al LDH nanoplates were controlled by growing time. The electrochemical performance of Co-Al LDH nanoplates were charaterized by cyclic voltammetry and galvanostatic charge/discharge in 2 M KOH solution at room temperature. Co-Al LDH grown for 2 hours has a specific capacitance of 1294 F/g at 2 A/g and 983 F/g at 50 A/g.

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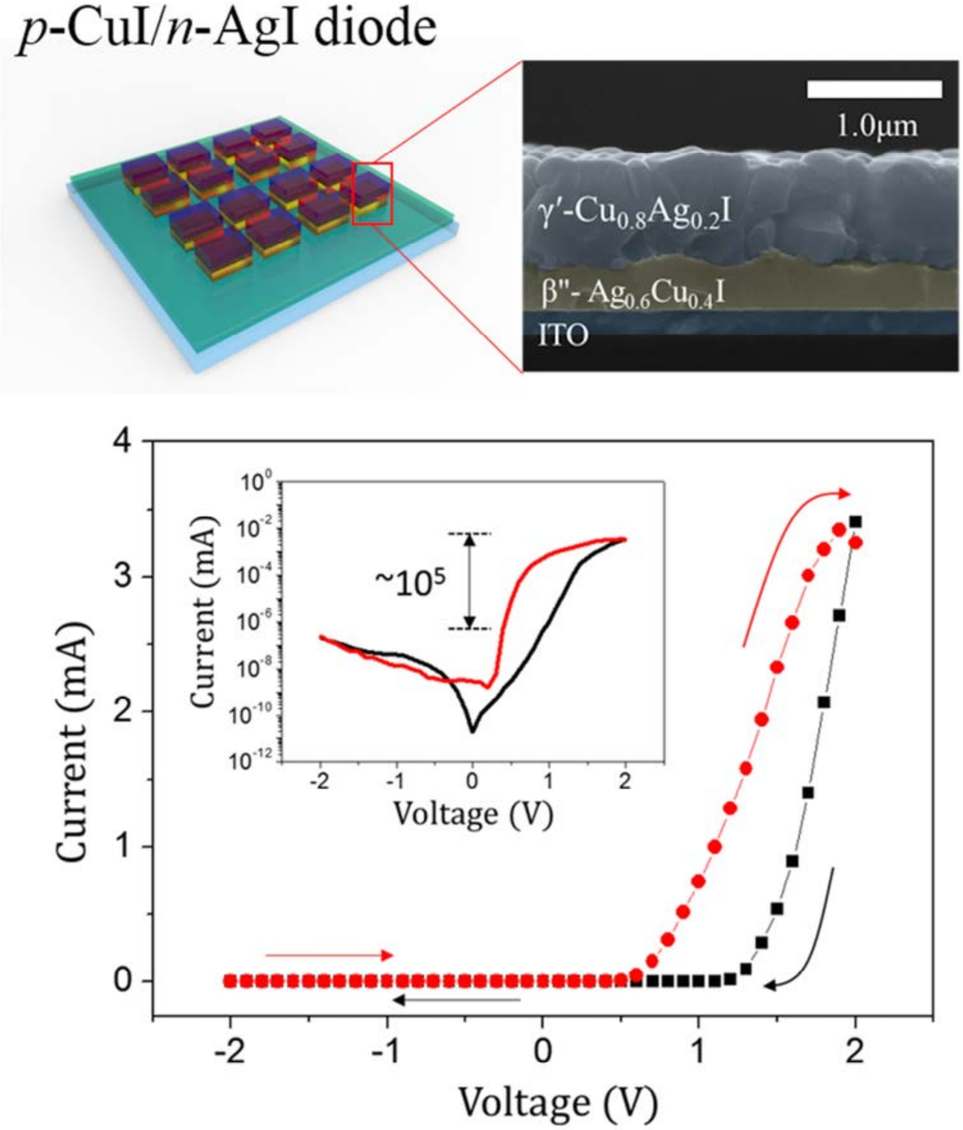
Metal Halide Thin Film Based Transparent Heterojunction *pn*-Diode

차지현 정덕영*

성균관대학교 화학과

The transparent AgI/CuI heterojunction on ITO substrates had been prepared by vapor phase iodization of metal thin films and show high rectifying diode behavior. We investigated the crystallographical and chemical characteristics of AgI and CuI thin films throughout the deposition sequences. In order to prepare the AgI/CuI heterostructure films on substrates, we should synthesize β-AgI as a bottom layer. In case of the CuI and Cu metal film as a bottom layer, uniform heterojunction films could not be obtained. Although elemental exchange between two layers were observed, the stacked films exhibited different crystal phases as well as chemical compositions. Moreover, we utilized the photodecomposition of AgI as patterning technique for thin films, as simple and fast patterning methodology superior to the general patterning techniques, such as photolithography and soft-lithography. The prepared AgI/CuI thin films exhibit a pn-diode behavior as rectifying ratio of 9.4×10^4 and turn-on voltage of 1V at room temperature.


p-CuI/n-AgI diode
1.0μm
γ′-Cu$_{0.8}$Ag$_{0.2}$I
β"- Ag$_{0.6}$Cu$_{0.4}$I
ITO
Current (mA)
Voltage (V)
4
3
2
1
0
-2
-1
0
1
2
~10^5
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}

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Photodynamic activites of multifunctional cobalt ferrite particles with various sizes

이규동 남준식 정진승*

강릉원주대학교 화학과

In addition to the increasing number of nanotechnology applications in medical diagnostics and therapeutics the utilization of nanomaterials in consumer products has recently become more important. Among them, the spinel ferrite materials have widely been paid attention due to their current and future applications not only in the field of catalysts but also in the field of biology and medicine, such as diagnostics, biosensing, therapeutics, drug delivery and targeting. In this study, biocompatible multifunctional particles ($CoFe_2O_4$@HP) of well-defined size (60,133,245,335 nm) were fabricated to be used as photodynamic therapeutic agents for cancer cells. The prepared $CoFe_2O_4$@HP particles with various sizes exhibit high water solubility, good magnetic resonance imaging (MRI) and biocompatibility without any cytotoxicity. This size dependent effect is determined by the particle specific surface area. These results indicate that $CoFe_2O_4$@HP are suitable for effective photodynamic therapy (PDT).

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Regiospecific growth of Au on a concave Pt nanocube through surface stabilization

황혜윤 박종식 이광렬*

고려대학교 화학과

For designing facet-controlled heteronanostructrues, regiospecific growth of heterophases on facet-controlled nanoparticles is studied due to physicochemical properties of heterostructured nanoparticles. The surface energy difference appears due to specific facets exposed on the surface and surface stabilizing moieties, leading to new structure-dependent properties. Growth of Au phase on a Pt-based concave nanocube in the absence or presence of surface binding moiety CO was observed how it affects the growth of the heteronanostructures. Concave surface of Pt nanocube was filled with Au in absence of CO via thermodynamic process while Au phase grows on the eight vertices of the Pt nanocube in the presence of CO via kinetic process. Herein, we report the successful regiospecific growth of Au on a concave Pt nanocube through facet-control using surface stabilizing moieties.

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Formation of double layer hollow nanostars of Pd/CuIr and Their Usage as Efficient Water Splitting Catalysts

이재영 윤동환 이광렬*

고려대학교 화학과

Hollow nanostructures with inherent high surface area per mass are attractive candidates for economically viable catalysts. Conceptually, a hollow nanostructure can be obtained by forming a desired material phase on a removable template and then by subsequently removing the template core. Herein we report the synthesis of unusual bilayer hollow nanostructure with a CuIr surface layer and a Pd inner-coating layer followed by a facile CuPd alloy phase formation and an outward movement of Cu phase under oxidizing condition. We also report the high catalytic performance of the hollow nanostructure in oxygen evolution reaction (OER).

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One pot Synthesis of hierarchical Pt nanohexapod nanocrystals

남경식 윤동환 이광렬*

고려대학교 화학과

Facet-controlled Pt nanoparticles are being recognized as an important class in catalysts for fuel cell electrode application. we demonstrate successful preparation of hierarchical Pt nanohexapod by combining the growth of a Pt hexapod. Lower coordination numbers at the branch tips give extremely high surface energy. For this reason branched growth is initiated at the tips under kinetic control. Interestingly, the subproduct within this sample grow dedrimers with different branching behaviors. This approach based on high surface energy of tips is potentially extendable to synthetic methodologies for the preparation of catalytic nanostructures.

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Facile synthesis of hollow PtCu@Ru octahedral nanocrystal via Pt seed-assisted formation of in situ removable Cu template

박수현 윤동환 이광렬*

고려대학교 화학과

A facile synthetic strategy has been developed for size-controlled PtCu@Ru nanorattle in the presence of Pt nanoparticles. The growth of the nanorattle structure is based on the fast nucleation of Cu on the preformed Pt nanoparticles. Subsequent decomposition of Ru precursors leads to the formation of Ru shell. The Cu layer between the core and shell of the intermediate PtCu@Cu@Ru nanoparticle, generated as a kinetic product, is in-situ removed by CTAB (cetyltrimethylammonium bromide)-induced destabilization process to yield a novel nanorattle structure with a Pt core and a porous Ru shell. The Pt nanoparticle surface is partially alloyed with the Cu phase to form CuPt alloy phase. The size of PtCu@Ru nanorattles could be conveniently controlled by varying the ratio of employed Cu and Ru precursors. The high surface area per mass of the hollow nanostructures would be greatly advantageous for catalytic performance.

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Rational synthesis of Facet-Controlled fcc Ru and Rh Nanoparticles: Seed-mediated heteronanostructures and their enhanced catalytic activity

진하늘 박종식 이광렬*

고려대학교 화학과

Facet-controlled nanoparticles have various surface energies depending on their structures, namely facets, edges and vertices, and unstable edges and vertices have been known the favored growth sites. In this work, we report a shape-controlled synthesis of M/Pt (M=Ru or Rh) nanoboxes (RUNB or RHNB) and octapods (RUOP or RHOP) by heteroepitaxially growing nanoplates on vertices of various shapes of Pt seeds. Such examples are very unique because of the difficulty in the facet controlled growth of heterophase and little understanding for the structural factors resulting in a conformal coating or a faceted crystal growth on vertices. In addition, the two similar, but distinct, nanoparticles show huge differences in oxygen evolution reaction by the combination effect of structural features and core-shell effect. We can also obtain fcc phase of Ru nanoparticles which are generally found hcp for the bulk state.

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Rationally synthesis of bimetallic hollow nanostructure and its mechanistic study

박종식 이광렬*

고려대학교 화학과

Metastable nanoparticle templates are being employed for the preparation of functional hollow nanostructures. The synthesis of hollow nanostructure requires the presence of pores in the newly grown shell on the metastable template, which would serve as the removal passage for the template content. Therefore, in principle, it should be possible to form a structural series from a core-shell nanoparticle to a hollow shell for a given set of core and shell materials. Herein, we describe the rational synthesis of novel bimetallic hollow nanostructure and its synthetic mechanism.

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Enhanced photocatalytic activity of ZnO-decorated CNTs prepared by high energy ball milling

오명은 최현철*

전남대학교 화학과

Ball milling is an effective method for the synthesis of nano-sized materials. During the ball milling, the impact and shear stress would cause the pulverization of materials. This process has been successfully applied to disperse or shorten carbon nanostructures. In this work, we demonstrate the efficient synthesis of the ZnO-decorated CNTs by high energy ball milling. The prepared sample was characterized by Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photocatalytic activities of CNT-ZnO were investigated with several dyes under ultraviolet light irradiation. The obtained results showed that ball milled CNT-ZnO displayed much higher photocatalytic activity compared to non-treatment material. In addition, ball milled CNT-ZnO exhibited excellent stability in the photocatalytic process.

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Preparation of SnO_2 nanoparticles by a precipitation method and their photocatalytic activity for methylene blue

김성필 최현철*

전남대학교 화학과

To investigate the characterization and photocatalytic activity of SnO_2 nanoparticle calcinated at various temperature, the three samples of SnO_2 nanoparticles were synthesized by a modified precipitation method from the $SnCl_2{\cdot}2H_2O$ precursor. The prepared SnO_2 nanoparticles were characterized by XRD, TEM, NEXAFS, and photocatalytic measurements. XRD analyses showed that the three samples have an average particle size of ~3 nm (sample A), ~5 nm (sample B), and ~7.2 nm (sample C). The Sn NEXAFS spectra of the three samples indicated that the prepared SnO_2 nanoparticles have tetragonal structures, and showed no noticeable change in the oxidation state of tin ions with rising calcination temperature. The photocatalytic properties of the SnO_2 nanoparticles were evaluated by photodegradation of MB and SnO_2 nanoparticle calcinated at 380°C has higher photocatalytic activity than the different catalysts and Blank.

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ZnO-decorated CNTs for photodegradation of Congo red

김은혜 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have received a considerable attention due to their unique chemical and physical properties, as well as their technological applications.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 Zinc oxide(ZnO) because of great surface area, oxide is a wide bandgap semiconductor (E_g ~ 3.4eV) with important technological applications in several fields. In this work, we demonstrate a novel and simple method for the synthesis of CNT-ZnO. The prepared CNT-ZnO was characterized by X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photocatalytic activity of CNT-ZnO was tested by congo red degradation process under ultraviolet light irradiation. The results showed that CNT-ZnO exhibited excellent stability in the photocatalytic process.

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Preparation of CNT-SnO_2 for the L-CySH sensor

김성필 최현철*

전남대학교 화학과

L-cysteine is a sulfur-containing amino acids which naturally contained with small quantities in a number of proteins and plays a important role in biological system. For example, it can be used as a prospective radiation protector, antioxidant, free radical scavenger, and cancer indicator. Its deficiency is associated with a number of clinical situations such as liver damage, skin lesions, hair depigmentation, edema, lethargy, muscle, fat loss, slowed growth, and AIDS. Due to the reasons above, sensitive detection of L-cysteine is practically important. In this study, we synthesized tin oxide decorated on thiolated carbon nanotubes (CNT-SnO_2). Morphology properties of the CNT-SnO_2 were investigated with transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Cyclic voltammetry (CV) and amperometry (at an applied potential of 0.45 V) were used to investigate electrochemical properties.

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Novel Alkoxyanthracene Donor and Benzothiadiazole Acceptor for Organic Thin Film Transistor and Organic Photovoltaic Cells

마재열 김윤희* 천예림 안은수

경상대학교 화학과

Novel alkoxy anthracene (ODA)-based polymeric semiconductors were designed for polymer solar cell applications. Alkoxyanthracene, which contains many p electrons and electron donating group, was easily synthesized. The copolymers, poly(alkoxy anthracene-alt-thiophene benzothiadiazole thiophene) poly(ODA-TBT) and poly(alkoxy anthracene-alt-benzothiadiazole) poly(ODA-BT), have been obtained by Suzuki coupling polymerization. Both polymers have ODA unit as a donor and benzothiadiazole as an acceptor. ODA-TBT has thiophene linkages between ODA and benzothiadiazole. The optical, thermal, and electrochemical properties have been investigated by UV?visible absorption, thermal gravimetric analysis, differential scanning calorimetry, and CV. The better device performance of poly(ODA-BT) is attributed to its charge transfer ability and enhanced mobility and crystallinity although poly(ODA-BT) does not have extended conjugation due to twisted structure compared with poly(ODATBT).

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The crystalline properties and performances of anthradithiophene-based devices are affected by solvent boiling point

박성종 김윤희* 하연희 안은수 김란 황재영[1]

경상대학교 화학과 [1]경상대학교 그린에너지융합연구소

We synthesized two new anthradithiophene derivatives : 9,10-di(4’-pentylphenylethynyl)-anthra[2,3-b:6,7-b’]dithiophene (DPPEADT) and 9,10-bi([9’,9’-dimethyl-fluoren-2-ylethynyl])-anthra[2,3-b:6,7-b’]dithiophene (DFEADT). We investigated the effects of the solvent boiling point on organic field-effect transistor (OFET) device performances in devices prepared using two newly synthesized materials: DPPEADT and DFEADT. We characterized the relationship between the molecular structures, film morphologies, and OFET device performances in devices prepared using solvents having one of three different boiling points (chlorobenzene, 1,2-dichlorobenzene, and 1,2,4-trichlorobenzene) 1,2,4-Trichlorobenzene, which provided the highest boiling point among the solvents tested and acted as a good solvent for DPPEADT, significantly improved the field-effect mobilities of DPPEADT devices up to 0.16 cm2/V by enhancing the crystallinity of the film. OFETs based on amorphous DFEADT films prepared using the three solvents did not provide enhanced electrical performances.

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Synthesis of Asymmetric alkylphenyl-substituted anthracene molecules for use in small molecule solar cells

안은수 김윤희* 마재열 천예림

경상대학교 화학과

We were designed and studied two symmetric asymmetric alkylphenyl- substituted anthracene for small molecule solar cells applications, NDHPEA and TNDHPEA. The first such molecule was 9,10-bis((4-hexylphenyl)ethynyl)-2-(naphthalen-2-yl)anthracene (NDHPEA), a small molecule containing an alkylphenyl-substituted-anthracene core unit with a naphthalene terminal unit. The second such molecule was 2-(9,10-bis((4-hexylphenyl)ethynyl)anthracen-2-yl)-5-(naphthalen-2-yl)thiophene (TNDHPEA), a small molecule composed of the core moiety used in NDHPEA, except for the introduction of a thiophene-bridged naphthalene arm unit. The two molecules differed only in the presence of a thiophene spacer. We focused on how the thiophene spacer influenced the nanoscale crystalline characteristics of the active layers and the resulting device performances. The asymmetric NDHPEA and TNDHPEA molecules were synthesized through the nucleophilic addition of a hexylphenylethnyl group, followed by a reduction reaction and a Suzuki coupling reaction. The thermal, photophysical, electrichemical properties have been investigated by thermal gravimetric analysis(TGA), differential scanning calorimetry (DSC), UV?visible absorption, and CV.

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B-Doped Graphene as a Metal-Free Cathode Material Compared to Pt over a Co(II)/Co(III) Electrolyte for Dye-Sensitized Solar Cell

정선민 고재중[1] 이재준[2,*] 김환규[3,*] 백종범[4,*]

울산과학기술대학교(UNIST) 에너지공학과 [1]고려대학교 소재화학과 [2]건국대학교 응용화학과 [3]고려대학교 신소재화학과 [4]울산과학기술대학교(UNIST) 에너지공학부

We report that B-doped graphene (BG) is prepared and tested as counter electrode (CE) in dye-sensitized solar cells (DSSCs) in conjunction with $Co(bpy)_3^{2+/3+}$ redox couple. The BG CE has lower charge-transfer resistance and surpassing electrochemical stability than Pt CE. As the result, the DSSC with BG CE exhibits higher power conversion efficiency than the DSSC with Pt CE, suggesting possibility to replace Pt CE in DSSCs.

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Synthesis of Size controlled Metal doped TiO_2 Hollow Spheres Using Polystyrene Core Materials

김재욱 배재영*

계명대학교 화학과

Metal doped TiO_2 hollow spheres (MTHS) that is synthesized by polystyrene (PS) core materials, various transition metals, and titanium tetraisopropoxide (TTIP) by core-shell structure. Defined MTHS diameter ranging from 132 to 423 nm, and shell thickness ranging from 12 to 27 nm. Transition metals are analyzed by X-ray photo electron spectroscopy (XPS). Result of TGA showed the removal temperature of PS. The XRD peaks showed Anatase structured and using N_2 sorption for BET surface area. Transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), Thermogravimetric Analyzer (TGA), analysis X-ray diffraction (XRD) and Brunauer-Emmett-Teller method (BET) are used to characterize the prepared MTHS.

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Synthesis of Mesoporous Silica Materials by using a Cationic Surfactant at Room Temperature

서원호 배재영*

계명대학교 화학과

Ordered hexagonal and cubic structured mesoporous silica materials were synthesized in presence of cationic surfactant and TEOS at room temperature. The resulting silica materials were characterized by fourier transform infrared spectrometer (FT-IR), X-ray diffraction (XRD), transmission electron microscope (TEM), and N_2 sorption isotherms. The FT-IR spectra confirmed the removal of surfactant after calcination and the occurrence of symmetric Si-O stretching. TEM images showed uniformed mesopores. XRD patterns indicated hexagonal and cubic structured. N_2 sorption isotherms indicated with high surface area.

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Synthesis of Amine Group Functionalized Mesoporous Silica with Cubic Structure for CO_2 Capture

구병진 배재영*

계명대학교 화학과

Functionalized ordered cubic mesoporous silica have been obtained by a post-grafting method using 3-aminopropyltriethoxysilane (S330,Osung) as modifying agent. The dependence of S330 concentration, and reaction time on average pore size, pore volume, superficial area, and morphology was studied. The modified silicas were characterized by powder X-ray diffraction (XRD), infrared spectroscopy (FT-IR), transmission electron microscope (TEM) and nitrogen adsorption?desorption experiments. According to the TEM results, no morphological changes were observed in the modified cubic mesoporous silicas by comparing with bare silicas. The gas absorption capability of the mesoporous silica absorbent show the highest performance of 4.08 mol CO_2/kg

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A solvent-free Diels-Alder reaction of graphite into functionalized graphene nanosheets

서정민 백종범[1,*]

울산과학기술대학교(UNIST) 에너지 및 화학공학부 [1]울산과학기술대학교(UNIST) 에너지공학부

A solvent-free Diels-Alder reaction was carried out by heating a mixture of graphite and a typical dienophile, maleic anhydride (MA) or maleimide (MI), in a sealed glass ampoule of argon. The functionalization of graphite with dienophiles was confirmed by various characterization techniques, suggesting the efficient functionalization and delamination of graphite into a few layers of graphiticnanosheets.

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Simple Preparation of Pd-NPs/Polythiophene Nanosphere Catalyst for Suzuki-Miyaura Coupling Reaction

배상은 김기정 허성*

한국외국어대학교 화학과

We developed a very simple preparation method of Pd-NPs decorated polythiophene nanospheres in an aqueous solution at room temperature. 2-Thiophenemethanol underwent polymerization to form polythiophene nanospheres in the presence of PdCl42- which was simultaneously reduced to Pd-NPs. There is no need for extra reducing agent and surface capping organic materials for the production of sub-10 nm Pd-NPs. Pd-NPs uniformly cover the polythiophene nanospheres whose dimension is about 100 nm. The Pd-NPs/polythiophene nanospheres were characterized by various methods such as scanning transmission electron microscopy (STEM) and scanning electron microscopy (SEM). The metallic face-centered cubic phase of Pd(0) was confirmed by powder X-ray diffraction (PXRD). The weight percentage of Pd species in Pd-NPs/polythiophene nanospheres was determined by inductively-coupled plasma atomic emission spectroscopy (ICP-AES). The Pd-NPs/polythiophene nanospheres were found to be an excellent catalyst for Suzuki-Miyaura coupling reaction for various substrates under mild reaction conditions.

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FeOF/Carbon Nanotube (CNT) Nanocomposites as a Cathode Material for Lithium-Ion Batteries

송희진 김종식*

동아대학교 화학과

Lithium-ion batteries (LIBs) are widely used as the most effective energy storage systems. However, the major challenges in the LIBs for wide applications are attributed to safety, toxicity, high cost, and limited specific capacities. Therefore, alternative cathode materials need to be developed to solve these problems. Iron oxyfluoride (FeOF) is considered to be one of the most promising candidates for the cathode material because of its abundance, low cost, low toxicity, and high theoretical specific capacities (about 590 mAh g^{-1} at 1.5-4.5 V and 295 mAh g^{-1} at 2.0-4.0 V, respectiviely). However, FeOF has low electroconductivity, poor capacity retention, and slow diffusion of lithium ions. In this study, FeOF/carbon nanotube (CNT) nanocomposites are fabricated by controlling the amount of about 10, 20, and 30 wt% of the CNT in the precursor solution ($FeSiF_6·6H_2O$). CNT is used to improve electroconductivity and alleviate drastic volume variation of FeOF during cycling due to its one-dimensional network structure. The oxygen containing functional groups of CNT act as nucleation sites of the FeOF precursor. FeOF synthesized by oxidation of $FeSiF_6·6H_2O$ on the CNT has fast electron transport and structural stability during charge-discharge cycles. The FeOF/CNT nanocomposites show improved cycling performances in the voltage ranges of 1.5-4.5 V and 2.0-4.0 V at a rate of 0.1 C, compared to bulk FeOF.

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Surface charge-dependent toxicity of gold nanoparticles

전현진 권영은* 이의연* 송남웅[1],*

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Biomedical applications of gold nanoparticles (AuNPs) are largely expanding nowadays due to their unique electronic and optical properties. AuNPs are often modified with various ligands in order to increase colloidal stability and to provide novel functions. While many applications require these modified AuNPs to come in contact with biological systems, little is known about their biocompatibility and biosafety. For this reason, we investigated how the modified AuNPs affect biological systems. We are especially interested in how surface charge and functional groups affect in vitro cytotoxicity of AuNPs. Various organic and peptide ligands were prepared and used to control the surface charge via place exchange reaction. The surface-modified AuNPs were characterized by dynamic light scattering (DLS), zeta potential measurement, and UV-Vis spectroscopy and used for live-dead assays and various functional assays. This work shows that the cytotoxic effect of surface-modified AuNPs are mainly influenced by the charge of the surface but also by the functional groups introduced. Generator of well-characterized, stable, and low toxic AuNPs will enable safer usage of AuNPs for biomedical applications.

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Light-triggered drug release from a gold nanorod contained composite membrane

조민철 김기범[1] LOGANATHANPALANIKUMAR[2] 박명환[*] 유자형[3,*]

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The development of a novel drug-delivery system with the ability to respond to a given stimulus has attracted much attention due to their enhanced therapeutic efficacy. We have developed the versatile delivery system using the dendrimer-gold nanorod composite membrane able to give a response to near-infrared (NIR) irradiation. The membrane was fabricated through dithiocarbamate (DTC) cross-linking of polyamidoamine (PAMAM) dendrimers to gold nanorods. The photothermal effect of a gold nanorod by NIR irradiation leads to rapid increase in temperature around the composite membrane, accelerating the release of drugs through the membrane. Scanning electron microscopy (SEM) was used to analyze surface morphology of the fabricated membrane and quantitative release of drugs by NIR irradiation was measured by UV-vis spectroscopy or fluorescence spectroscopy.

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A Novel Alkoxy naphthalene and Quarterthiophene copolymers for OTFTs

김형남 김윤희* 김란 안은수 **LIU XIANQING**

경상대학교 화학과

A quarterthiophene and Alkoxy naphthalene copolymers were synthesized by a Suzuki coupling reaction. The copolymers showed good solubility in common solvents such as chloroform and toluene, etc. It's optical, thermal and electrochemical properties and organic thin film transistor characteristics were characterized. The structure confirmed using 1H NMR, FT-IR spectroscopy. The weight average Mw of PQTHN and PQTON were found to be 9200 with polydispersity of 1.2 and 30600 with that of 2.39, respectively. Solution processed OTFTs using PQTON exhibited 6.96 x 10^{-4} cm^2 V^{-1} s^{-1} as mobility with an on/off ratio of 2.46 x 10^4

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Preparation and characterization of covalently cross-linked SPEEK/Cs-MoSiA/CeO2 composite membranes for water electrolysis

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Covalently cross-linked SPEEK/Cs-MoSiA/Ceria (SPEEK: sulfonated poly ether ether ketone) composite membrane was prepared for the polymer electrolyte membrane in water electrolysis. Cs-MoSiA (Molybdosilicic acid substituted with Cs) was added to the SPEEK to enhance proton conductivity. CeO2 was used to scavenge free radicals which were generated from operation in water electrolysis and to improve the durability of the membrane. The composite membrane featured the electrochemical properties such as 0.104S/cm of proton conductivity at 25℃, and over 1000 hours of oxidative durability in Fenton test.

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TPD-Based Copolymers with Strong Interchain Aggregation and High Hole Mobility for Efficient Bulk Heterojunction Solar Cells

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경상대학교 화학과

A?D?A type conjugated polymer, PTPD-TVT, containing thienopyrroledione and thiophene?vinylene?thiophene(TVT) units was synthesized as an electron donor for organic photovoltaic devices. It has a small bandgap ,excellent coplanarity and high hole mobility. To enhance the interchain interactions between the polymerchains, selenophene?vinylene?selenophene (SVS) unit was introduced. Devices made from PTPD-TVT and PTPD-SVS have rather promising power conversion efficiencies (PCEs) of 4.87 and 5.74%, respectively. The higher PCE value for solar cells based on PTPD-SVS was attributed to an enhanced carrier mobility resulting from stronger interchain aggregation in the BHJ active layer. These results show that the incorporation of a vinylene unit in TPD-based polymers is an effective way to reduce the bandgap and thereby improve charge transport for efficient photovoltaic devices.

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Portable Sponge/Polymer Brush Composites for Environmental Remediation

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Due to advancement of industrial development, heavy metal ions in waste water are daily flowing into ground surface and water resources. Cases of serious side effects have been reported since they are accumulated in the human body along the food chain. Because of effectiveness of adsorption process, numerous adsorbents have been proposed for efficient removal of heavy metal ions or organic pollutants in waste water. However, previously reported adsorbents and adsorption process are not suitable for small scale enterprise and individual user. Development of a portable heavy metal ion remover which can be used even by untrained user is highly demanded. Sponge is portable, easy to use, and ubiquitous materials. Polymer brushes possess advantages of numerous reaction sites and pH-responsive behaviors for control of adsorption/desorption. Thus, highly porous sponge composites decorated with polymer brushes was developed for fast and efficient removal of heavy metal ions or organic pollutants in waste water or drinkable water.

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Fabrication of Polyurethane Sponge Composites for Selective Oil Absorption from Oil/Water Mixture

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With the Increasing industrial oily wastewater and the frequent oil spill accidents, selective removal of waste oils from oil/water mixture continues to be the hot issue of research. Various materials such as sponges, metal meshes, and fabrics have been used for oil/water separation. Although considerable efforts have been focused on fabricating sponge composites for oil/water separation, development of novel approaches to enhance the performance is still necessary. In this respect, polyurethane (PU) sponge was used as templates and coated with carbon nanotube (CNT), polydopamine (PDA), and hydrophobic CaCO3 in order for fabricating sponge composites. These stepwise coating led to the increase in specific surface areas and flame retardant property of the PU sponge composites. Our sponge composites possessing flame retardant property were successfully used for application in selective oil absorption from oil/water mixture.

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Visible Light-Driven Photocatalyst/Cu Mesh Composites for Oil/Water Separation and Pollutant Purification

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Superhydrophobic surfaces were fabricated on Cu mesh templates by controlled oxidation method and subsequent chemical modification with low surface energy materials. Initial chemical etching of the Cu substrates resulted in the formation of micro-pit structures which contribute to a significant increase in trapped air in the nanostructures. Various types of surface morphologies such as needle-like, hairy-like, basket-like, and needle-pine-like structures were formed on Cu mesh surfaces by varying the experimental conditions. To endow visible-light driven photocatalytic function, polymer/Ag/AgX layers were subsequently developed on Cu/CuO mesh. A combination of the filter layer (Cu/CuO mesh) and the photocatalyst layer (Cu/CuO/polymer/Ag/AgX mesh) was demonstrated to be used for oil/water separation and pollutant purification.

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Control over pore size distribution of halloysite nanotube by systematic variation of pH

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The halloysite is well known for its many applications as nanoreactors or nanotemplates, catalysts, and capillaries. It becomes important to control the effective lumen size or diameter of the halloysite. The simplest method to control the size of the halloysite is to change the pH of the system, because the functional groups of the external or internal surface of the halloysite can readily be affected by changing the pH. In the present work, we have modified the external surface from silanols to carboxylic acids. Untreated halloysite showed good dispersibility only at basic condition, but carboxylate-modified halloysite dispersed well at both acidic and basic conditions. These results are confirmed by dynamic light scattering (DLS), Fourier-transform infrared spectroscopy (FT-IR), and scanning electron microscopy (SEM).

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New efficient fused-ring spiro[benzoanthracene-fluorene] dopant materials for blue fluorescent organic light-emitting diodes

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New blue fluorescent spirobenzoanthracene-type dopant materials, 3,9-di(di-p-tolyl)aminospiro[benzo[de]anthracene-7,9'-fluorene] (DTSBAF) and 3,9-di(di-4-biphenyl)aminospiro[benzo[de]anthracene-7,9'-fluorene] (DBSBAF) were designed and successfully prepared by an amination reaction of 3-bromo-9-chlorospiro[benzo[de] anthracene-7,9'-fluorene] with di(p-tolyl)amine and di(4-biphenyl)amine, respectively. The EL characteristics of 1,10-dinaphthylspiro[benzo[ij]tetraphene-7,9'-fluorene] (DNSBTF) as the blue host material doped with the above blue dopant materials was evaluated. The electroluminescence spectra of indium tin oxide (150 nm)/N,N'-diphenyl-N,N'-bis[4-(phenyl-m-tolyl-amino)phenyl]-biphenyl-4,4'-diamine (DNTPD, 60 nm)/N,N,N',N'-tetra(1-biphenyl)-biphenyl-4,4'-diamine (TBB, 30 nm)/SBTF hosts: SBAF dopant (30 nm, 5%)/9,10-di(naphthalene-2-yl)anthracen-2-yl-(4,1-phenylene)(1-phenyl-1H-benzo[d]imidazole) (LG201, 20 nm)/LiF (1 nm)/Al (200 nm) with DNSBTF as a host material show a blue emission band with a full width at half maximum of 50 nm and a λmax = 472 nm. The device obtained from DNSBTF doped with DTSBAF showed a good color purity (0.141, 0.254), high luminance efficiency (10.12 cdA-1 at 5 V) and high external quantum efficiency (6.02%). Abstract text goes here. The abstract should be a single paragraph that summarises the content of the article.

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New All Fused Ring Spiro Blue Host and Dopant System: Application in Sky-Blue Fluorescent Organic light-emitting materials

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Highly efficient sky blue organic light emitting devices (OLEDs) have been fabricated with a spirobenzo[c]fluorene-7,9'-fluorene]-core based fluorescent dopant (D3) and fused ring spiro host materials, 1,10-di(2-naphthyl)spiro[benzo[ij]tetraphene-7,9'-fluorene] (H1) and 1-[1-(4-biphenyl)]-10-phenylspiro[benzo[ij]tetraphene-7,9'-fluorene] (H2). Typical blue fluorescent OLEDS with the configuration of ITO/N,N’-diphenyl-N,N’-bis[4-(phenyl-m-tolyl-amino)phenyl]-biphenyl-4,4’-diamine (DNTPD)/N,N,N’,N’-tetra(1-biphenyl)-biphenyl-4,4’-diamine (TBB)/SBTF hosts: D3/9,10-di(naphthalene-2-yl)anthracen-2-yl-(4,1-phenylene)(1-phenyl-1H-benzo[d]imidazole) (LG201)/LiF/Al was investigated. The device using H1: 5%D3 showed an electroluminescence emission at 472 nm and an efficiency of 6.91 cd/A and an external quantum efficiency of 4.56% at 107.84 mA/cm2 with a sky blue CIEx,y coordinates of (0.150, 0.217) at 7447 cd/m2.

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The Development of Hollow Nanostructure with Exfoliated Ruthenium Oxides and Titanium oxide for the Energy Storage Applications

장수진 백승민*

경북대학교 화학과

Hollow spheres with high surface area are advantageous for achieving high capacity and coulombic efficiency due to the short diffusion length of lithium cations in the energy storage applications. Also, the transition metal oxides such as ruthenium oxides with high conductivity could have better energy storage properties as anodes in rechargeable lithium-ion batteries, in comparison with those of carbon-based materials. Titanium dioxides have high capacity, low-voltage and low production cost. And ruthenium dioxides have high electrical conductivity, excellent chemical and electrochemical property. In this study, we are successfully synthesized heterostructured hollow sphere composed of exfoliated titanate and ruthenate. According to the transmission electron microscope analysis coupled with energy dispersive X-ray spectroscopy, alternate layers of titanate and ruthenate were shown. The charge/discharge capacity of hollow nanostructure was significantly larger than those of layered titanate, showing the synergistic effect of hybridization.

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Silver loading on poly(ethylene terephthalate) fabrics using silver carbamate via thermal reduction, and their properties

곽완규 공명선*

단국대학교 나노바이오의과학과

Silver-coated poly(ethylene terephthalate) (PET) fabrics were prepared though the deposition of silver nanoparticles (AgNPs) generated from thermal reduction of silver 2-ethylhexylcarbamate. The PET fabrics modified with 3- mercaptopropyltriethoxysilane, which acts as an anchor for the Ag-NPs, were paddedwith a solution of silver 2-ethylhexylcarbamate in methanol, and were then reduced for in situ generation of Ag-NPs only by heating at 130 °C. The PET/Ag fabrics were characterized via scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive X-ray (EDX), X-ray photoelectron spectroscopy (XPS), water contact angle analysis, and by measuring the electrical conductivity and antibacterial activity. A continuous layer of Ag-NPs with a size between 30 to 100 nm was assembled on the PET fabrics. The PET/Ag imparts high conductivity to the textiles with an electric resistance as low as 3.44 ± 0.12 Ω, and the antibacterial effects of the treated PET fabric against Escherichia coli O157:H7 (ATCC 43889) and Staphylococcus aureus (ATCC 25923) were examined and were found to be excellent.

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Fluorous Solvent-Soluble Materials for Photolithography containing Anthracene Moieties

손종찬 김영태 이진규*

인하대학교 고분자공학과

Conventional patterning ways for inorganic electronic devices is photolithography using organic solvents for coating, develop, strip. Differing from Inorganic ones, Organic devices can’t use organic solvents because of desorption on organic components beneath photoresist film. Furthermore, debris following decomposition reaction by UV irradiation to photoresist and photo acid generator can be threat causing deterioration of devices’ performance. In order to resolve these problems, we designed a highly fluorinated photoresist polymer [copolymerization of 6-(anthracene-9-yl)hexyl methacrylate (AHMA) and semi-perfluorodecyl methacrylate (FDMA)] taking advantage of orthogonal patterning. Through merits of orthogonal process that minimizes chemical interaction between fluorous solvents and organic devices and photo-dimerization without photo acid generater, we examined photolithography on organic electronic devices. Synthesis of P(AHMA-FDMA) by random radical polymerization and Lithographic evaluation was reported. Finally, P(FDMA-AHMA) and fluorous solvents were applied to the photolithographic patterning of OLED pixels.

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Solution processable highly fluorinated dielectric hybrid nanocomposites for dielectric layer

김영태 손종찬 이진균*

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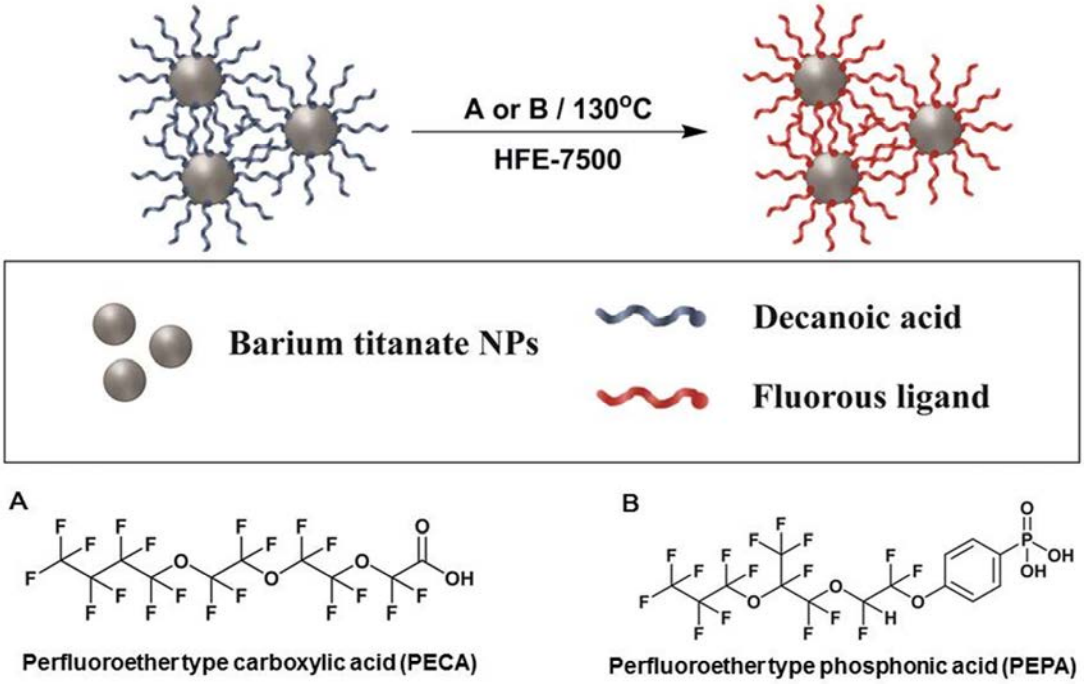
다양한 전자소자의 발전은 유기물을 이용한 대면적화, 유연화와 함께 비용절감에 대해 초점이 맞춰지는 듯하다. 이에 대한 여러가지 시도가 이루어지고 있으며, 설비가 비교적 간단하며 저온 조건에서 진행할 수 있는 solution process 가 적합한 방법 중 하나로 뽑히고 있다. 여러 전자소자 중 OTFT(Organic thin-film transistor) 제작에 관하여 solution process 를 활용하고 있으며, 특히 절연층(dielectric layer)에 사용되는 dielectric materials 에 대해서도 solution process 가 가능하도록 다양한 연구가 시도되고 있다. 유기물을 이용한 dielectric materials 는 낮은 dielectric constants 를 갖는 단점이 있으며, 무기물을 이용한 dielectric materials 는 용액공정에 대한 어려움이 존재한다. 이런 단점들을 보완하기 위해 Inorganic oxide 와 같은 무기물의 표면에 TOPO(Trioctylphosphine oxide)나 Oleic acid 와 같은 유기물을 ligand 로 도입한 유·무기 hybrid nanocomposites 에 대한 연구가 진행되고 있다. 하지만 이러한 nanocomposites 의 경우 일반적인 유기용제를 사용하여 박막을 제작하기 때문에, 상·하부의 유기층에 대한 손상을 일으켜 소자의 성능을 저하시킬 수 있다. 우리는 이를 해결하고자 유기물질과 화학적으로 상용성이 없어 상·하부의 유기층에 대한 손상을 일으키지 않는 불소계 용제를 이용한 용액공정에 대한 연구를 진행하였다. 높은 dielectric constant 를 갖는 수 nm 크기의 $BaTiO_3$ 입자표면에 유기물 ligand 대신 고불소계 ligand 를 결합하여 불소계 용제에 분산이 가능한 고불소계 dielectric nanocomposites 을 합성하였다. Decanoic acid 에 의해 안정화된 $BaTiO_3$ 를 합성한 후 리간드 치환을 진행하여 입자 표면에 두 가지 형태의 고불소계 ligands 를 도입하였으며, 불소계 용제에 우수하게 분산할 수 있었다. 또한 분산시킨 용액은 spin coating 을 이용하여 우수한 유전상수를 갖는 소자로 제작할 수 있었다.


A or B / 130^{o}C
HFE-7500
Barium titanate NPs
Decanoic acid
Fluorous ligand
A
Perfluoroethertype carboxylic acid (PECA)
B
Perfluoroethertype phosphonic acid (PEPA)

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Carbazole-Triazine Derivatives for Efficient Thermally Activated Delayed Fluorescence(TADF) materials

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A carbazole-triazine derivatives were used as dopant materials for the preparation of highly external quantum efficiency blue organic light emitting diodes based on the themally activatied delayed fluorescence. The sky blue emitting compounds 9-(2-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-carbazole (Cz-Trz), 9-(2-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-3,6-dimethyl-carbazole(MCz-Trz) and 3,6-di-tert-butyl-9-(2-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-carbazole(tBCz-Trz) were successfully synthesized. A sky blue device consisting of PEDOT(60nm)/TAPC(20nm)/mCP(10nm)/mCP:Dopant(25nm)/TSPO1(5nm)/TPBi(30nm)/LiF(1nm)/Al(200nm) was used. The EL emissions of the devices are observed at 470nm(Cz-Trz), 484nm(MCz-Trz), 480nm(BCz-Trz), respectively. In optimized structure, the best performance of MCz-Trz based blue emitting devices exhibits a current efficiency of 30.9 cd/A and external quantum efficiency of 14.7% at 100 cd/m2.

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Silk / polyurethane Fiber 제조 및 특성 조사

홍석민 공명선[1,*]

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

천연고분자는 독성이 없는 생분해성, 생체적합성이 좋은 제품을 개발하고 이에 따라 손상되고 병든 장기를 조직재생공학 방법으로 개발하여 대체 하고 있습니다. 이에 최근에는 천연고분자, 실크 피브로인(SF), 과 같이 두 개 이상의 분해 가능한 물질을 합성하여 좀 더 생체에 적합한 인공장기를 만들어 사용하고 있습니다. 본 연구에서는 폴리우레탄의 인장력이 좋은 장점과 실크피브로인(SF)의 견고성 그리고 두 물질의 공통적인 특징으로 생체적합성, 생분해성, 무독성, 우수한 기계적 특성을 이용하여 합성 하였다.폴리우레탄을 합성하기 위하여 약산에 강하고 독성이없는 polyalkylene carbonate diol(PCD)과 생분해성 역할을 하는 Dianhydro-D-glucitol (Isosorbide)과 Hexamethylene diisocyanate(HDI)를 축합중합하여 PU(PCD : Isosorbide : HDI / 2 : 8 : 10)을 합성하였다.실크는 불용성 피브로인과 수용성 세리신으로 구성되어있는데 세리신은 약 알칼리성 용액으로 처리하면 제거되고 피브로인만 남는다. 실크 수용액을 만들기 위해서는 염화칼슘과 에탄올을 사용하여 용해한 뒤 투석하고 동결건조 한 후에 원하는 수용성 실크를 얻을 수 있다. 본 연구에서는 합성을 확인하기 위해서 FT-IR 을 사용하였고 열적특성을 확인하기 위해서 TGA 및 DSC 를 사용하여 측정하였다. 인장강도 및 인장률을 특성을 확인하기 위해 Instron universal testing machine 을 측정하였다. 전기방사실험을 통해서 나노파이버의 표면과 두께를 SEM 을 통해 측정하였다. 접촉각을 측정하기 위하여 Contact angle 을 측정하였다. 인체 내에서 분해 정도를 확인하기 위해서 생 분해성 실험을 해보았다.

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Si-WS_2 hybrid as advanced anode material for lithium ion Batteries

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It is well known that Si accommodates lithium up to 4.4 Li^+ atoms per Si atom, which is equal to a capacity of 4000mAh/g. However, Expansion and contraction is occurred while the charge and discharge process, and it lead to pulverization. As a result, Capacity fades rapidly.To overcome this problem, Si-WS_2 hybrid material was fabricated by exfoliation and reassembling reaction. The X-ray diffraction analysis showed that Si particles were successfully attached onto the surface of WS2 nano layer. The electrochemical performance of the obtained hybrid material was examined by the charge and discharge process. Compared to the specific capacity of the pure Si particles, Si-WS_2 hybrid material exhibited much higher Capacity.

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Enhanced photocatalytic activity of titanium oxide via electron beam irradiation

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Titanium dioxides have highly attracted research interests because of their exceptional applications especially photocatalytic hydrogen evolution reaction. In this study, we tried to increase photocatalytic activities of titanium dioxide via soft chemical method including electron beam irradiation. According to UV-vis diffuse reflectance spectra, the subband was formed in electron beam irradiated titanates, which led to the enhanced photocatalytic activities in hydrogen evolution reaction. The energy dispersive X-ray spectroscopy showed that the nitrogen and chlorine atoms were included in electron beam irradiated titanates. And the X-ray photoelectron spectroscopy indicated that the nitrogen and chlorine atoms exist in lattice of electron beam irradiated titanates. This synthetic methodology could be the fabrication of new photocatalysts with enhanced activities.

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Crystal Structure and Electrochemical Properties of New Li-containing Phosphate Compounds

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아주대학교 에너지시스템학부

New lithium-containing phosphates, $\mathrm{LiMg_3(PO_4)P_2O_7}$ and $\mathrm{Li_2Sr_2Al(PO_4)_3}$ were prepared by a solid-state reaction, and their structure were characterized by an *ab-initio* structure determination method on the basis of X-ray diffraction data. $\mathrm{LiMg_3(PO_4)P_2O_7}$ was found to be orthorhombic (space group *Pnma*) with lattice parameters a = 9.0387(1) Å, b = 10.6072(1) Å, c = 8.3065(1) Å, and V = 796.39(1) $\mathrm{Å^3}$. The structure features infinite $[\mathrm{Mg_3O_{10}}]_\infty$ layers that are parallel to the *bc* plane and that are interconnected along the *a* axis by $\mathrm{PO_4}$ and $\mathrm{P_2O_7}$ groups. This gives rise to a three-dimensional framework that contains large tunnels along the directions [100] and [010]; the Li ions are stabilized in these tunnels. $\mathrm{Li_2Sr_2Al(PO_4)_3}$ crystallizes in the monoclinic space group *P21/n* with Z = 4 in a cell of dimensions, a = 4.945(1) Å, b = 22.088(3) Å, c = 8.632(2) Å, and β = 91.47(1)°, V = 942.5(3) $\mathrm{Å^3}$. The structure can be described as an alternation of two types of sheets denoted as $_{\infty}^{2}[\mathrm{LiAl(PO_4)_2}]_2$ and $_{\infty}^{2}[\mathrm{LiSr_2PO_4}]^{2+}$.The measurements of impedance allowed us to determine bulk ionic conductivity in the various temperature range. Temperature dependency of the bulk ionic conductivity shows Arrhenius behavior. The highest conductivities of $\mathrm{LiMg_3(PO_4)P_2O_7}$ and $\mathrm{Li_2Sr_2Al(PO_4)_3}$ were found to be $\sigma = 3.40 \times 10^{-5}$ S/cm at 769 K and 1.30×10^{-4} S/cm at 667 K with activation energy $E_a = 1.17$ eV and 1.02 eV, respectively.

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Ionic conductivity of Zinc-doped perovskite-type strontium aluminates, $Sr_3(Al_{2-X}Zn_X)O_{6-0.5X}$

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Oxide ion conducting solids are needed to reduce the operating temperature of solid-oxide fuel cells. Oxide mobility in solids is associated with defects. Doping is the most effective method for improving the defect concentration of compound. The structure of $Sr_3Al_2O_6$ can be related to that of the perovskites, ABO_3. The formula should be rewritten as $Sr_{7/8}\square_{1/8}(Sr_{1/4}Al_{3/4})O_{9/4}\square_{3/4}$. The oxygen vacancies are ordered in such a way that all the Sr(B) atoms are coordinated to 6 oxygens, keeping the octahedral coordination characteristic of the perovskite structure, whereas all the AI atoms are coordinated to 4 oxygens. In this study, Oxygen defect-induced samples of the perovskite-type $Sr_3(Al_{2-X}Zn_X)O_{6-0.5X}$ (X = 0 to 0.3) compound were prepared by pechini sol-gel method. The lattice parameters exhibit linear dilation with increasing zinc contents. Ionic conductivities have been investigated for zinc-doped perovskite-type strontium aluminates of the $Sr_3(Al_{2-X}Zn_X)O_{6-0.5X}$ (X = 0 to 0.3) series. The conductivity at 900 °C was estimated to be 1.45×10^{-5} S cm^{-1} for $Sr_3(Al_{1.8}Zn_{0.2})O_{5.9}$.

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Structure and Ionic Conductivity of $Na_2SrSi_2O_6$ and $Na_2CaSi_2O_6$

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아주대학교 에너지시스템학부

Sodium ion electrolytes, $Na_2SrSi_2O_6$ and $Na_2CaSi_2O_6$ have been synthesized by conventional solid state reaction at various temperature (800-950℃). The crystal structure of $Na_2SrSi_2O_6$ and $Na_2CaSi_2O_6$were characterized by X-ray diffraction. Rietveld refinements were performed with the FULLPROF package. The compound crystallizes hexagonal crystal symmetry with space group *R*-3*m*. The structure of $Na_2SrSi_2O_6$ belongs to the group of cyclosilicates and is isotypic with $Na_2CaSi_2O_6$. The structure has a six-membered ring of SiO_4 tetrahedra. Linkage between the rings is provided by four symmetrically independent M-sites occupied by sodium/alkaline earth atoms (Sr, Ca). The alkali and alkaline earth atoms are coordinated by six to nine oxygen ligands. Alternatively, the structure can be described as a defect ABO_3 perovskite with 12.5% vacancies in the A-substructure and 25% oxygen vacancies. The ionic conductivity of $Na_2SrSi_2O_6$ and $Na_2CaSi_2O_6$was measured in the frequeny range of 2MHz ~ 1Hz with temperature ranges between 40℃ and 300℃.

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Synthesis of New Alternating Copolymer for Organic Solar Cell

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경상대학교 화학과 [1]경상대학교 그린에너지융합연구소

We have synthesized a new conjugated polymer, according to the weak donor/strong acceptor strategy and investigated its optical and electrochemical properties. The weak donor is alkanoyloxy-substituted benzodithiophene (BDT) and the strong acceptor is benzothiadiazole (BT). The CO-BDT-DTBT polymer was found to have a deep HOMO energy level (-5.62 eV), which produces an impressive open circuit voltage in a BHJ polymer solar cell. This copolymer was used as an electron donor in combination with the fullerene derivative (PC71BM) as an electron acceptor for the fabrication of BHJ polymer solar cells. Our preliminary CO-BDT-DTBT:PC71BM solar cells were found to exhibit a PCE of 1.46% with a high VOC of 0.89V, a moderate JSC of 3.6 mA/cm2 , and FF of 31.6%. The PCE was then further improved to 1.53% by processing the CO-BDT-DTBT:PC71BM blends in the presence of 3 vol% of the additive DIO. This increase in the PCE is attributed to the enhanced JSC value that results from improved light conversion properties and the improved crystallinity of the copolymer phase. These results show that the new copolymer is a useful material for organic photovoltaic applications.

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A Novel Strategy for Maintenance of Catalytic Activity by Using Wrinkled Silica Nanoparticle (WSN) Support for FT-Synthesis

정동욱 이연* 이진규*

서울대학교 화학부

Recently, Fischer-Tropsch (FT) synthesis has been receiving much attention again for the conversion of natural gas, coal, and biomass-derived synthesis gas into liquid, due to the increasing crude oil price and the demand for clean fuels. Cobalt catalysts immobilized on the porous solid support are preferred for the FT synthesis because of their high productivity, high selectivity for linear long chain hydrocarbons, and also low activity in the water-gas shift reaction. However, catalyst deactivation, the decrease of catalytic activity and selectivity over time, is a problem faced in industries. Sintering which is one of the deactivation factors can be induced by the harsh temperature and pressure conditions of the FT synthesis and leads to a loss in the active surface area of catalysts through aggregation of cobalt particles. Consequently, the sintering process can reduce catalytic properties such as activity and life time and preventing Co particles from agglomeration during FT synthesis is important to industry. Herein, we synthesized cobalt catalysts supported on the hierarchical mesoporous silica nanoparticles with a wrinkle structure (WSNs), WSN-Co, for the FT synthesis. The wrinkle structure can isolate adjacent Co catalysts from each other and prevent them from sintering. Therefore, WSN-Co can maintain initial catalytic activity and increase life time of catalyst.

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The Partial Cation Exchange of Djurleite to Wurtzite $CuInS_2$ through Incorporation of Indium

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아주대학교 분자과학기술학과 [1]아주대학교 응용생명화학공학부

The bulk material of wurtzite copper indium sulfide(wz-$CuInS_2$) is metastable phase at room temperature, but it is stable phase at high-temperature(1045-1090℃). Until now only a few studies have shown that nanocrystal-sized wz-$CuInS_2$ is stable at ambient condition. This study is to fabricate stable wz-$CuInS_2$ by cation exchange(CE) method. The CE method has become an emerging technique recently. Especially, this is useful tool for synthesis of nano-sized materials. The CE method has the advantages to conduct at low temperature and enable metastable structure to be synthesized. This study shows that djurleite is transformated to wz-$CuInS_2$, alloyed material. The transformation to wz-$CuInS_2$ was proved by X-ray diffraction analysis(XRD), transmission electron microscopy(TEM), elemental analysis, optical measurement. So we confirmed incorporation of In^{3+} into djurleite($Cu_{1.94}S$). The synthetic product showed remarkable optical properties. It is thought that this synthesized nanocrystal can be used as potential material for solar cell.

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Nanoporous cobalt oxides for efficient oxygen evolution catalysts

박세흠

한국과학기술연구원(KIST) 연료전지센터

We report a synthesis of nanporous cobalt oxide catalyst for oxygen evolution reaction (OER). Compared to as-prepared cobalt catalyst, a novel nanoporous cobalt catalyst with annealing process shows higher activity and stability in alkaline media. The crystal structure, morphology, and electronic state of catalyst were characterized by XRD, TEM, XPS and XAFS data. In addition, the electrochemical data were obtained with cyclic voltammetry (CV) and OER. The enhanced performance could be attributed to the difference in electronic state of as-prepared and annealed catalyst. This newly synthesized nanoporous cobalt catalyst is expected to contribute in fuel cell field with high OER activity and durability.

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H_2O_2 Sensing using Peroxy Lucifer 1 Conjugated Nanoparticle

백경내 김형섭 박명환*

삼육대학교 화학과

Reactive oxygen species(ROS) generated by normal metabolism of oxygen have important roles in cell signaling and homeostasis. Because the excess of ROS can be a cause of many diseases such as Alzheimer, Asthma, Heart diseases, damaging of immune system and cancer, real time detection of ROS is very important. A excess hydrogen peroxide(H_2O_2) that is one of the ROS can cause oxidative stress resulting in many diseases. In this study, we have synthesized the H_2O_2-sensitive fluorophore conjugated poly(urethane acrylatenonionmer)(PUAN) nanoparticles. H_2O_2 levels will be quantitatively estimated by ratiometric fluorescence intensity using our H_2O_2-sensitive nanoparticles.

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Synthesis and Crystal Structure of the New Mixed Metals Quaternary Selenogermanate, $Cs_{1.57}(Fe_{1-x}Ge_{1+x})Ge_2Se_8$. (x=0.23)

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The new mixed metals quaternary selenogermanate, $Cs_{1.57}(Fe_{1-x}Ge_{1+x})Ge_2Se_8$(x=0.23), has been synthesized by using reactive alkali metal halide fluxes and structurally characterized by single crystal X-ray diffraction techniques. The title compound is closely related with the well known stoichiometric phase $Cs_2FeGe_3Se_8$. It crystallizes in the space group *C2/m* with a formula unit in cell dimensions, a=13.9013(7) Å, b=7.5716(4) Å, c=16.4574(8) Å, β=109.438(2)°, and V=1633.49(9) $Å^3$. In the crystal structure of the title compound, both Fe and Ge atom are surrounded by four Se atoms in the tetrahedral fashion. These polyhedra are combined to from the two-dimensional anionic layers, $_{\infty}^{2}[(Fe_{1-x}Ge_{1+x})Ge_2Se_8{}^{1.57-}]$, and alkali metal cations, Cs^+ staying in the van der Waals space between the layers through electrostatic interactions. The classical charge valence can be described as $[Cs^+]_{1.57}([Fe^{2+}]_{1-x}[Ge^{4+}]_{1+x})[Ge^{4+}]_2[Se^{2-}]_8$.

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A New Layered Mixed-metallic Thiophosphate, $Ag_{0.89}(Ta_x/Zr_{1-x})PS_6$ (x=0.14)

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In the middle of searching for new soluble inorganic polymers using the reactive halide-flux technique, a new mixed-metallic thiophosphate, $Ag_{0.89}(Ta_x/Zr_{1-x})PS_6$, has been found and the crystal structure has been determined by single crystal X-ray techniques. $Ag_{0.89}(Ta_x/Zr_{1-x})PS_6$ is composed of the one-dimensional chain, $^{1}\infty[MPS_6]^{-}$. This chain is constructed with dodecahedral MS_8 and tetrahedral PS_4 units by sharing common sulfur atoms. MS_8 units are linked by sharing three S atoms and PS_4 unit is bridging these MS_8 units. The chains are linked one another by Ag^+ ions to build a two-dimensional double layers. These layers stack on top of each other with van der Waals gaps. The classical charge valence of the compounds should be described as $[Ag^+]_{0.89}[Ta^{5+}]_x[Zr^{4+}]_{1-x}[P^{5+}][S_2^{2-}][S^{2-}]_4$.

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Stabilization of the New Chromium Thiophosphate Ion, $Cr_2P_2S_{12}^{4-}$ via Hybrid Solid-Solution Synthetic Routes

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A new quaternary thiophosphate, Cs_2CrPS_6 has been synthesized with alkali metal halide flux. The compound contains the binuclear $[Cr_2P_2S_{12}]^{4-}$ cluster which are well separated from each other by Cs^+ cations. The anionic cluster is composed of pair of edge-sharing Cr-centered octahedra and two P-centered tetrahedra. The cluster anion, $[Cr_2P_2S_{12}]^{4-}$ is stabilized through the electrostatic interactions with the alkali metal cation, Cs^+. In order to isolate the anionic species, Cs_2CrPS_6 has been dissolved in the polar solvents. The Cs_2CrPS_6 crystals rapidly dissolved in NMF and $(PPh_4)^+Cl^-$ has been added. Green needle-shaped crystals were obtained at room temperature and the crystal structure has been determined by single-crystal X-ray diffraction techniques. The compound is proved to be $(PPh_4)_2Cr_2P_2S_{12}(C_2H_4N)_2(H_2O)_2$. In this compound, half of the Cs^+ cations has been replaced with $(PPh_4)^+$ cations. The compound is made up of a zero-dimentional $[Cr_2P_2S_{12}(C_2H_4N)_2]^{2-}$ anionic clusters, separated by $(PPh_4)^+$ cations and water molecules. We propose that these anionic organic-inorganic hybrid clusters are stabilized through the electrostatic interactions with the organic counter cation, $(PPh_4)^+$

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Synthesis of Electromagnetic absorbing film using iron oxide/GO hybrid particle

정병문

재료연구소 복합재료연구본부

Graphene have attracted considerable attention in recent years because of their unique physical properties. Graphene have potential for plate type template. However, graphene have poor dispersion property due to chemically inert nature and pi-pi interaction of sp2 carbons. Graphene oxide (GO) is common candidate for functional applications due to their abundant chemical linker and good solubility to water. Recently, metal particles have attracted considerable attention because of their potential applications for the electromagnetic (EM) interference and absorbing materials. However, the conventional metal particles of flaky or spherical shape have some drawbacks. For instance, the various shapes and sizes of particles can cause an inhomogeneous distribution in the polymer composite system. In order to fully realize the potential of metallic fillers as EM absorbing materials, it is necessary to develop the flat structure of the fillers which can provide uniform distribution in the composite materials. In this work, we synthesized ferrite/GO composites using redox reaction between ferric ion and graphene oxide and controlled the crystalline phase, size and distribution of ferrite nanoparticles. In the reaction, ferrite particles attached to GO surface and plate-like hybrid particles were fabricated. The hybrid particles were investigated by SEM, XRD and VSM. Near-field absorption properties of electromagnetic wave were investigated by composite film of hybrid particles and polymer.

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Boron Nitride 박리에 의한 나노시트 제조에 관한 연구

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Hexagonal BN nanosheet 는 그래핀과 화학 구조가 매우 유사하며, 열전도도와 기계적 강도 또한 유사한 성질을 가지고 있다. h-BN nanosheet 는 그래핀과 달리 절연성 물질로 화학적, 열적 안정성이 매우 뛰어난 장점을 가진 소재이기도 하다. 고분자 수지와 나노 두께를 가지는 h-BN nanosheet 유기-무기 층을 코팅하여 계면 공극 완화 및 고분자 수지와 결합을 유발하여 열전도도를 향상 시킬 수 있다. 본 연구에서는 열전달 필러소재로 사용되는 세라믹 소재 Boron Nitride 를 사용하여 나노시트 박리기술, 형상, 표면제어 등을 통하여 나노시트의 두께 및 형상을 관찰하였다. 특히, 분산용매 및 박리시간에 따른 나노시트의 SEM, TEM, PSA, XRD 등을 평가하였다.

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Development of colorimetric sensor for nitric oxide utilizing gold nanoparticles

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포항공과대학교(POSTECH) 화학과

AuNPs have highlighted as promising material as a biological sensor. Herein, we designed NAM-AuNPs for the detection of nitric oxide (NO) by inducing aggregation of AuNP. NO is a free radical gas, and has various biological functions such as cell proliferation, neurotransmission and antibacterial activity depending on concentration of NO. To design NO sensor utilizing AuNPs, we synthesized NO reactive N-(2-aminophenyl)-8-mercaptooctanamide (NAM) for modifying the surface of AuNPs. Amide-substituted benzotriazole intermediate was formed by the reaction between NO and NAM, which induced aggregation of AuNPs via electrostatic interaction. NAM-AuNPs was enabled to analyze NO quantitatively utilizing UV-vis absorption spectra. The calculated detection limit was determined as 0.2 μM. In addition, color change of AuNPs with increase of concentration of NO was easily identified with a naked eyes. The size change of NAM-AuNPs was determined by TEM and DLS. The present study demonstrates that NAM-AuNPs has a potential as promising colorimetric sensor and detection tool.

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Incorporation of *Angelica gigas* Nakai root extract with 2-dimnensional layered inorganic materials

김태현 오제민*

연세대학교 화학및의화학과

We have incorporated 2-dimensional layered inorganic material (layered double hydroxide; LDH) with *Angelica gigas* Nakai root extract through dehydration-rehydration process which called reconstruction. Pristine LDHs were prepared by conventional coprecipitation followed by hydrothermal treatment having well-ordered 2-dimensional hydrotalcite-like crystal structure and average size ~ 250 nm. The natural extract of *Angelica gigas* Nakai, which have been utilized in the treatment of inflammation and female disorders as herbal medicine, were treated with methanol to obtain extract. For the incorporation, LDHs were calcined at 400 ^{o}C for 8 hours to obtain mixed metal oxide (layered double oxide; LDO), which was further dispersed into 40 wt% methanol extract solution with various LDO/extract weight ratio, 0.11, 0.21 and 0.43. The extract contents in hybrid increase upon increasing LDO/extract ratio, showing highest contents of ~ 12% at LDO/extract ratio of 0.43. The surface charge of LDH shifted from +44 mV to +20 mV upon extract incorporation, which was attributed to the adsorption of negatively charged extract moiety on LDH surface. The scanning electron microscopic results showed that the hybrid had house-of-card structures, resulting form random stacking of LDH nanolayers during dehydration process. We quantified the amount of active ingredients in *Angelica gigas* Nakai such as flavonoid, polyphenol, decursin and decursinol angelate by UV-vis spectroscopy. It was revealed that the active ingredients were effectively concentrated in the hybrids by 1.2-3.0 times.

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Antimicrobial property of natural extract-nanoclay hybrids and their film coating

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연세대학교 화학및의화학과

We prepared natural extract-nanoclay hybrids having antibacterial activity by simple hybridization method. In order to supply porosity to nanoclays, three kinds of mineral materials such as illite (IL), holrate (HO) and scoria (SC) were treated with 6M HCl at 60^{o}C for 6hrs. For the preparation of natural extract, Paeonia suffruicosa Andrews (PS) and Agrimonia pilosa Ledeb (AP) were extracted using thermally treatment at 60^{o}C deionized water. The antibacterial activity of PS, AP and PJ was determined by paper disc diffusion assay on both Gram positive Bacillus subtilis and Gram negative Escherichia coli bacteria. Three kinds of nanoclays and two natural extracts were hybridized in aqueous media to produce 6 nano-bio hybrids. We determined contents of the natural extract in each nano-bio hybrids by weighing method and select nano-bio hybrids with natural extract above 10 wt% for further study. Through the power X-ray diffraction patterns, scanning electron microscopic images and zeta potential measurement, we confirmed that natural extracts were mainly adsorbed on the surface of nanoclays. Thermogravimetric and differential thermal analyses results suggest the molecular rearrangement of natural extract in the hybrids. In order to evaluate the antibacterial activities of the hybrids we carried out bacterial colony count method. The nano-bio hybrid showed similar or enhanced antibacterial activity compared with natural extract alone. In order to introduce the antibacterial activity with polyethyleneterephthalate (PET) film, PET film was coated with polyurethane and nano-bio hybrid mixed solution. We measured the transparency and antibacterial activity of nano-bio hybrid component coated film.

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Highly enhanced hole injection of quantum dots light emitting diodes by insertion of PANI:PSS interlayer

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We report on the improved electrical and electroluminescent performance of quantum dot light emitting diodes (QD-LEDs) with a polyaniline-poly (p-styrenesulfonic acid) (PANI:PSS) hole-transport interlayer. Insertion of the PANI:PSS between poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and poly(N-vinylcarbozole) (PVK) results in highly improved device characteristics. UPS results showed that the insertion of the PANI:PSS layer remarkably shifted the electronic energy levels of the PVK layer, which induced the energy barrier reduction of the hole traveling to the QD layer. These results suggested that the reduced hole-injection barrier at the QD layer/PVK interface prevented carrier charging and imbalanced carrier injection, such that the QD-LEDs exhibited much enhanced electric and electroluminescent characteristics.

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Near-infrared emissive aza-Boron-Dipyrromethene dyes by functional group substitution

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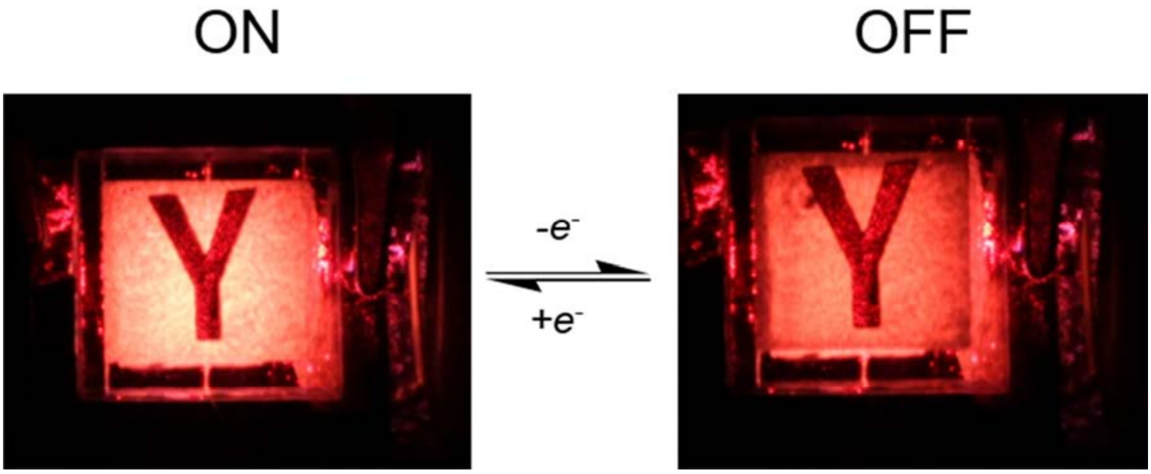
연세대학교 화공생명공학과

Aza-Boron-dipyrromethene (aza-BODIPY) dyes substituted with electron donating or withdrawing group at 1/7, 2/6, 3/5 positions showed sharp NIR absorption and emission band. The electrofluorochromic (EF) device based on the reversible electrochemistry of the electroactive materials, was prepared with aza-BODIPY dyes to demonstrate NIR EF switching. To examine the EF properties of the dyes, the optical properties were characterized by UV/Vis and fluorescence spectroscopy, and their electrochemical behavior was measured by cyclic voltammetry (CV). NIR EF switching was visually observed through light cut-off filters and the EF switching was continued over 1000 cycles with ~ 30 % loss. The NIR EF switching was visually observed through a visible light cut-off filter, featuring high fluorescence contrast.



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Physicochemical properties of food grade nano-sized iron and zinc supplement in solid and aqueous suspension

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Nano-sized food additives are used for food additives. iron and zinc supplements were commonly contained such as yogurt, daily products and beverages etc. In previously literature, control over morphology is important for many of the biological and food applications since health risks can be induced by particle size and shape. In this study, we investigated physicochemical properties of sunactive Fe-P80(Taiyo kagaku., Co) and sunactive Zn-P240 (Taiyo kagaku., Co), used for food additive as iron and zinc supplements, in various solutions. We confirm the morphology and size distribution by the scanning electron microscopy (SEM). In the X-ray diffraction (XRD) patterns, we confirm the crystal structure sunactive Fe-P80 and sunactive Zn-P240 which have amorphous and wurtzite. From the surface chemistry analyses such as FT-IR, XPS and XAS, we found that functional group at the metal surface, metal oxidation state and local structure. Through the CHN elements analysis and ICP-AES, we can confirm the organic matter and metal contents. In various solutions, we investigated surface charge and hydrodynamic size. AcknowledgementThis research was supported by a grant (14162MFDS135) from Ministry of Food and Drug Safety in 2014

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Simple synthesis of urchin-like Pt-Ni bimetallic nanostructures as enhanced electrocatalyst for oxygen reduction reaction

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Proton exchange membrane fuel cells (PEMFCs) are considered as one of the promising renewable energy technologies to solve problems with the exhaustion of fossil fuel and oil. Platinum group metal (PGM)-based materials have been a dominant class of electrocatalyst for efficient electrochemical energy conversion devices. However, the commercialization of PEMFCs has been hindered due to the slow kinetics of the oxygen reduction reaction (ORR), decreasing the overall performance. In addition, the scarcity and high cost of Pt metal drive up the cost of manufacturing fuel cells. Therefore, a majority of fuel cell research has focused on finding the optimized catalysts showing the decrease of the amount of Pt and the enhancement of the catalytic activity for the ORR. In order to address these requirements, several approaches have been developed. One of them, Stamenkovic et al. demonstrated that Pt-Ni bimetallic material is one of the most promising candidates showing enhanced performance for the ORR. Although there are many papers exploring the activity of Pt-Ni bimetallic nanoparticles with different shapes, the study on shape and composition of Pt-Ni bimetallic nanoparticles is still challenging due to the difficulty of their control. We herein report on the facile synthesis of urchin-like Pt-Ni nanostructures through one-pot synthesis utilizing a heat-up method. In order to achieve control of the composition of our synthesized Pt-Ni nanostructures, the molar ratios of the precursors were adjusted. We demonstrate that urchin-like PtNi nanostructures exhibit 15.4 times higher specific activity compared to commercial Pt catalyst.

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Highly efficient blue fluorescence and red phosphorescence hybrid white organic light-emitting diodes

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가톨릭대학교 화학과

DAnP was synthesized and electrical properties were characterized. The PL maximum value of DAnP is 469nm in solution state and 480nm in film state. DAnP was used as non-doped emitting layers (EMLs) in OLEDs with the following structures: ITO/2-TNATA (60 nm)/NPB (15 nm)/DAnP (35 nm)/Alq3 (20 nm)/LiF (1 nm)/Al (200 nm). The EL maximum value is 480nm, which is similar to the result for the PL maximum value. The luminescence efficiency was 5.45 cd/A and power efficiency was 2.71 lm/W. A efficient multilayer white organic light-emitting diode(WOLED) with the structure of ITO/NPB (30 nm)/CBP: 3 wt% Ir(piq)3 (8 nm)/DAnP (40 nm)/TPBi (40 nm)/ LiF (1 nm)/Al (200 nm) was fabricated and characterized, where DAnP and tris(1-phenylisoquinoline) iridium (Ⅲ) [Ir(piq)3] were used as a blue fluorescent dye and a red phosphorescent dye respectively. A WOLED showed luminance efficiencies of 5.08 cd/A, power efficiencies of 2.55 lm/W, and CIEs of (0.35, 0.36).

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Study on Synthesis and Characterization of red phosphor K_2SiF_6:Mn^{4+} for single packaged white LEDs

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In this study, we synthesized and characterized red phosphor K_2SiF_6:Mn^{4+} in order to improve the color rendering index (CRI) of white light-emitting diodes (LEDs). The two-step processes to synthesize red phosphor K_2SiF_6:Mn^{4+} were used in the co-precipitation method. The phosphor was precipitated from H_2SiF_6 solution with K_2MnF_6 and KF. Obtained red phosphor K_2SiF_6:Mn^{4+} has five narrow bandwidth peaks and dominant wavelength (DWL) of K_2SiF_6:Mn^{4+} is 631 nm. To improve the color rendering index (CRI) at white light-emitting diodes, we used single packaged phosphor converted-LED (pc-LED) that combined with green silicate phosphor and red K_2SiF_6:Mn^{4+} on InGaN blue LED. Synthesized red-emitting K_2SiF_6:Mn^{4+} phosphors were characterized using photoluminescence (PL), scanning electron-microscopy (SEM) and x-ray diffraction (XRD). The realized single packaged white light-emitting diodes (LEDs) were characterized using electroluminescence (EL).

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Synthesis of Zn-Ag-In-S quantum dots for multi-packaged white light emitting diodes with high color rendering index

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Non-toxic element based Zn-Ag-In-S (ZAIS) alloyed quantum dots (QDs) were synthesized by using a colloidal hot injection method. ZAIS QDs were suitable for color convertor with blue light emitting diodes (LEDs) because of broad band-width (~ 100nm) of photoluminescence (PL) and emission color tunability. To realize the white-LED with high color rendering index, green and red emissive ZAIS QDs were obtained with broad band-width as 85 and 95, respectively. The quantum yields (QY) of green and red ZAIS QDs were 45% and 55%, respectively. Green and red ZAIS QDs based monochromatic LEDs were fabricated by packing the ZAIS QD&silicone binder composite on the blue LED cup and covering the long-wavelength pass dichroic filter (LPDF), which can pass the long-wavelength and reflect the short-wavelength in the visible regions, on the LED package. The electroluminescence (EL) optical properties of obtained white-LEDs were 40~50 lm/W, ~90 of CRI value at 3500 ~ 5000 K. The structural properties of green and red ZAIS QDs were observed by transmission electron microscope and X-ray diffraction (XRD). The optical properties of ZAIS QDs and ZAIS QDs based multi-packaged white-light emitting diodes were characterized by UV-vis spectrometer, PL, and EL.

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Combined fabrication of 2D photonic crystal assisted $Lu_3Al_5O_{12}$:Ce ceramic plate phosphor and free-standing red film phosphor for white LEDs

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The combination of a two-dimensional (2D) SiN_x photonic crystal layer (PCL)-assisted $Lu_3Al_5O_{12}$:Ce (LuAG:Ce) green ceramic plate phosphor (CPP) and a free-standing (Sr,Ca)$AlSiN_3$:Eu red film phosphor were fabricated in order to enhance luminous efficacy, color rendering index (CRI), and special CRI (R_9) of LuAG:Ce CPP-capped white light-emitting diodes (LEDs) for high-power white LEDs. By introducing the 2D SiN_x PCL, the luminous efficacy of the 2D LuAG:Ce CPP-capped LEDs was improved compared to that of the LuAG:Ce CPP-capped LED, while maintaining low color rendering properties. The adding of the free-standing red film phosphor in the flat CPP-capped, and the 2D PCL-assisted CPP-capped LEDs led to enhancement of the CRI and the special CRI (R_9) for white LEDs.

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Fabrication of multi-package white LEDs using green emitting QD-CIGS and red emitting QD-CIS

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Core-alloyed shell structured green-emitting $CuIn_xGa_{1-x}S_2$-ZnS (CIGS-ZS), and red-emitting $CuInS_2$-ZnS (CIS-ZS) quantum dots (QDs) were synthesized using a colloidal hot injection method in order to make the white light emitting diodes (WLEDs) with high color rendering index. WLED was realized using red CIGS-ZS, green CIS-ZS QD-based LED and InGaN blue LED. The quantum yields (Q.Ys) of CIGS-ZS and CIS-ZS QD were 60%,65% and dominant wavelength of QDs were 525nm, 610nm. The three-package WLEDs showed high luminous efficacy (90.23lm/W) and good color rendering index (83) at 3000K The optical and structural properties of the green-emitting CIGS-ZS QDs and red-emitting CIS-ZS were measured using photoluminescence (PL), UV-vis spectroscopy, scanning electron-microscopy (SEM) and x-ray diffraction (XRD). The optical properties of InGaN blue LED, green, red QD based LEDs and three-package WLEDs were measured using electroluminescence (EL) with applied current of 60mA and 180mA.

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Comparison of white-LEDs based on TOP-capped and OA-capped Zn-Ag-In-S

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Yellow emitting $AgIn_5S_8$-ZnS/ZnS (AIS-ZS/ZS, core-alloyed shell/shell) quantum dots (QDs) were synthesized using a colloidal hot injection method with a capping agent of trioctylphosphine (TOP) and oleic acid (OA) respectively. It’s hard to make red-shift of dominant wavelength (DWL) by using TOP. The emitting wavelength of AIS-ZS/ZS QDs can be easily tuned by using OA as a capping agent instead of TOP. The quantum yield (Q.Y.) of TOP-capped AIS-ZS/ZS QDs is 56.8% and DWL is 548nm. When OA-capped AIS-ZS/ZS QDs were synthesized at same temperature with TOP-capped that, the Q.Y. is 40% and DWL is 564nm. We packed yellow emitting AIS-ZS/ZS QDs and silicone binder composite on blue-LED chips for white-LEDs. The correlated color temperature (CCT) and luminous efficacy (LE) of white-LED packed with TOP-capped AIS-ZS/ZS QDs were 4294K and 71lm/W, respectively, at 60mA (3.15V). In case of white-LED packed with OA-capped AIS-ZS/ZS QDs, the CCT and LE were 2786K and 59lm/W, respectively, at the same applied current. At the point of longevity, the relative efficiency of white-LED packed with TOP-capped AIS-ZS/ZS QDs decreased 56%. On the other hand, that of white-LED packed with OA-capped AIS-ZS/ZS QDs decreased 36%. AIS-ZS/ZS QDs using OA as a capping agent was better about tuning colors and longevity at white-LEDs. The optical properties of white LED packaged with the QDs were measured using an electroluminescence (EL) system.

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PLGA nanoparticles co-encapsulated ovalbumin and poly I:C induce an enhanced immune response in dendritic cell based cancer immunotherapy

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Dendritic cells (DCs) are specialized antigen-presenting cells (APCs) that capture, process and present antigens and induce an antigen-specific cytotoxic T lymphocyte (CTL) response. Nanoparticles (NPs) can deliver antigens and toll like receptor (TLR) ligands to antigen presenting cells (APC). NPs encapsulated antigens with adjuvant are efficiently presented on MHC class I molecules of dendritic cells and stimulate strong cytotoxic and T helper cell responses. In this study, we developed poly(lactic-co-glycolic acid) (PLGA) NPs encapsulated with ovalbumin as an antigen and poly I:C as an adjuvant, which could co-delivery of antigen with adjuvant into DCs and induce an enhanced immune response in DC based cancer immunotherapy. NPs synthesized by double-emulsion solvent evaporation method. Size of PLGA NPs ranged from 180 to 210 nm and zeta potentials were negative charge, from -25 to -18 mV. Ovalbumin was encapsulated in NPs with a loading efficiency of 80 %. Loading efficiency of poly I:C encapsulated in NPs was 45 %. DCs treated with PLGA-NPs showed higher maturation and pro-inflammatory cytokine secretion compared to control ($p < 0.05$). Moreover, DCs treated with PLGA-NPs demonstrated higher CD8+ T cell activation and proliferation by cross-presentation compared to control ($p < 0.05$). DCs treated with PLGA-NPs were significantly inhibited tumor growth in EG-7 tumor-bearing mice compared to control ($p < 0.01$). Mouse immunized DCs maturated by NPs were higher antigen specific CTL response compared to control ($p < 0.005$). Here, we developed novel nanoparticles co-encapsulated with model antigen and adjuvant, to enhance maturation and intracellular delivery efficiency into DCs, and leading that antigen presenting efficacy of DC treated with PLGA-NPs was enhanced.

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Critical parameters governing energy density of Li-storage cathode materials diagnosed by confirmatory factor analysis

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Up to date, a devotion to high energy density (ED) Li ion batteries (LIBs) has been carried out via rather one-by-one confirmation of a relationship between electrochemical properties and materials traits without a general, reliable, and comprehensive model. Therefore, although such a scrutinized investigation on a specific cathode material has elicited significant scientific findings, the sensitive dependence of electrochemical properties on crystallographic and elemental properties made the generalization of such findings difficult. Density functional theory (DFT) calculation could compensate for these shortcomings to some extent. However, DFT is also far from complete in understanding the overall trend of reported experimental data, indicating a necessity of a new systematic approach that can prospect a whole experimental data a quantum-leap innovation in material designs. In this work, we data-mine the cathode materials of LIBs through confirmatory factor analysis (CFA). Both layered and spinel structures are data-mined separately. By collecting accurate structural and electrochemical data of the both types, we prepared a systematic data set and utilized it in the CFA through principal component analysis (PCA) and a simple linear regression. The data sets that we adopt for CFA are huge in size, i.e., 19 X 40 for layered structure and 16 X 33 for spinel. The CFA reveals that, while the control of a few crystallographic parameters is critical for layered cathodes of high ED, some of intrinsic properties of constituent elements govern the ED in spinel structures. The CFA also disclose that the cyclability of the both is irrelevant to the parameters we selected, implying that the electrochemical conditions during C-D are crucial factors for the least capacity (Q) fading. The acquisition of these conceptual understandings with human cognition capability is practically impossible without a smart statistical approach like CFA.

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Restrained Cr disproportionation in an Al doped O3-type $NaCrO_2$ cathodefor sodium ion batteries

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The extensive use of Li ion batteries (LIB) in large-scale systems is unrealistic because of the limited amount of lithium as a natural resource [1]. Recently more interest has been shifted to a low-cost alternative, and room temperature sodium ion battery (SIB) has come to the fore as a suitable technology. Layered A_xMO_2 (A=Li and Na, M= transition metal) type metal oxides have been widely studied as cathode materials for LIB/SIB applications. Among these, layered Cr-based R-3m type layered transition metal oxides such as $LiCrO_2$ and $NaCrO_2$ are widely studied due to their relative higher capacity. However, these layered metal oxides; $NaCrO_2$ in particular suffers from severe capacity loss when used as a SIB cathode. The main reason for the capacity fading can be attributed to the disproportionation reaction that occurs in the redox reaction process of Cr, where the Cr^{3+} migrates from the octahedral to the narrow tetrahedral site after oxidation, blocking the diffusion of Na ions. Substituting/doping a suitable metal ion can effectively subdue this phenomenon and result in enhanced cyclic stability and capacity retention. In this work, Al doped $NaAl_xCr_{1-x}O_2$ ($0.0 < x < 0.1$) were successfully synthesized by a solid state method. The XRD studies reveal that the substitution of Cr^{3+} with Al^{3+} ions did not alter the crystal structure, and maintains an O3- phase of pristine $NaCrO_2$. Although a minor loss in capacity was incurred, an optimized Al substitution results in good cyclic stability and enhanced capacity retention, which is an outcome of the suppression of the disproportionation reaction.Reference[1] S. Komaba, C. Takei, T. Nakayama, A. Ogata, N. Yabuuchi, *Electrochem. Commun.* 12 (2010) 355-358.

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Capillary force lithography : micro pillar substrates fabrication and various application

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There are various method to fabricate nanostructure such as electron-beam and dip-pen lithography, capillary force lithography (CFL). Among these lithography techniques, capillary force lithography is a versatile tool and cost effective. Micro pillar quartz substrates was fabricated By capillary force lithography on quartz substrate. This micro pillar quartz substrates can use various application such as gas sensing, UV-vis measurement and solar cell.Three-dimensional hierarchical strutures have been introduced as effeicient structures for gas sensor applicaiotn due to large surface areas and fast gas diffusion. To increase the sensitivity of gas sensor, SWNTs were synthesized on the micro pillar structure due to the whole surface of SWNTs can absorb gas molecules and quick gas diffusion.

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Chitosan nanoparticles to targeting dendritic cells in vivo for enhancing immune response

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Dendritic cell (DC) based cancer immunotherapy has been vigorously developed in clinic. However, it has hurdled for maintain procedure and culture condition of DCs in situ. Therefore, to reduce maintain procedure in situ, we designed direct DCs targeting system in vivo after injection of nanoparticles (NPs). To effective delivery of antigen and adjuvant, we prepared chitosan NPs (CH-NP) incorporated with both ovalbumin (OVA) and polyinosinic:polycytidylic acid (poly IC). Intracellular delivery of CH-NP was confirmed by flow cytometry and confocal microscopy, resulting that CH-NP was highly uptake into DC. In addition, we confirmed endosomal escape of CH-NP by buffering effect after uptake of CH-NP into endosome, leading that CH-NP promote cross presentation of DCs, and induced CD8+ T cell activation. Moreover, therapeutic efficacy for CH (OVA+poly IC)-NP was significantly increased in EG7 tumor bearing mice compared to control ($p < 0.05$). These results suggest that the CH-NP was potent delivery method of antigen and adjuvant to DCs in vivo.

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Enhancement of Electrochemical Performance in optimized SnO_2/graphene framework for LIBs

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In a reduction reaction (discharge) of SnO_2, Sn can be alloyed with 4.4 of Li, after a conversion reaction to Li_2O and Sn. Sn have the pulverization resulted from irreversible volume expansion during the alloy reaction causes a great amount of irreversible capacities and capacity fading with cycling. However, SnO_2 can realize a high capacity anode in Li ion batteries, theoretically. Because of this advantage, studies on various kinds of nanometric structures or composites were conducted to make it reliable and commercially viable. To solve these disadvantages in our lab, we are conducting the experiment, in which the SnO_2 nanoparticles are confined between covalently linked graphene layers (framework). The tightly cross-linked framework is expected to prevent crack formations, because it buffers the volume expansion. Our group has already reported that the reversibility of SnO_2 could be enhanced by confining the SnO_2 nanoparticles within graphene frameworks (Journal of Power Sources 240 (2013) 683-690). The capacity fading, however, was not satisfactory, showing the low Coulombic efficiency maintained throughout the entire number of cycles (50 cycles). In this work, we optimized the amounts of cross-linker and the conditions of framework synthesis for stable capacity retention and rate performance during extended charge/discharge cycles, by comparison with previous SnO_2 nanoparticles within graphene frameworks.

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Porous silicon surface analysis utilizing microscopic FT-IR

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공주대학교 화학과

Recently porous silicon has been found to serve as a biosensor by modifying the surface with biomolecules. Porous silicon is a material obtained by electrochemical dissolution of a single-crystal silicon wafer in HF containing electrolyte which has been intensively investigated for a variety of applications such as optical interferometer, microelectronic circuit, Bragg reflector, Rugate filters, integration of signal processing circuitry, photonic devices, immunotherapy, biocompatible material and bone tissue engineering, as well as in vivo gene and drug delivery payload due to its biodegradable nature. Porous silicon can be used for immobilization of biomolecules such as protein, hemoglobin, DNA, and enzymes like glucuronidase, urease, tyrosinase, glucose-oxidase, ascorbate-oxidase, azurine and laccase proved be a promising material for optoelectronics, photonics and biosensors applications. The changes in photoluminescence and refractive index are used as a tool for determination of analytes on the porous silicon surface. We have explored the effect of different etching time on the variation of the surface functional groups employing the microscopic FT-IR analysis while the presence of analytes on the surface were found by the optical and surface analysis.

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Influence of a dense stacking on the electrochemical behavior of an amorphous $CoSnO_3$/ graphene composite for high performance anode in LIB

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Among the possible candidates for Li ion battery (LIB) anodes, Sn based metal oxides or ternary Sn based metal oxides have received much attention due to their very high theoretical capacity and ternary Sn based metal oxides namely $CoSnO_3$, in particular has received special attention due to its ability to relieve the internal stress of the electrode from isotropic volume change upon cycling [1]. Amorphous $CoSnO_3$ is more effective in this regard in comparison to the crystalline structure. Besides the intrinsic benefits, amorphous $CoSnO_3$ still suffers from volume changes inevitably leading to electrode pulverization and rapid capacity fade. So, ensuring the battery integrity over many charge/discharge (C/D) cycles is a formidable challenge for this category of electrodes. Coating of the metal oxide with carbon based material, in particular graphene has been proven effective to suppress this volume change. In this work, we present a new method to develop a densely stacked $CoSnO_3$/graphene composite. An electrostatic aligning of positively charged amine functionalized graphene (GN) with Co^{2+}/Sn^{2+} anchored graphene oxide (CSG) in an acidic solution results in a tightly stacked composite (CSG/GN) sandwiching amorphous $CoSnO_3$ between graphene layers. The pre-aligned stacks after thermal treatment (r(CSG/GN) results in an amorphous structure and exhibit very large reversible capacity and improved cyclic stability. When cycled at a current density of 100 $mA.g^{-1}$, the composite delivers very high capacity of 1360 $mAh.g^{-1}$ during 50 C/D cycles in contrast to thermally reduced r(CGG) (consisting a similar amorphous structure), which displayed rapid fading and delivers a capacity of 620 $mAh.g^{-1}$ under identical cycling conditions. Other composites synthesized by varying the metal ion concentration show identical C/D profiles with minor variation in the observed capacity, relative to the active material content. The origin of the sustained high capacity in optimized r(CSG/GN) composite is proposed to be arising from

enhanced reversibility of the conversion reaction stabilized by the compact structure, which is facilitated by the pre-aligning process. Pre and post-cycling investigative studies conclude that the dense stacking of graphene was a key factor and contributes immensely to the enhancement and cyclic stability of amorphous $CoSnO_3$.References[1] Z. Wang, Z. Wang, W. Liu, W. Xiao, X. W. Lou, Energy Environ. Sci. 6 (2013) 87.

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Synthesis and characterization of a layered fullerene/graphene composite for secondary battery applications

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Ambient temperature sodium ion batteries are considered the next best alternative to lithium ion battery (LIB) technology for large scale energy storage. Graphite or graphene based anodes are very popular in the LIB technology owing to its ability to intercalate Li ions reversibly. However, the application of the same is unfavorable in sodium ion battery (SIB) due to the inability of graphite to accommodate relatively larger Na ions (1.02 ?) [1,2]. Hence regulating the d spacing is a promising strategy to accommodate Na ions. The careful regulation of the d-spacing and the graphitic domain size could enhance the Na storage capability.In the present work, we present a new strategy to prepare a fullerene (FU) intercalated graphene (FIG) composite. The FU behaves as a spacer between graphene layers, regulating the d-spacing. Initially, FU was functionalized with ethylenediamine to produce amine functionalized FU (FN). UV-Vis and FTIR studies confirmed the successful functionalization of FU, XRD and UV-Vis results also revealed that the structure of FU was retained during the reaction. In an acidic solution, positively charged FN was electrostatically aligned with oppositely charged graphene oxide (GO). The pre-aligned composite was then thermally treated to produce FU intercalated graphene. XRD analysis of FIG shows that the FU structure was intact implying that the synthesis method did not jeopardize the structure of FU and the FU was intercalated between graphene layers. The FIG composite was tested as an anode for LIB and SIB, where interfacial type storage was evidenced in both cases, validating the regulated spacing. References1 . D. A. Stevens and J. R. Dahn, J. Electrochem. Soc., 148 (2001) A803 2 . Y. Wen, K. He, Y. Zhu, F. Han, Y. Xu, I. Matsuda, Y. Ishii, J. Cuming, C. Wang, Nature commun 5 (2014) 4033.

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Synthesis and Electroluminescent Properties of Organic Emitters including Electron Donor and Acceptor in a Molecule

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가톨릭대학교 화학과

New OLED materials such as DPAT-Ph, DPAT-Na, and DPAT-An were synthesized by through boronylation, bromination, Suzuki aryl-aryl coupling reaction and Buchwald-Hartwig amination. DFT calculation using PBE0/6-311G(d) was used to investigate the optimized chemical structure of the synthesized compounds. As a result, DPAT-An showed the largest hydrogen repulsion between a core group and a side group and the most twisted structure. Each compound has dipoles because it has electron donor and acceptor in a molecule and showed solvatochromism. Although there was no big change in the UV-visible spectra, the more the solvent polarity was increased in the PL spectra, the more PL maximum value was red-shifted. While DPAT-Ph and DPAT-Na emitted strong light in a solution state with the naked eye, DPAT-An emitted very weak light in a solution state, but strong light in a thin film state. As a result of taking an AIE active test, it was identified that DPAT-An uniquely showed AIE phenomenon. Three compounds showed high thermal stability of 342～370℃ in Td. DPAT-Ph showed the peak EL wavelength of 469nm in a sky-blue region. It showed 3.71cd/A, 2.07lm/W and E.Q.E of 3.61%. DPAT-Na and DPAT-An exhibited the peak EL wavelength of 502 and 547nm which is yellow to yellowish green range. Two compounds showed the high luminance efficiency of 8.09 and 17.97cd/A and E.Q.E of 3.10 and 5.20%. They also showed 3.74 and 8.20lm/W. DPAT-An which had showed high thermal stability exhibited long device lifetime of 1380 hours, which is about 10 times longer than Alq3, a standard green fluorescent material commercially used.

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Fluorescence modulation in nanoporous AuAg bimetallic skeletons

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Plasmon metal nanoporous skeleton consisted of gold and silver bimetallic components were fabricated by a series of electrochemical routes. Firstly, AuAg alloy composition was electrochemically deposited, and then Ag phase was completely removed by nitric acid, which resulted in nanoporous gold skeletons. Then very thin Ag nanofilm was deposited on the nanoporous Au skeleton by electrochemical deposition. In this study, we could precisely control the pore size and fabricated Ag coated nanoporous Au bimetallic film. We finally studied fluorescence intensity, wavelength, and lifetime modulation of introduced dye molecules on and in the bimetallic plasmonic metal skeletons as a function of the overcoated Ag film thickness.

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$LiNi_{0.5-x}Mn_{1.5+x}O_4$ (x < 0.5) for Fine Tuning of Electrochemical Performance of Spinel Cathodes

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$LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) shows great promise of a high energy cathode material for Lithium ion batteries. A numerous papers have been published during the past decade, because, while LNMO retains a fast lithium ion transport property of $LiMn_2O_4$ via three-dimensional channels, high voltage redox of $Ni^{2+/4+}$ provides a high energy density. However, the capacity of LNMO degrades relatively fast with repeated cycling, hampering commercial viability of LNMO. In this study, we investigated electrochemical properties with Ni content in $LiNi_{0.5-x}Mn_{1.5+x}O_4$ synthesized by sol-gel (S-G) method and $LiNi_{0.5-x}Mn_{1.5+x}O_4$ prepared by simple mixing $LiMn_2O_4$ and $LiNi_{0.5}Mn_{1.5}O_4$together. Preliminary results revealed that $LiNi_{0.5-x}Mn_{1.5+x}O_4$ synthesized by S-G shows significantly improved capacity retention and the absence of an abrupt voltage drop between Ni and Mn redox regions. We expect for $LiNi_{0.5-x}Mn_{1.5+x}O_4$ to deliver a high energy density after long-term cycling, mainly due to better capacity retention. The reason of the difference between synthesized and mixed materials will be presented.

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Fabrication of anti reflective moth-eye nano pattern film on glass substrate for reducing the light reflectance

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A new anti-reflection film was fabricated on glass substrate via moth eye nano-structure consisting of hexagonal-closed-packing array. These moth eye nano-structure which was fabricated by a combination of polystyrene (PS)-based nanosphere lithography (NSL) and reactive ion etching (RIE) deceased the reflectance of the glass and increased the transmittance. Using the NSL, hexagonal-closed-packing PS array was used as etching mask. From the RIE process, the moth eye pattern was fabricated. The structural of the moth eye nano-structure was investigated by scanning electron microscope (SEM). The reflectance and transmittance were measured by reflectance and transmittance spectroscopy.

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Is it possible to detect early stage of a cancer by a simple, cheap and quick method?

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부경대학교 화학과

The purpose of this study is fabrication of an inexpensive, simple and sensitive biosensor using multi wall carbon nanotubes (MWCNTs, diameter 20 nm length 5 μm) and micro pore filter paper (pore size 0.45 μm). For detection of prostate specific antigen (PSA), the carboxylated CNTs were activated with PSA antibody (monoclonal antibody of the prostate specific antigen) by using N-(3-dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride (EDC) and N-hydroxysulfosuccinimide sodium salt (NHSS). The activated CNTs were deposited on micro pore filter paper, which were used for fabrication of biosensor with 5 × 2 ㎜^{2} size. Sensing signal of the biosensor increased to 148.9 % of base signal along with the increased concentration of PSA.

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Enhanced light extraction of $Lu_3Al_5O_{12}$:Ce ceramic plated phosphor with 2D SiN_x photonic crystal

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In this study, we introduce a two-dimensional (2D) SiN_x photonic crystal layer (PCL)-assisted $Lu_3Al_5O_{12}$:Ce (LuAG:Ce) green ceramic plate phosphor (CPP) in order to enhance light extraction efficiency of LuAG:Ce CPP. The 2D SiN_x PCL was fabricated by nanosphere lithography (NSL) with polystyrene (PS) beads and reactive-ion-etching (RIE) method. The optical properties of the LuAG:Ce CPPs and 2D SiN_x PCL-assisted LuAG:Ce CPPs on an InGaN blue light-emitting diodes (LEDs) were measured under an applied current of 350 mA. By introducing the 2D SiN_x PCL, the luminous efficacy of the 2D LuAG:Ce CPP-capped LEDs was improved compared to that of the LuAG:Ce CPP-capped LEDs with a thickness of 0.10 mm and 0.15 mm, respectively.

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Thin Indium Seed Layer Assisted Growth of ITO Nanorods using RF-Magnetron Sputtering System

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High density ITO nanorods were fabricated via thin indium seed layer using RF-magnetron sputtering system. In order to enhance the density of ITO nanorods, we coated thin indium layer on conventional ITO glass substrates by thermal evaporator. After depositing thin indium layer, the substrates were treated in 500 °C in order to convert thin indium layer into innumerably increased small indium clusters. Each of these clusters acts as a growing site for ITO nanorod. These high density ITO nanorods were used as a large surface area electrode for supercapacitor. Structural and morphological properties were investigated by scanning electron microscope (SEM), electrical properties including sheet resistance and cyclic voltammetry curve were measured by four-point probe and potentiometer. Transmittance was measured by UV-visible spectrometer.

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Field effect transistor based on Au modified MWCNT for non-enzymatic carbohydrates detection

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부경대학교 화학과

An effective and facile reduction approach for the fabrication of nanocomposite Au nanoparticle attached multiwall carbon nanotube (Au-MWCNT) is demonstrated. HAuCl4 is used as Au precursor chemical for the formation of Au nanoparticles (AuNPs) on MWCNT. This method involves a simple mixing procedure followed by a mild heating process without any reducing agent, linker chemical or electric current. This approach does not need the exhaustive surface oxidation process of MWCNTs by the strong acid. The diameter of AuNPs on surface MWCNT is 10~50 nm confirmed by TEM and XRD. The structure and intrinsic properties of MWCNT do not change before and after the attaching AuNPs by thermal decomposition. Raman spectroscopy indicates that the defect of MWCNT due to attachment of AuNPs was decreased. Electronic device application will be investigated by fabrication of the field effect transistor (FET) based on Au-MWCNT for non-enzymatic carbohydrates detection.

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Highly selective luminescence sensors for mercury ions based on BSA-gold nanoclusters on the 3D Networks of CNT

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한양대학교 화학과 [1]한양대학교 나노과학기술연구소

Clusters of noble metals such as gold and silver have been of recent interest due to their interesting properties such as photo-luminescence, non-photobleachability, photon anti-bunching. It was used the PL quenching assay for monitoring Hg2+ using bovine serum albumin (BSA) capped gold nanocluster (BSA-Au NCs) has excellent selectivity over metal ions and anions. Carbon nanotubes (CNTs) have attracted much attention because of their excellent electrical and mechanical properties. Especially, it is expected that three dimensional (3D) networks of CNTs of high density is useful for highly sensitive sensors. Three dimensional networks of the CNTs on porous Si substrates can be produced by simple chemistry. So, 3D Network of CNTs conjugated BSA-Au NCs were used for detection capability as a convenient portable devices of Hg2+.

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Polydiacetylene Vesicle Coated Three Dimensional Network of CNTs for Sensitive alpha-cyclodextrin Sensor

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The importance of the signal amplification is arising in the sensor field for the accurate and instant analysis. A PCDA vesicle has double bond chain in the middle of the vesicle and when a signal is applied on the conjugated polymer, the back bone chain’s energy band gap is changed and the chain emits intensive red fluorescence light. There are several resources that can give signals to the PCDA vesicles and only alpha-cyclodextrin has a specific ring size that can change the structure of the vesicle which leads to color change.Many attempt has been tried to develop a platform for PCDA on 2D substrate, but the previously studied 2D based platforms have extremely low fluorescence signal. In this study, PCDA vesicles are uniformly coated on the three dimensional structure which has larger surface area than the two dimensional substrate. The fluorescence intensity from the PCDA coated three dimensional structure has 2.5 times higher than the fluorescence intensity from the two dimensional substrate. This result will contribute to the development of a highly sensitive sensor.

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The reduction of 4-nitrophenol by Pd-decorated graphene oxide as a catalyst

김지당 최현철*

전남대학교 화학과

Graphene is a two-dimensional material with a single atomic layer of carbon atoms arranged in a hexagonal lattice. Due to its unique structure, graphene exhibits unusual optical and electronic properties. In this study, we prepared Pd-decorated graphene oxide by introducing thiol groups on graphene surfaces. Surface thiolation is an effective way to obtain dispersed metal nanoparticles on the surface of graphene. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The reduction kinetics of 4-nitrophenol is also investigated by ultraviolet-visible (UV-vis) measurement.

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Preparation of Ag-decorated graphene oxides and investigation of its catalyst activity

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전남대학교 화학과

Silver (Ag)-based compounds have high catalytic activity for various chemical reactions. However, their high surface energy makes them highly reactive and susceptible to aggregation into large particles, which results in the deterioration of their unique chemical properties and the loss of their catalyst activities. In an effort to overcome these problems, nanocomposites composed of Ag nanoparticles dispersed on suitable substrates have been intensively studied. In this study, we report a simple and effective process to prepare Ag-decorated graphene oxide by depositing Ag nanoparticles on thiolated graphene surfaces. Thiol groups were utilized as linkers to secure the Ag nanoparticles without agglomeration. The samples mainly were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The Ag-decorated graphene oxide exhibits high catalytic activities for the reduction of 4-nitrophenol.

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Formation of controllable hexagonal disk of NaLuGdF4:Yb,Er by hydrothermal process

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창원대학교 화학과

Yb3+ ion is possessed of large absorption cross section around 980 nm and involves the efficient energy transfer (ET) to other Er3+ ions. Therefore, Yb3+ ions play a role of sensitizer for infrared-to-visible upconversion (UC) process. We have prepared successfully Yb3+, Er3+-doped NaLuGdF4 nanoparticles by hydrothermal method. The morphology and structure of the UC nanoparticles were investigated by using scanning electronic microscopy (SEM) and X-ray powder diffraction (XRD). The uniformity and thickness of nanoparticles were influenced mainly by precursors concentration and reaction time. Under a 980 nm excitation from laser diode, the upconversion spectra consist of an intense emission band centered at ~540 and 660 nm. It was revealed that the upconversion process of Yb3+,Er3+-doped NaLuGdF4:Yb,Er is a two photon process. The ET mechanism was discussed in detail.

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Up-conversion luminescence properties of oxy-fluoride glass ceramics

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창원대학교 화학과

Recently, infrared-to-visible up-conversion in rare-earth doped oxy-fluoride glasses has been extensively investigated, due to their potential applications for visible lasers, optical data storage, color display, under-sea optical communications and sensors. Among rare-earth ions, Er3+ ion is one of the important active ions because of its convenient energy level structure exploitable in up-conversion processes. On the other hand, Yb3+ ion has only two spin?orbit states (2F7/2 ground state and 2F5/2 excited state), which guarantee a large cross section around 980 nm. Therefore, Yb3+ ion can act as a sensitizer that can be pumped efficiently by laser diodes at 980 nm, thus allowing for an efficient energy transfer from Yb3+ to Er3+ ions. We have observed greatly enhanced up-conversion efficiency of rare-earth ions in Er3+/Yb3+-codoped glasses through energy transfer. The up-conversion efficiency was strongly dependent on the characteristics of the glass host materials. The oxy-fluoride glasses are attractive hosts because they include the advantages of both oxide and fluoride glasses with, higher chemical and mechanical stability and lower phonon energy as well.We have prepared the Er3+/Yb3+ codoped SiO2?Al2O3?CaF2 oxy-fluoride glasses by melt and quenching method. The intense green (524 and 541 nm) and red (660 nm) up-conversion photoluminescence were obtained by the 980 nm laser diode excitation. The up-conversion is occurred based on two photon absorption either by the energy transfers from Yb3+ ion or by the excited state absorption. As increasing Yb3+ concentration, the red emission was increased by one photon process. It can be explained by a weak blue emission. The excitation power dependences and temporal behaviors of up-conversion were investigated for understanding up-conversion mechanism. The up-conversion processes in Er, Yb codoped oxy-fluoride glasses were explained by the energy transfer (ET) and energy back transfer (EBT) between Yb3+ and Er3+.

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Synthesis and Characterization of New Blue Emitting Material for OLED

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경상대학교 화학과 [1]경상대학교 그린에너지융합연구소

We designed and developed a new limb-structured anthracene derivative comprising an anthracene core with phenyl units at itsthe 9 and 10-positions and fluorene units at its 2 and 3-positions. This blue-emitting material was synthesized via the Suzuki cross-coupling reaction and its structure was confirmed by using FT-IR,1H NMR,13C NMR, and mass spectroscopy. The optical, electrochemical and thermal properties of the material were investigated.

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One-step hydrothermal synthesis of NaLuGdF4:Yb3+/Er3+ upconversion nanoparticles

GerelkhuuZayakhuu B.T.Huy 정종원 이용일*

창원대학교 화학과

Upconversion (UC) is an unique type of photoluminescence in which lower-energy excitation is converted into higher-energy emission via multi-photon absorption processes. The facile synthesis of Yb3+/Er3+-doped NaLuGdF4 upconversion nanoparticles (UCNPs) coated with malonic acid (MA) and polyacrylic acid (PAA) were accomplished by one-step hydrothermal method. The UCNPs capped with the carboxylic group (COOH-) of MA/PAA on the surface make the UCNPs water soluble. The visible green, blue and red emissions are observed from the UCNPs upon near-infrared (NIR) excitation. The characterizations of NaLuGdF4:Yb3+/Er3+ were performed by using photoluminescence (PL), scanning electron microscope (SEM), Fourier-transform infrared spectroscopy (FT-IR) and X-ray diffraction (XRD). FT-IR spectra was measured to confirm the successful capping of MA/PAA ligands on the surface of UCNPs. It was revealed that were the nanoparticles were spherical with a uniform size of 50-70 nm in SEM images. In addition, these high quality UCNPs have prominent potential applications for optical nanodevices and bioanalytic sensing.

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Preparation of an upconversion hollow fiber Y2SiO5:Yb,Er by electrospinning method

최혜원 B.T.Huy 이용일*

창원대학교 화학과

Upconversion (UC) nanoparticles have the ability to convert near infrared radiations with lower energy and long wavelength into visible radiations with higher energy and short wavelength. There are various synthesis methods of UCPs including co-precipitation method, thermal decomposition method, hydrothermal/solvothermal method, and electrospinning method. Among these methods, electrospinning method has an advantage to make nanofibers under the influence of high electrical voltage.By controlling the viscosity of polymer, the voltage and, distance between tip and collector, various types of Y2SiO5:Yb,Er UC hollow fibers were obtained. Hollow shape has many advantages because the surface area is extended to inside as well as outside. The characterizations of UC hollow fiber were performed by using photoluminescence (PL) and Field mission scanning electron microscope (FE-SEM). Under 980 nm excitation wavelength, the UC spectra consist of two bands located at about 540 and 660 nm. These bands originate from Er3+ emissions. The mechanism of upconversion process will be discussed.

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Synthesis and Characterization of Conjugated Polymers for Organic Solar Cell Applications

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경상대학교 화학과

Low bandgap polymers with dithienylquinoxaline moieties based on 6H-phenanthro[1,10,9,8-cdefg]carbazole were synthesized via the Suzuki coupling reaction. Alkoxy groups were substituted at two different positions on the phenyl groups of the quinoxaline units of these polymers: in the para-position (PPQP) and in the meta-position (PPQM). The two polymers showed similar physical properties: broadabsorption in the range of 400?700 nm, optical bandgaps of 1.8 eV, and the appropriate frontier orbital energy levels for efficient charge transfer/separation at polymer/PC71BM interfaces.

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A Study on La2O3- based insulators prepared by Atomic Layer Deposition: Growth Condition and Material Properties

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Thin films of rare earth metal oxides are interesting materials for many technology applications, which requires a method for controlled growth of such films. La2O3 is the promising insulator for the next-generation high-k gate insulators to achieve higher drivability as well as lower gate leakage. In this work, we report a thermal atomic layer deposition(ALD) process for growing high-κ oxide, La2O3. The thin films were grown by ALD including La-precursor (alkoxides, alkylmides, cyclopentadienyls) and H2O as oxygen source, respectively. It was dependence of the film thickness(cycle number) and the growth rate on the deposition temperature. Additionally, such grown films were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), atomic force microscopy current?voltage (I-V) and capacitance?voltage (C-V) measurements. This study will be used to improve the design techniques of new high-k gate insulators and products for next-generation flexible electric devices

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Catalytic behaviors of Rh/α-Fe_2O_3 submicron spherical particles for CO oxidation

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The size-controlled magnetite spherical particles were synthesized from $FeCl_3$, sodium acetate trihydrate, and ethylene glycol using the solvothermal reduction method. The magnetite particles were calcined to transform into the α-Fe_2O_3 phase. The α-Fe_2O_3 spherical particles were found to have an average diameter of ca. 420 nm and internal space in them . Rh metal particles were embedded in the α-Fe_2O_3 submicron spherical particles and the Rh-loaded oxide system was tested as catalyst for CO oxidation. α-Fe_2O_3 fine powder and Rh-loaded α-Fe_2O_3 fine powder as reference materials were prepared to examine as catalysts for CO oxidation. Kinetic measurements on the catalytic CO oxidation were performed in a flow reactor using an on-line gas chromatography system operated at atmospheric pressure. The Rh/α-Fe_2O_3 submicron-spheres catalyst has been found to be highly active for the CO oxidation. Kinetic data obtained for the Rh/α-Fe_2O_3 submicron-spheres were compared to those obtained for the α-Fe_2O_3 fine powder, the α-Fe_2O_3 submicron-spheres, and the Rh/α-Fe_2O_3 fine particles. The catalytic processes were discussed according to the kinetic results. The catalysts were characterized using XRD (X-ray powder diffraction), FE-SEM (field emission-scanning electron microscopy), HR-TEM (high resolution-transmission electron microscopy), and N_2 sorption measurements.

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Synthesis and Structural Properties of Platinum Nanodots Assemblies Core-Silica Shell Nanoparticles

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한림대학교 화학과

Platinum (Pt) nanodots assembly (m-Pt) core-silica shell nanosystems (m-Pt@SiO2 NPs (spherical nanoparticles) and m-Pt@SiO2 NChs (nanochains)) were successfully synthesized by the reverse microemulsion (water-in-oil) based method. The reverse microemulsion substance was composed of surfactant (Brij35), co-surfactant (n-hexanol), organic solvent (cyclohexane) and water. The morphologies and structural properties of the core-shell nanoparticles were being controlled and characterized by mean of the transmission electron microscopy (TEM) and the scanning electron microscopy (SEM). We are expecting these novel nanomaterials can be applied for the plasmon-induced energy transfer or photosynthesis systems.

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Synthesis and application of Flower-like Ni-based Coordination Polymer Particles and NiO Microparticles

유효종[*] MAIDUYHIEN

한림대학교 화학과

In this report, we described a high-yielding method to fabricate flower-like NiO microparticles with high porosity showing great prominences in varied applications. The flower-like NiO microparticles were thermally converted from the pre-synthesized Ni-based coordination polymer particles. It is noteworthy that the thermal-converting step results in a substantial enhancement in estimated BET surface area, which is evidenced by N_2 adsorption isotherms. This is mainly owing to the formation of new mesoporous systems resulting from the eradication of organic linkers. As revealed from SEM and TEM images and powder X-ray diffraction data, NiO microparticles show monodisperse flower-like topologies assembling from numerous nano-sized plates and high degree of crystallinity, respectively. The morphology and size of flower-like NiO microparticles were further investigated by varying concentration of monodentate ligands, known as modulators, and surfactant, molar ratio of Ni^{2+} to organic linkers, temperature, and amount of additives (e.g. HCl, or NH_4OH). It is well-documented that metal oxides have been exploited as solid supports to make biosensors due to the high compatibility, less toxicity, strong adsorption capability, and fast electron transfer. In this report, we successfully deposited flower-like NiO microparticles onto ITO electrodes and investigated their electrochemical characteristics using cyclic voltammogram. The CV data displays well-defined peaks with high current density, indicating the applicability of flower-like NiO microparticles to be employed as solid supports in biosensing.

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Facile fabrication of highly porous nickel oxide and its application in amperometric urea biosensor

유효종* **MAIDUYHIEN**

한림대학교 화학과

In this report, we describe a facile method for the fabrication of Ni based coordination polymer nanoparticles using modulators (e.g. acetic acid, benzoic acid, or pyridine) to control their size. The resultant coordination polymer nanoparticles were then calcinated at controlled temperature to produce highly porous nickel oxide nanoparticle. The SEM and TEM show NiO nanoparticles with regular shape while powder X-ray diffraction data shows a high degree of crystallinity. Moreover, BET data of nickel oxide nanoparticles exhibit relatively high specific surface area (112 m^2/g) with well-defined pore size (10 nm), showing great potentials in various applications.We also successfully deposited NiO nanoparticles onto an indium tin oxide (ITO) serving as an efficient matrix for the immobilization of urease (Ur) for urea detection. The prepared bioelectrode (Ur/NiO/ITO/glass) is employed for urea sensing using cyclic voltammetry (CV). As shown in preliminary CV data, the prepared electrodes show a high sensitivity and linear relationship between current and urea concentrations with short response time. The next step is to assess how the sensitivity and precision of urea biosensors can be affected by interferants (e.g. glucose, uric acid, cholesterol, lactic acid, ascorbic acid) simultaneously existing in human serum.

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Synthesis, structure, and ligand exchange of a copper(II)-based molecular helix with 2,6-pyridinedicarboxylates

유효종* 이상돈

한림대학교 화학과

An one-dimensional (1-D) metal-organic polymer, $[Cu_2(PDA)_2(DMF)_2]_n$ (PDA = 2,6-pyridinedicarboxylate, DMF = dimethylformamide), was synthesized by reaction of copper(II) nitrate hemi(pentahydrate) and 2,6-pyridinedicarboxylic acid in DMF. The complex shows a molecular helix structure consisting of five-coordinate Cu(II) building blocks with distorted square pyramidal geometry. Tridentate chelating PDA, DMF, and an oxygen from the carboxylate of the adjacent Cu(II) building unit are coordinated to the copper(II) center. The weakly coordinated DMF groups in $[Cu_2(PDA)_2(DMF)_2]_n$ easily exchange with a pyridine to generate a pyridine-coordinated non-helical 1-D metal?organic polymer with six-coordinate pseudooctahedral Cu(II) units.

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Synthesis and Coordination Polymerization of Cobalt Cluster-based Supramolecular Triple-Stranded Helicates

유효종

한림대학교 화학과

A cobalt cluster-based supramolecule, $Co_8(PDA)_6(PTA)_3(DMF)_2(H_2O)_4$ (1) (PDA = 2,6-pyridinedicarboxylate, PTA = benzene-1,3-dicarboxylate, DMF = dimethylformamide) was successfully synthesized by the reaction of cobalt nitrate hexahydrate ($Co(NO_3)_2 \cdot 6H_2O$), 2,6-pyridinedicarboxylic acid (H_2PDA), and benzene-1,3-dicarboxylic acid (H_2PTA) in DMF. Two tetranuclear cobalt clusters are diagonally linked through three PTA ligands to form a novel inorganic supramolecular triple-stranded helicate with left-handed helical geometry containing eight cobalt atoms, six PDAs, and three PTAs. Reaction of excess cobalt(II) acetate tetrahydrate ($Co(OAc)_2 \cdot 4H_2O$) with H_2PDA and H_2PTA in DMF yields the one-dimensional coordination polymer $[Co_8(PDA)_6(PTA)_3(DMF)_2(H_2O)_4\text{-}(Co(OH_n)_2)]$ (n = 1 or 2) (2), which is composed of 1 as the basic building blocks and tetrahedral cobalt (II) ions as linkers. Due to the left-handed helical motif of complex 1, coordination polymer 2 shows a left-handed, S-helix geometry with two S-helices intertwined to form a double-stranded helix. This synthetic result is an unusual example whereby a secondary helical coordination polymer is fabricated by the polymerization of a primary cluster-based supramolecular building block.

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Tailored Solution-Phase Synthesis of Au Nanofibers by using Mixed Surfactants

유효종* 최순

한림대학교 화학과

Anisotropic gold nanostructures, especially gold nanofibers, have recently received tremendous attention due to their unique optical properties which could be employed in a wide variety of applications. However, nanofibers, in most cases, are fabricated mainly using electrospinning method requiring high-tech equipment or hard-templated synthesis. Herein, we describe a facile method to produce gold nanofiber with high monodispersity in a solution-phase. Moreover, by adjusting mixed surfactants of CTAB and Brij35 which function as both reducing and shape-directing agents, the aspect ratio and formation yield were successfully manipulated. Eventually, the synthesized Au nanofibers were hybridized with Pt nanoparticles, showing great prominence in a variety of catalytic applications.

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Controllable Fabrication of Star-shaped Gold Nanoparticles (Au SSNPs) with Multi-branches and Their High Catalytic Performance

유효종* <u>최순</u>

한림대학교 화학과

Star-shaped gold nanoparticles (Au SSNPs) which have multi branches and sharp tips were successfully synthesized in high yield through a facile seed-mediated method using cetyltrimethylammonium bromide (CTAB), Brij35, Au seed nanoparticles, Ag+ ions, ascorbic acid, and salicylic acid. It is noteworthy that the lengthes of each branch of Au SSNPs were finely tuned by adjustment of molar ratio of surfactants, and in particular by the change of salicylic acid. The Au SSNPs show significant surface enhanced Raman spectroscopy (SERS) promising for a variety of optical applications. The formation mechanism of star-shaped topologies is proposed and further proved by time-resolved SEM images.In order to evaluate the applicability of the synthesized Au SSNPs, 4-nitrophenol reduction and ethanol electrooxidation were employed as model reactions. We also investigated the catalytic performance of Au SSNPs with different length of branches and found that the longer length lead to the higher catalytic activity.

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Synthesis of Highly Fluorescent Amine-Stabilized Gold Nanoclusters

유효종* 최순

한림대학교 화학과

Gold (Au) nanoclusters (NCs) comprising several tens of atoms exhibit remarkably strong emission, which mainly originates from their molecular-type transition properties. A variety of synthetic approaches to the production of fluorescent NCs has been reported, the majority of which employed specific templates. In an endeavor to develop more effective synthetic strategies for the production of highly fluorescent and useful Au NCs using small molecules as a template, we could synthesize highly emissive Au NCs by means of stabilization with small organic molecules with amine functional groups using a thermal synthetic strategy. The optimization of synthetic procedure to yield the Au NCs with high quantum yields will be presented.

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Synthesis, characterization, and Catalytic Activity of Raspberry-Like Gold Nanoparticles (Au RLNPs) and Au RLNP@SiO2nanoparticles

유효종* 문영서 MAIDUYHIEN 최순

한림대학교 화학과

Raspberry-like gold nanoparticles (Au RLNPs) synthesized through reduction of $HAuCl_4$ by using Brij35 surfactant and NaOH show high catalytic activities in the reduction of 4-nitrophenol and ethanol electrooxidation. The enhanced catalytic activities of Au RLNPs are mainly due to their high surface roughness. However, Au RLNPs are easily changed to spherical or aggregated nanoparticles by treatment with acids, thiols, and cationic surfactants (e.g., CTAB), making it difficult to sustain the catalytic activity. To improve the stability and applicability in a wide range of environments without degrading the original Au RLNP morphology, silica-coated Au RLNPs (Au RLNP@SiO_2 NPs) were successfully synthesized through a sol-gel process using poly(vinylpyrrolidone) (PVP) as a primer. In comparison with Au RLNPs and other Au nanoparticles, Au RLNP@SiO_2 NPs are more easily recovered and recycled in repeated catalytic reactions.

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Synthesis of Tridentate 2,6-Bis(imino)pyridyl Ruthenium(II) Complexes with N-Heterocyclic Carbene Ligands: Activation of Imidazolium Salts

유효종* <u>이상돈</u>

한림대학교 화학과

Low-valent Ru(0) complexes, [η^2-N_3]Ru(η^6-Ar) or {[N_3]Ru}$_2$(μ-N_2), where Ar = C_6H_6 or C_6H_5Me, and [N_3] = 2,6-(2,4,6-$(CH_3)_3C_6H_2N{=}CCH_3)_2C_5H_3N$, activate C-H bonds in imidazolium salts to produce bis(imino)pyridyl ruthenium-(imidazolidin-2-ylidene) complexes, [N_3]Ru(H)(X)(NHC) (1) (X = halides and tosylate). Formation of 1 is most likely to proceed via C-H oxidative addition, followed by anion coordination, which is expected to be a useful pathway in synthesizing new complexes with both N-heterocyclic carbene (NHC) and hydride ligands. A zwitterionic ruthenium complex with an ylidic ligand, bis(imino)pyridyl ruthenium-(2-methyleneimidazoline) complex, 2, was also successfully isolated and fully characterized. The ^{1}H NMR spectra and the solid-state structure confirm that complex 2 is an ylidic transition-metal complex with both NHC and hydride ligands, which was formed through the activation of imidazolium salts.

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Oxidized carbon nitrides: Water-dispersible nano-dots and their bioimaging applications

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인하대학교 화학과 [1]인하대학교 화학-화학공학 융합학과

To realize the great promise of two-dimensional (2D) allotropes of various 3D materials, it is highly important to develop routes for the production of 2D C3N4 materials, which are one-atom thick, in order to understand their intrinsic properties and identify their possible applications. In this work, water-dispersible, atomically thin, and small carbon nitride nano-dots were produced using the chemical oxidation of graphitic C3N4. Various analyses, including X-ray diffraction, X-ray photoelectron, Fourier-transform infrared spectroscopy, and combustion-based elemental analysis, and thermogravimetric analysis, confirmed the production of 3D oxidized C3N4 materials. The 2D C3N4 nano-dots were successfully exfoliated as individual single layers; their lateral dimension was several tens of nanometers. They showed strong photoluminescence in the visible region as well as excellent performances as cell-imaging probes in an in vitro study using confocal fluorescent microscopy.

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Controlled Fabrication of DNA-Silica Hybrid Materials with Self-Assembled DNA Nanostructures

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DNA exhibits the unique hydrogen bonding property for self-assembled nanostructures which were the naturally evolved products in order to carry the secret code of genetic information. Based on the fact, DNA has been used for the formation of nanomaterials as a fundamental building block or seed material for mineralization. DNA origami is an example of exquisite assemblies at nanometer scale in the collaboration with computational calculation, and has enabled the design of 2D or 3D DNA nanostructures. Despite the impressive achievements of DNA origami, there has been a great need for harnessing DNA nanostructures to synthesize unprecedented hybrid materials in a controlled manner. In this context, we proposed a templated fabrication of DNA-silica hybrid materials on the basis of self-assembled DNA nanostructures. Resulting DNA-silica hybrid materials would be applied to the development of multi-functional nanodevices for nanobioapplications, such as drug delivery, catalysis, and bioimaging.

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Double Locked Silver-coated Silicon Nanoparticle/Graphene Core/Shell Fiber for High-Performance Lithium-Ion Battery Anodes

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We present a fabrication of a scalable coaxial core/shell silicon-graphene fiber prepared by dual-nozzle-induced wet-spinning assembly for high-performance silicon anode. Over 50 wt% of silicon nanoparticles mixed with graphene oxide suspension can be incorporated in the core with using outstanding dispersive property of unique silver-coated silicon nanoparticles in aqueous media. This core fiber is further encapsulated by graphene shell which not only provides conducting pathways, but also alleviates severe volume expansion of silicon core. This novel core/shell silicon anode double locked with graphene architecture delivers more stable cycle performance and superior rate capability than anodes composed of simple mixture of silicon-graphene composites.

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Phase-pure FeCr2Se4 and FeCr2S4 nanocrystals synthesis via wet chemistry method with high conductivity

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A novel facile synthetic route for iron-based ternary NCs, i.e., FeCr2Se4 and FeCr2S4 was introduced using a wet chemistry method. Narrow bandgap Fe ? based ternary semiconducting nanocrystals (NCs) offer a promising conductivity for electronic structure with different doping. Importantly, their higher potential to be industrialized in solar cells differs from Cd and Pb ? based compounds due to non-toxicity of inherited materials. General synthetic route of the ternary compounds passes through mixing and reacting different elemental powders in evacuated silica ampoules to consume long time under high temperature (700 - 1000 °C) but resulting in uncontrolled size and morphology of colloidal NCs. In the suggested method, the morphology of NCs was simply controlled using solvent and heating temperature where oleylamine was multi-utilized as surfactant, solvent, and reducing agent. The synthesized NCs possess excellent monodispersity of size and shape without any aggregation and the conductivity of the deposited layer of FeCr2Se4 and FeCr2S4 NCs shows 3.25μA and 2.33μA, respectively. Therefore, our iron-based NCs may substitute current chalcogenides that are environmentally toxic and low efficiency of energy transfer.

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Catalytic Vapor Assisted Growth of Uniform Nano-crystalline Graphene on Insulating Substrate

이재현* 김민성[1]

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We report a simple and direct growth of uniform single layer graphene on dielectric SiO_2 surface by utilizing CMOS compatible germane gas. Crystalline and structure of graphene is easily controlled by tuning gas ratio. Raman spectra and XPS conform that as grown graphene is consist of sp^2 hybridized carbon structures. Without wet etching process, we are able to fabricate graphene field effect transistors. The present results demonstrate a promising graphene growth technique for current Si based CMOS technology.

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Study on Photothermal Effect of Gold Nanorods with Different Morphology

심규동 장의순*

금오공과대학교 응용화학과

금속 나노입자의 Surface plasmon resonance (SPR) 현상은 다양한 분야에 응용되고 있으며 특히 SPR 조건을 만족시키는 Wavelength 의 빛이 Gold 나노입자에 조사되었을 때 여기된 전자들이 Gold 원자와의 충돌로 인해 발생되는 열을 이용하여 암을 치료하는 기술이 세계적으로 큰 관심을 받고 있다. 특히, Gold nanorod (GNR)는 의학적으로 응용 가능성이 큰 근적외선 영역에서 광열효과 (Photothermal effect)가 매우 우수하다고 알려져 있다. 본 연구에서는 GNR 을 합성하는 일반적인 방법인 Seed-mediated growth method 의 합성조건을 달리 하면서 끝부분이 둥근 일반적인 GNRs 과 Dog-bone 모양의 GNRs (DB-GNRs)를 합성하였으며 이들의 입자 모양에 따라 광열효과가 달라지는가를 살펴보았다.

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A Three-Dimensional π-Electron Acceptor Bearing Benzoquinone Units: Synthesis, Characterization and Application Towards Solar Cells

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가톨릭대학교 화학과 [1]서울대학교 재료공학부

para-Benzoquinone-based π-electron acceptor molecule with a 3D molecular structure (triptycene tris(1,4-benzoquinone) (TT)) was synthesized and its chemical structure was fully characterized. The thermal, optical and electrochemical properties of TT were investigated as well as its potential for photovoltaic applications.

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Ni(dmamb)$_2$를 사용한 MgO 기질 위의 NiO 박막의 MOCVD

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NiO 는 p 형 투명 전도성 막으로서 광학적 및 전기적 특성이 우수한 물질이다. 우리는 Ni(dmamb)$_2$ [nickel bis(1-dimethylamino-2-methyl-2-butanolate)]를 선구물질로 사용하여 MgO(100) 기질 위에 NiO 박막을 CVD 방법으로 칭착시켰다. Ni(dmamb)2 는 상온에서 액체이며 증기압이 75 ℃에서 213 mTorr 로 충분히 높다. 기질의 온도는 250-400 ℃ 구간에서 25 ℃ 간격으로 변화시켰다. 박막의 특성을 X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), reflection high-energy electron diffraction (RHEED), scanning electron microscopy (SEM)로 조사하였다.

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Synthesis and characterization of 2-naphthol and thiazole-based excited-state intramolecular proton transfer (ESIPT) molecules for fluorescent zinc sensors

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Because zinc ion plays various kinds of important roles in human physiopathology, development of sensitive and noninvasive ion sensing technique is important to trace and visualize free zinc ions. However, most of the attention has been focused to the detection of endogenous free zinc ions using typical structure of a fluorescent zinc sensors which is composed of a conventional fluorophore and a well-known zinc-specific receptor such as di(2-picolyl)amine (DPA), N,N-di(2-picolyl)- ethylenediamine (DPEN), tris(2-picolyl)amine (TPA), or N,N,N′-tris(2-picolyl)ethylenediamine (TRPEN). In this work, we have designed and synthesized novel kinds of sensing materials which are based on excited state intramolecular proton transfer (ESIPT) fluorophore, that results in the formation of two tautomeric forms in the excited state of the probe, normal and tautomer forms are very successful for the design of probes with dual fluorescence. For orange-red emitting sensing part, naphthol and thiazole-based ESIPT fluorophore, 3-(4,5-diphenylthiazol-2-yl)naphthalen-2-ol, was synthesized and zinc-selective di(2-picolyl)amino (DPA) unit was introduced as a receptor part.

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Study on antimicrobial mechanism of ZnO nanoparticles under dark condition and UV light irradiation

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ZnO 는 우리 주변에서 가장 흔하게 사용되는 반도체 물질로써 그램 음성균, 양성균 전반에 걸쳐 높은 항균력을 갖는다고 알려져 있다. 지금까지 제안된 암실조건에서 ZnO 의 항균 메커니즘은 산소 결함 위치에서 발생한 활성산소, 수용액 상에서 ZnO 로부터 방출된 Zn 이온, ZnO 와 세포벽의 정전기적 상호작용, 크게 이 세 가지로 설명된다. 하지만, 암실조건에서 ZnO 의 항균 메커니즘은 아직까지 명확하게 규명되지 않은 상황이다. 본 연구에서는 서로 다른 모양의 ZnO 나노입자를 이용하여 그램 음성균과 양성균을 대상으로 암실조건에서 항균력을 테스트하였으며 이를 바탕으로 암실조건에서 ZnO 나노입자가 갖는 항균 메커니즘에 관하여 자세히 살펴보았다. 또한, 자외선 조사 조건에서 서로 다른 입자모양을 갖는 ZnO 나노입자들로부터 활성산소 발생양의 차이를 확인하고 항균특성을 향상시키기 위한 ZnO 나노입자의 조건에 대하여 고찰하였다.

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Development of Ag nanoparticles coated ZnO nanoplates and study on its antimicrobial activity

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최근에 유기계 항균제에 내성을 보이는 슈퍼바이러스의 탄생으로 전 세계적으로 큰 위협요인이 되고 있으며 이로 인해 새로운 항균제 개발에 관한 연구가 큰 관심을 받고 있다. 그러나 항균제 개발에 필요한 막대한 연구비에 비하여 시장성이 크지 않기 때문에 제약회사들은 새로운 항생제 개발에 소극적인 자세를 취하고 있는 현실이다. 따라서 기존에 오랜 기간 사용되어온 유기계 항생제를 항균성이 있다고 잘 알려진 무기물질들로 바꾸려는 시도는 막대한 연구비를 투자하지 않고도 새로운 항생제 또는 항균제를 개발할 수 있다는 점에서 학계와 산업체에서 세계적으로 많은 관심을 받고 있다. 본 연구실에서는 이전 연구에서 (0001)면이 발달한 ZnO nanoplate 가 자외선 조건에서 다른 모양의 ZnO 나노입자 보다 가장 우수한 항균성을 나타내는 것을 확인한 바 있다. 본 연구에서는 ZnO nanoplate 의 항균 특성을 더욱 향상시키기 위하여 항균성이 우수하다고 알려진 Silver 나노입자를 ZnO nanoplate 와 Hybrid 시키고 ZnO nanoplate 와 비교하여 항균력이 얼마나 향상 되는가를 확인하였다.

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Recovery/recycling technology of glycosylated enzyme using the magnetic composite for lignocellulosic bioethanol production cost savings

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지구 온난화 및 석유자원 고갈에 따른 차세대 친환경 에너지원 확보가 이슈화되어 목질계 바이오매스와 같은 비식용원료를 활용하는 바이오에탄올 생산 기술에 대한 연구가 최근 큰 관심을 받고 있다. 목질계 바이오에탄올 생산에 있어 당화효소가 생산 비용에서 차지하는 비율은 약 30-50%로 특정회사에서 독과점으로 생산되고 있는 당화효소를 전량 수입해야 하는 국내 환경에서 효소 생산 공정의 개선 없이는 목질계 바이오에탄올의 생산비용 절감이 어려운 상태이다. 따라서 본 연구에서는 자기적 특성이 우수한 자성복합체[(Graphene Oxide(GO)-Magnetic Nanoparticle(MNP)]를 개발하고 이를 이용하여 당화효소를 회수/재활용함으로써 목질계 바이오에탄올 생산단가를 절감시킬 수 있는가를 탐색하였다. 합성한 자성복합체는 TEM 이미지와 입도분석 등으로 확인하였으며 당화과정을 모색하여 흡광도를 통해 생성된 글루코오스의 농도를 측정하였다. 실험 결과, 자성복합체를 이용하여 당화효소를 재활용한 경우와 자성복합체를 이용하지 않고 재활용하여 5 차례 비교하였을 때 5 번째 재활용 과정에서 당화수율이 5.7 배이상 높았으며 소용량 보다 대용량 조건으로 당화효소를 재활용할 경우 더욱 우수한 당화수율을 얻을수 있었다. GO-MNP 와 같은 자성복합체를 이용한 목질계 바이오에탄올 생산을 위한 당화효소 회수/재활용 기술은 세계 최초로 시도되는 것으로써 관련기술 분야에서 기술적 우위를 선점할 수 있으며 공정비용을 획기적으로 절감할 수 있는 차별화된 당화 시스템을 구축하여 국내 목질계 바이오에탄올 시장의 활성화를 가져올 수 있을 것으로 기대된다.

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Study on Photothermal and Magnetothermal Effect of Urchin-like Fe3O4@Au Core@Shell Nanostructure

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Fe3O4 자성체는 RF 유도전류에 의하여 형성된 자기장에서 Fe3O4 의 자기모멘트(Magnetic Moment)의 회전과 나노 입자 자체의 회전에 의해 열이 발생하며 이를 자성 나노 입자의 자화열 효과 (Magnetothermal)라고 한다. 한편, 금 나노입자의 경우 표면 플라즈몬 공명 (Surface plasmon Resonance)과 일치하는 파장의 빛을 조사해 주면 금속의 자유 전자들이 빠른 속도로 진동하면서 원자와 부딪히게 되고 이에 따라 열이 발생하게 된다. 이를 광열효과 (Photothermal)이라 한다.성게구조의 Fe3O4@Au 코어@쉘 나노입자는 자화효과를 갖는 Fe3O4 나노 입자와 광열효과를 갖는 Au layer 가 결합된 형태를 갖는다. 따라서 성게구조의 Fe3O4@Au 코어@쉘 나노입자는 광열효과와 자화열 효과를 동시에 적용할 수 있으며 각각의 단일효과를 이용한 암 치료 기술과 비교하여 보다 효과적으로 암을 치료할 수 있는 기술을 개발 할 수 있을 것으로 예상된다. 본 연구에서는 이러한 아이디어를 바탕으로 성게구조를 갖는 Fe3O4@Au 코어@쉘 나노입자에 빛과 유도전류자기장을 동시에 조사하면서 Fe3O4@Au 코어@쉘 나노입자로부터 발생된 열이 단일 빛과 유도전류자기장을 각각 가하였을 때 보다 얼마나 향상되는가에 대하여 자세히 살펴보았다.

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Development of transparence coating materials with super-hydrophobic property

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국내시장에서 판매되는 대부분의 발수 코팅제는 발수 능력이 검증된 Fluorine 계 또는 Silane 계 폴리머를 사용하고 있으나 오랜 기간 유사한 물질들을 이용해 왔기 때문에 제품의 기술력에 큰 차이를 보이지 않고 있으며 높아져 가는 사용자들의 요구를 충족시키기 위해서는 더 우수한 발수 능력이 요구된다. 한편, 학계에서는 다양한 나노입자를 이용한 초발수 코팅 물질들이 연구되어져 왔으며 대표적으로 실리카 나노입자를 이용한 초발수 코팅 기술이 있다. 그러나 실리카 나노입자의 경우 초발수 성능을 도출하기 위해서는 기판 위에 균일하며 밀집된 구조체를 유지해야 하며 따라서 기존의 불소계 발수코팅제와 같이 스프레이 형태의 제품을 구현하기 어렵다는 단점이 있다. 본 연구에서는 Fluorine functionalized silane 을 실리카 원료로 사용하여 실리카 나노입자를 합성하였으며 합성된 실리카 나노입자는 표면에 도입된 Fluorine 으로 인해 매우 우수한 초발수 성능을 나타냈으며 스프레이 형태로 코팅하였을 때 실리카 나노입자들이 Networking 된 구조를 형성하면서 두껍게 코팅하지 않아도 초발수 능력이 나타났다. 따라서 투명성에서도 기존의 실리카 나노입자를 이용한 초발수 코팅제와 비교하여 매우 우수하게 나타났다.

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Influence of poly(vinyl alcohol) on pore structure of mesoporous SBA-15: Mesopore connectivity, surface area and micropore size distribution

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In 1998, Stucky`s group reported a new class of mesoporous materials synthesized at low pH and with non-ionic surfactant as templates. The hexagonally ordered materials of this class was called SBA-15 and displays mesopore structure similar to that MCM-41, however, SBA-15 shows larger cylindrical, hexagonal pore diameters and wall thicknesses and its mesopores are connected by micropores. In this study, effect of poly(vinyl alcohol) (PVA) in the synthesis on pore structure of mesoporous SBA-15 was investigated. It was found that, by addition of PVA, the surface area and porosity of SBA-15 is increased, while the structure and size the mesopores changed. Nitrogen adsorption-desorption measurements indicate that PVA introduces additional pores with pore sizes of around 2 nm into the mesopore wall. Thus, this may be due to the improved connectivity of mesopores by the reaction of hydrophilic PVA, which was added during synthesis, and triblock copolymer P123 with PEO chains and/or the presence of PVA itself. Accordingly, the mesoporous SBA-15 formed in the present study were confirmed to have improved the specific surface area and micropore volume through the PVA loading.

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Design and synthesis of fluorescent chemosensors based on naphthalene and thiadiazole-containing excited-state intramolecular proton transfer (ESIPT) molecules

문혜린 박상혁*

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Fluorescent chemosensors are continuously being designed and developed due to their wide range of applications. Among them, fluorescence chemosensors which are based on excited-state intramolecular proton transfer (ESIPT) materials have an advantage of the uncomplicated detection due to their large Stokes' shift by the result of intrinsic 4-level photocycle scheme of the ground and excited states of two different tautomers. For instance, 2-(20-hydroxyphenyl)benzoxazole (HBO) preferentially adopts the enol (E) form stabilized by intramolecular hydrogenbonding in the ground state. Upon photoexcitation at 320 nm, the excited enol (E*) is quickly converted into the excited keto (K*) tautomer by ESIPT on a subpicosecond time scale, which gives rise to an emission band (~510 nm) with a large Stokes shift. However, up to now, core unit of ESIPT chemosensors are limited to several well-known molecules such as benzoxazole, sulfonamide, and hydroxyflavone. In this work, we have designed and synthesized novel class of ESIPT-based chemosensor molecules by the introduction of naphthalene- and thiadiazole group instead of benzene and benzoxazole unit. Anion detection using the new materials will be presented in this work

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Foldecture as a Core Material with Anisotropic SurfaceCharacteristics

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The synthesis of microscale, polyhedrallyshaped, soft materials with anisotropic surface functionalityby a bottom-up approach remains a significant challenge.Herein we report a microscale molecular architecture(foldecture) with facet-dependent surface characteristicsthat can potentially serve as a well-defined catalytictemplate. Rhombic rod shaped foldectures with six facetswere obtained by the aqueous self-assembly of helical β-peptide foldamers with a C-terminal carboxylic acid. Ananalysis of the molecular packing by X-ray diffractionrevealed that carboxylic acid groups were exposedexclusively on the two (001) rhombic facets due toantiparallel packing of the helical peptides. A surfaceenergy calculation by molecular dynamics simulation wasperformed to provide a plausible explanation for thedevelopment of anisotropy during foldecture formation.The expected facet-selective surface properties of thefoldecture were experimentally confirmed by selectivedeposition of metal nanoparticles on the (001) facets,leading to a new class of sequentially constructed,heterogeneous “foldecture core” materials.

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Controlled Coloration of β-FeOOH Yellow pigments

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Red-Yellow color akagneite (β-FeOOH) and red color hematite (α-Fe_2O_3) have attracted much interest owing to eco-friendly pigments. Especially, rod type β-FeOOH is easily tuned color change from redness to yellowness through various length. This work describes aspect ratio control of β-FeOOH nanorods by regulating the concentration of $FeCl_3.6H_2O$. Concentration of chloride ions of $FeCl_3.6H_2O$ solution is the key parameter to control the growth and aspect ratio of β-FeOOH nanorods. We studied the relation of growth mechanism and coloration of β-FeOOH nanorod. The length of the nanorod could be varied from 100 to 600 nm. We confirmed that light yellowness (*b**) of β-FeOOH improved with increased length. In addition, their physical properties were evaluated through analysis of coloration, reflectivity and shape.

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Catalytic Performance of Binary Copper-Manganese Oxide Coated on Porous Ceramic Supports

변미림 이희숙 김세희 한양수*

(주)세일에프에이 연구소

Binary copper manganese oxide catalyst supported on granule-type porous ceramic supports was prepared and the catalytic activity for carbon monoxide removal at ambient temperature evaluated. For the preparation of Cu-Mn coating solution, precursory Cu-Mn slurry (30wt%) prepared by redox precipitation was dispersed in various media, organic solvent such as cellusovle and acetylaectone and inorganic binder solution such as colloida silica, water-glass solution, boehmite colloid, and clay suspension. Such prepared Cu-Mn-containing dispersion was coated on porous ceramic supports by dip process, followed by drying at 120℃ and heating at 280 ~ 300℃ under an ambient atmosphere. The catalytic activity of the supported Cu-Mn catalyst for carbon monoxide removal at ambient temperature was evaluated, which will be discussed in detail on the basis of XRD, XRF, nitrogen isotherm analysis results.

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New Preparation Method of Botallackite-type Basic Copper Acetate

이지호 윤주영 이희숙[1] 한양수[1,*]

(주)나노스페이스 연구소 [1](주)세일에프에이 연구소

In the present study, attention has been focused on the new synthetic method of anion-exchangeable layer structured compound. The basic copper hydroxide acetate, $Cu_2(OH)_3(CH_3COO)\cdot H_2O$, with a botallackite-type layer structure, was prepared by a simple refluxing process of copper acetate aqueous solution at >70 ℃ under ambient atmosphere. According to X-ray diffraction analysis (XRD) and scanning electron microscopy (SEM) observation thus prepared $Cu_2(OH)_3(CH_3COO)\cdot H_2O$ has a basal spacing (d_{001}) of 9.2 Å and a well-developed hexagonal plate-like shape, respectively. The interlayer acetate ions are located between the positively charged copper hydroxide layers could be exchanged with both organic intercalants like sodium dodecyl sulfate and inorganic ones like MnO_4^-.

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Preparation of Dipeptides Containing Layer Nanocomposites by Solid State Intercalation Process

<u>변미림</u> 최진주[1] 윤주영[1] 한양수[1,*]

(주)세일에프에이 연구소 [1](주)나노스페이스 연구소

Layered nanocomposites of expandable clay (montmorillonite, Kunipia G, CEC ~120mequiv./100g) and dipeptide molecules were prepared by a simple solid state intercalation method. 5 kinds of dipeptide compounds (Paromomycin, Fusaricidin, Q3, Q4, AP-25) were used as guest molecules. In the typical preparation, desired amount of clay and dipeptide powder were just mixed with a few drops of solvent(methanol) in agate mortar, and ground softly for 30min, followed by heating at 100℃ for 1hs.Above process could be repeated, it necessary, to obtain single phase intercalated product. It was observed that the dipeptide molecules are successfully intercalated between the silicate layers to form dipeptide-silicate layer complexes with the basal spacing (d001) of 12.3~17.1Å depending on the guest molecules.

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Preparation of Mn-pillared Layer Copper Hydroxide by Coprecipitation Process

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(주)나노스페이스 연구소 [1](주)세일에프에이 연구소

The manganese species (MnO_4^-) pillared layer copper hydroxide, $Cu_2(OH)_3(MnO_4)$, was prepared by a direct coprecipitation process. In a typical preparation, copper acetate solution and KMnO4 solution were titrated simultaneously into the pH-controlled base solution, which resulted in the formation of Mn-species intercalated copper hydroxide layer with basal spacing (d_{001}) of 7.2 Å. It was found that the solution pH, reaction temperature and period played an important role in the preparation of Mn-pillared compound. Higher pH (pH >10), higher reaction temperature (>60 ℃) and extend reaction time (>6 hr) cause the collapse of layer structure into crystalline CuO and other amorphous-like products within our experimental conditions.

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Airborne Molecular Contamination, and Electrical Transports through ITO-based van der Waals Interface

공규돈 김미소 윤효재*

고려대학교 화학과

This poster focuses on electrical characterization of van der Waals interface formed with ITO (tin-doped indium oxide) using EGaIn (eutectic gallium indium alloy) microelectrode. For developing optoelectronic devices ITO-based van der Waals interfaces are produced inevitably, but it is experimentally difficult to investigate them. We studied how electrical characteristics of ITO-based van der Waals interface responds to the degree of contamination of the ITO surface by using ITO//Ga_2O_3/EGaIn junctions. Comparisons of current densities for ITO//Ga_2O_3/EGaIn junctions prepared with differently cleaned (with UV light, ozone, and/or organic solvent rinsing) ITO surfaces indicated that UV/ozone surface cleaning of ITO surface enhances the electrical conductance of the van der Waals interface up to 10^3, and improves the accuracy and reproducibility of performance of ITO electrode.

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Role of a Surfactant in Tailoring Shape Evolution of 3D Molecular Architecture

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한국과학기술원(KAIST) 화학과

There have been tremendous efforts to control the three-dimensional (3D) shapes of nano/microstructures, since the shape is one of the most important parameter determining physicochemical properties of materials. Therefore, both tailoring shapes and understanding the mechanism of morphogenesis have been of great interest to material scientists in order to elicit the targeted functions. For example, using surfactants is a common method to control the shape of a wide variety of organic and inorganic crystals. In most precedent studies, surfactant molecules are known to adsorb preferentially onto the specific crystal facets to stabilize surface energy and inhibit the growth. However, quantitative investigation of the interactions between crystal facets and surfactant has been recognized as a challenging task. Here, we report the role of ionic surfactant cetyltrimethyl ammonium bromide (CTAB) in shape evolution of 3D molecular architectures obtained from the self-assembly of a β-peptide foldamer. Shape evolution tendency and molecular packing structures of the self-assembled structures were analyzed by electron microscopy and diffraction experiments. Moreover, molecular dynamics simulation provided a plausible explanation for the role of surfactant molecules in crystal growth mechanism and interactions between surfactants and building block peptides in detail.

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Ultra-Sensitive Bragg-Reflective Photoluminescent Porous Silicon for Explosive Vapors

박미애 손홍래*

조선대학교 화학과

Novel photoluminescent Bragg-reflective porous silicon (PBR PS) exhibiting dual optical properties, both optical reflectivity and photoluminescence, were developed and used as explosive sensor. PBR PS samples were prepared by an electrochemical etch of n-type silicon under the illumination with a 300 W tungsten filament bulb for the duration of etch. The etching solution consisted of a 1:1 volume mixture of aqueous 48% hydrofluoric acid and absolute ethanol. Typical etch parameters for the generation of PBR PS involved using a periodic square wave current with 55 repeats. PBR PS exhibits strong red color reflection at 620 nm and strong red photoluminescence at 650 nm. The optical properties of free-standing PBR PS were investigated. The front side surface of PBR PS shows both reflectivity and photoluminescence, however the back side surface of free-standing PBR PS shows only reflectivity without PL. Surface and cross-sectional morphology and optical characteristic were determined by using scanning electron microscopy and optical spectroscopy. Both reflectivity and PL were simultaneously measured under the exposure of explosives. Quenching of luminescent by electron deficient nitroaromatic explosives, such as trinitrotoluene (TNT), pentaerythritol tetraanitrate(PETN), cyclotrimethylenetrinitramine (RDX).This research was supported by Agency for Defense Development.

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Porous Silicon Nanowires Prepared from an Electrochemical Etching and Metal-Assisted Chemical Etching

정대윤 손홍래*

조선대학교 화학과

We report the synthesis of porous silicon nanowires through a metal-assisted chemical etching of porous silicon in a solution of hydrofluoric acid and hydrogen peroxide. The morphology of porous silicon nanowires was characterized by scanning electron microscopy, and transmission electron microscopy. The etch-rate of porous silicon nanowires is faster than that of silicon nanowires but slower than that of porous silicon. The porous silicon nanowires distribute uniformly on the whole porous silicon layer and the tips of the porous silicon nanowires congregate together. The porous silicon nanowires whose diameters are less than 5 nm showed a SAED pattern without lattice fringe indicating that they retain a single crystalline and a sponge-like porous structure.This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Enlarged pore size distribution and High Pore Volume of Graphene Flakes for Hybrid Electric Car

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성균관대학교 화학과 [1]성균관대학교 화학과, CSMM

Supercapacitors consisting of electrical double layer capacitors offer fast charging-discharging rates and the ability to operate for millions of cycles. These devices can be applied for power hybrid electric vehicles and portable electronic equipment. In order to obtain a high performance supercapacitor, there are several factors that must be achieved including high specific surface area (SSA), high electrical conductivity, and high diffusion rate of the electrolyte due to an appropriate pore volume. Herein, we report a high performance supercapacitor using activated non-stacked reduced graphene oxide (a-NSrGO) that has a high SSA (up to 999.75 $m^2\ g^{-1}$) with intrinsic graphene conductivity and a fast diffusion rate of the electrolyte. Due to the high total pore volume (5.03 $cm^3\ g^{-1}$) and wide pore size distribution from macro- to micropores (main pore width: 0.61 - 0.71 nm) in the a-NSrGO sheets, the as-prepared a-NSrGO electrode shows high specific capacitance (105.26 F g^{-1}) and short relaxation time (τ_0 = 1.5 s) in a propylene carbonate (PC)-based organic electrolyte. The maximum energy density of 79.8 Wh kg^{-1} and power density of 67.6 W kg^{-1} were estimated in full packaged coin cell. The high performance of the a-NSrGO supercapacitors is attributed to their specific appearance and enlarged pore distribution with high SSA. This is expected to find application in conventional supercapacitor devices.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of HF Gas Based on an Oxidized DBR Porous Silicon Interferometer

박주천 손홍래*

조선대학교 화학과

Detection of HF gas is important since it is highly toxic (the Occupational Safety and Health Administration, OSHA, limit for human exposure to HF in the gas phase is 3 ppm) and used in large quantities in industrial environments, in particular in the semiconductor and petroleum refining industries. Three different devices are used to measure toxic gases in an industrial environment. Fourier transform infrared spectroscopy (FTIR) is accurate but it has a high cost and there is a delay between the collection of the gas samples and their analysis. Solid state metal oxide sensors allow measurement of gas through changes in their electrical conductivity. They are inexpensive and have a very long lifetime (up to 10 years), but their selectivity is low. Finally, the most commonly used sensing technique is electrochemical. In these sensors, gas diffuses through a membrane and reacts at an electrolyte-catalyst interface creating a current which is proportional to the gas concentration. The detection limit is 0.1 ppm of HF in 1 min. A major problem with electrochemical sensors is selectivity, in as far as these devices can respond to gases other than those they are designed to measure. For example, it is not possible to differentiate HF and HCl. The new HF detection technique that we demonstrate in this work is cheap and specific for HF. The oxidized distributed Bragg reflector porous silicon (ODBR PSi) has been successfully prepared and used for sensing HF in the gas phase. Under white light illumination ODBR PSi displays Bragg interference, which has been used as a sensitive transducer in HF gas sensors. In this paper, we show that ODBR PSi interferometers are sensitive to dissolution of SiO2 in the inner pore structure and can be used to detect HF in the gas phase. For detection of HF, the reaction of the silicon oxide with HF gas, results in a decrease of the refractive index of ODBR PSi. A decrease in refractive index is resulting from the conversion of the SiO2 to SiF4, which is volatile under the conditions of the experiment. Detection of HF gas was achieved by monitoring the shift of the Bragg peak versus the exposure time of the ODBR PSi film.This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Carbon Quantum Dots: A Fluorescence Turn-on Sensor for Explosives

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조선대학교 화학과

Blue photoluminescent carbon quantum dots were successfully prepared by tuning the carbonization of citric acid from the pyrolysis reaction. Optical characterization of carbon quantum dots was investigated by UV-vis and fluorescence spectrometer. Quantum efficiencies of carbon quantum dots were obtained from fluorescence spectroscopy. Morphologies of carbon quantum dots were obtained using TEM. TEM image displays the carbon quantum dots with the size of about 5 nm. Carbon quantum dots were used to detect explosives such as nitroaromatic, nitramine, and nitrate ester compounds. An increase of photoluminescence from carbon quantum dots as a fluorescence turn-on sensor was measured upon the exposure of explosive compounds. The sensing mechanism of carbon quantum dots was investigated.This research was supported by Agency for Defense Development.

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Ultra-Sensitive Porous Silicon Quantum Dots As an Explosive Sensor

kimjinsoo 조보민 손홍래*

조선대학교 화학과

Photoluminescent(PL) porous silicon were prepared by an electrochemical etch of n-type silicon under the illumination with a 300 W tungsten filament bulb for the duration of etch. The red PL emitting at 650 nm with an excitation wavelength of 360 nm was due to the quantum confinement effect of silicon quantum dots in porous silicon (PS). Hydroxy-terminated red luminescent PS was obtained by an electrochemical treatment of fresh PS with the current of 150 mA for 60 seconds in water and sodium chloride. As-prepared PS was fractured by ultra-sonication and centrifuged in toluene solution to obtain PL silicon quantum dots. Chloromethyltetraphenylsilole exhibiting an emission band at 520 nm was reacted with hydroxy-terminated silicon quantum dots to give a silole-capped silicon quantum dots (SiQDs).As prepared silole-capped SiQDs were exposed to two different phases of TNT, RDX, and PETN for sensing which resulted in noticeable quenching of PL. For vapor sensing, silole-capped SiQD was coated on a lens, which then was illuminated by a light excitation source. Vaporized analytes were blown onto the coated lens and was monitored by a complementary metal?oxide?semiconductor (CMOS). PL intensity was recorded by a computer, which showed that when the vapor of the analytes contacted the sensor membrane, PL from the lens quenched promptly and recovered when the supplying of the vapors stopped due to presumably via electron transfer mechanism. This revealed that real time detection of explosive vapors with high sensitivity was feasible.Sensing liquid phase of the analytes was carried out by using UV-vis and fluorescence spectrometer to investigate the changes in fluorescence when different concentrations of analytes are added. By employing stern-volmer constant, we could see that it detected the analytes reliably and rapidly.Lifetime was measured to observe changes in their optical behavior of pre/post-reaction and when introduced to the TNT solution. The result of pre/post-reaction lifetime comparison showed that silole-capped SiQD resembled as-prepared SiQD. With the increase of TNT concentration in silole-capped SiQD solution, the intensity of PL increased however, their lifetime did not change significantly. This research was supported by Agency for Defense Development.

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H-terminated and HO-terminated Silicon Quantum Dots Showing an Extraordinary High Quantum Yield

조보민 손홍래*

조선대학교 화학과

Photoluminescence properties and surface morphologies of porous silicon were investigated by controlling of etching times and applied current densities. FE-SEM image of porous silicon surface indicated that the porous silicon prepared at currents below 200 mA/cm2 exhibited very stable and even surface. However the porous silicon prepared at currents above 300 mA/cm2 displayed the cracked surface of porous silicon. This cracked surface was collapsed to give cracked domains at currents over 500 mA/cm2. Photoluminescence of porous silicon was investigated by controlling of etching times and applied current densities in the range from 50 sec. to 900 sec. and from 50 mA/cm2 to 800 mA/cm2, respectively. Photoluminescence intensity of porous silicon increased gradually during etching process, reached maximum, and then decreased as the etching time increased. Porous silicon showed the best photoluminescence efficiency was prepared at currents of 200 mA/cm2 and etching time of 300 sec. Silicon quantum dots were obtained from the as-prepared porous silicon by using ultrasono-method. Quantum yields for the H-terminated and HO-terminated silicon quantum dots were measured and extraordinary high quantum yields for both silicon quantum dots were obtained.This research was supported by Agency for Defense Development.This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Artesunate-layered zinc hydroxide nanohybrid with enhanced oral bioavailability

김지영 양재훈 최진호*

이화여자대학교 화학.나노과학과

Low bioavailability of artesunate (AS), anti-malaria drug, is attributed to its low solubility in water. In order to overcome this problem, the novel drug delivery vehicle system with sustained release property was successfully demonstrated by intercalating AS into layered zinc hydroxides (ZBS) via co-precipitation. According to the powder x-ray diffraction analysis, the basal spacing of AS-ZBS nanohybrid was determined to be 2.88 nm, indicating that AS was successfully incorporated into the ZBS layers, which was also confirmed by 1-D electron density mapping analysis and TEM analysis. The fourier transformed infrared spectra revealed that AS molecules were deprotonated and electrostatically incorporated between cationic zinc hydroxide layers without any structural change. Through CHNS analysis, TG analysis and HPLC analysis, the contents of AS for AS-ZBS nanohybrid was determined to be 45.8 wt%. Furthermore, AS-ZBS nanohybrid was coated with Eudragit- L100 (anionic polymer) for the pH-dependent dissolution property (AS-ZBS-L100). AS-ZBS-L100 nanohybrid showed the greatly enhanced dissolution rate of AS in simulated intestinal condition (pH 6.8) compared with the intact AS. *In vivo* pharmacokinetic study was performed in rats via oral administration to compare the absorption of artesunate for AS-ZBS-L100 nanohybrid and intact AS. According to the plasma concentration-time curve, the pharmacokinetic data such as AUC and C_{max} values for the AS-ZBS-L100 nanohybrid (AUC = 177.2 ± 30.1 h mg/L and C_{max} = 51.1 ± 14.8 μg/mL) were remarkably larger than those of intact AS (AUC = 23.3 ± 3.4 h mg/L and C_{max} = 20.1 ± 4.3 μg/mL). Therefore, AS-ZBS-L100 nanohybrid system has a great potential as a malaria drug formulation with enhanced bioavailability.

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Self-Assembled Amphiphlic Graft Poly(organophosphazene) Micellar Host with Hydrophobic Guest

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A facile soft chemical route to resveratrol-polyphosphazene micelle (RSV-PPZ) was demonstrated on the basis of guest molecule mediated self-assembly. We synthesized a new type of amphiphlic graft PPZ ($[NP(MPEG550)_{1.5}(GlyPheLeuEt)_{0.5}]_n$) modulated by varying the balance of hydrophilicity and hydrophobicity to induce tunable morphology in a micellar structure. RSV, the highly hydrophobic polyphenolic compound, was encapsulated with newly designed PPZ by hydrophobic-hydrophobic interaction. RSV medicated PPZ micelles were stable in very low critical micelle concentrations (~20 mg/l) with spherical morphology and average size 14 nm of RSV-PPZ. And an attempt was also tried to understand an effect of micelle structure of RSV-PPZ on solubility enhancement and reducing toxicity. Therefore, we can conclude hydrophobic guest molecule mediated micelle could be a potential candidate for drug delivery system.

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Polymer-Based Photonic Crystals Replicated from DBR Porous Silicon

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Synthesis of nanostructured materials has emerged as a useful and versatile technique to provide the use of encoded materials for chemical and biological sensors, high throughput screening, and controlled release drug delivery. Since the discovery of porous silicon (PSi) from silicon wafer, research has been associated with emerging technologies, such as photonic crystals for optical band pass filters and micro chemical reaction applications in micro chemical and micro fuel cells. DBR PSi is an attractive candidate for building nanostructured composite materials because the porosity and average pore size can be tuned by adjusting the electrochemical preparation conditions that allow the construction of photonic crystals. DBR PSi can be generated by applying a computer generated two-distinct current densities. DBR PSi exhibits unique optical properties. The resulting DBR PSi films can be lifted off from the silicon substrate to obtain a free-standing DBR PSi films. For many applications, free-standing DBR PSi is limited by its chemical and mechanical stability because these free-standing films are very brittle. Here, we have prepared polymer replicas showing a desired reflectivity by the casting of polymer solution onto a porous silicon dioxide multilayer and provides the means for the construction of complex photonic structures with polymers. The photonic polymer replicas showing a desired reflectivity by casting of polymer solution onto a porous silicon dioxide multilayer have been prepared. The photonic polymer replicas are robust in ambient condition and exhibit an excellent reflectivity in their reflective spectra. The photonic band gaps of replicas are narrower than that of typical semiconductor quantum dots. The means for the construction of complex photonic structures with polymers have been provide.This work was supported by the Human Resource Training Program for Regional Innovation through the Ministry of Education and National Research Foundation of Korea (NRF-2012H1B8A2026282)

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Porous amino acid-layered double hydroxides and their CO_2 uptake behaviors

최고은 양재훈 최진호*

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A soft chemical route to amino acid layered double hydroxide (LDH) nanohybrids was demonstrated on the basis of an intercalative ion-exchange reaction. Two different amino acids, phenylalanine and glutamic acid, were intercalated and stabilized in the interlayer space of a 2-dimensional double hydroxide lattice by electrostatic interaction. An attempt was also made to understand the effect of the intracrystalline structure of the amino acid in the LDH on the specific surface area, porosity, and gas sorption properties of the hybrid. According to the X-ray diffraction analysis, the basal spacings of LDH intercalated with phenylalanine and LDH intercalated with glutamic acid were expanded to 1.80 and 1.22 nm, respectively, relative to that of the pristine $Mg_2Al\text{-}NO_3$-LDH (0.88 nm), which indicates that amino acid molecules were successfully intercalated into the LDH. Fourier transform infrared spectra for both samples confirmed that the carboxylic acid group in the amino acid is anionic carboxylate under basic conditions and it eventually interacts with the positively charged LDH surface. From N_2 adsorption/desorption analysis, the BET specific surface area of the LDH intercalated with phenylalanine was found to be twice as large as that for the LDH intercalated with glutamic acid. However, the CO_2 adsorption capacity of the former was determined to be three times more enhanced than that of the latter, due to an enhanced specific surface area and effective amine sites to form carbamates.

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Effect of Molybdenum Sulfide on the Electrocatalytic Activity of Pd Nanoparticle in Alkaline Electrolyte

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In this study, we report the effect of molybdenum sulfide (MoS_2) on the electrocatalytic activity of Pd nanoparticles in alkaline media. First, Pd/MoS_2 sample was synthesized by ultrasound-assisted polyol synthesis for 3 h. Structural characterizations showed that our sample have several nanosized Pd particles which are highly dispersed on MoS_2. Electrochemical analysis of Pd/MoS_2 was carried out by rotating disk electrode (RDE) measurement in alkaline media. We found that Pd/MoS_2 have suitable oxygen reduction reaction (ORR) and ethanol oxidation reaction (EOR) activity compare with commercial Pt/C. Furthermore, we also found that Pd/MoS_2 have enhanced electrochemical durability than Pt/C. Based on the electrochemical results, we demonstrated that strong metal-support interaction (SMSI) between Pd and MoS_2 leads the enhanced electrocatalytic activity and durability.

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PEMFC용 고효율 및 고내구성 전극촉매 기술 개발

김해리

오-덱(주) 기술연구소

본 연구는 PEMFC 용 고효율 및 고내구성 전극촉매를 위하여 성능에 영향을 미치는 백금의 분산성 향상기술, 내구성 향상을 위한 담지체 적용 기술 등 전극촉매에 적합한 합성기술을 개발하는 데 목적이 있다. 또한 개발된 전극촉매의 연료전지 자동차 적용을 위한 대량생산 기술을 개발하는 데 목적이 있다.전극촉매의 경우 백금의 담지량이 매우 높아 담지체인 카본 위에 고르게 담지시키기는 매우 어렵다. 백금을 고르게 담지시키기 위하여 합성과정 중 첨가제를 추가로 투입하거나 추가 분산공정을 도입하여 분산도를 높이는 등의 연구가 진행되고 있지만 이와 같은 방식으로는 담지체에 분산성을 높여 담지할 수 있는 백금량에 한계가 있다.이와 같은 백금 분산성과 담지량의 한계 문제를 해결하고자 백금 전구체와 카본과의 흡착방법 및 전구체 환원조건을 조절하여 효과적인 합성방법을 연구하였다. 개발된 전극촉매의 합성방법은 백금을 카본에 2 단계에 걸쳐 담지시키는 방법으로 자체 개발한 전극촉매용 백금 전구체를 이용하여 카본표면에 1 차적으로 물리적 고착을 진행하고 2 차적으로 화학적인 고착기술을 적용하여 원하는 백금 함량을 가지는 촉매를 제조하는 형태이다. 이와 같은 방법으로 합성된 전극촉매의 표면분석을 통해 고담지량의 촉매임에도 담지체 위에 2~3nm 정도의 미세한 입자로 고르게 분산되어 있음을 확인하였으며 또한 전기화학적 활성평가(I-V curve)에서 1350mA/cm$_2$@0.6V(25cm$_2$ MEA)의 성능으로 상용촉매와 동등이상의 성능을 보이고 있음을 확인 할 수 있었다.위 합성방법을 이용하여 전극촉매의 대량생산 기술을 개발하였다. 20L 급 Pilot scale 을 통하여 대량생산 공정개선이 진행되었으며, Scale up 을 진행하여 50L 급의 합성 System 구축 및 대량생산 공정을 안정화 하는데 성공하였다. 현재 합성 1 회당 Cathode 300g, Anode 160g 의 촉매 생산 용량을 만족하며 이는 국내 최대 규모의 전극촉매 합성 시스템이다.이외에도 전극촉매의 내구성 향상을 위한 Pt-

TiO_2 촉매기술개발, 전극촉매의 백금량 저감을 위한 PtPd alloy 촉매 개발 등 연료전지 상용화를 위한 촉매 기술을 지속적으로 개발 중에 있다.

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Electrochemical growth of flat Pt films with an unusually high surface area

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백금은 다양한 반응에 대해 전기화학적 촉매활성이 좋은 금속으로 널리 알려져 있다. 특히 평평한 나노다공성 구조체를 형성하고 있는 백금의 경우 매우 큰 표면적을 가지는 특성 때문에 순수한 백금보다 더 우수한 전기촉매적 활성을 보인다. 이를 형성하는 다양한 방법들 중에서도 전기화학적 석출법은 비교적 간단하게 구조체를 형성할 수 있다는 장점이 있다. 본 연구에서는 환원제 또는 주형을 이용하여 구조체를 형성하는 선행연구들과 달리 매우 간편한 방법인 전기화학적 석출법만을 이용하여 큰 표면적을 가지는 평평한 백금 구조체를 형성하였다. 또한 전기화학적 석출법에서 조작 가능한 변수에 따라 형성되는 구조의 차이를 주사 전자 현미경과 전기화학적 방법을 통해 관찰하였으며, 큰 표면적의 원인이 되는 기공의 존재여부는 투과 전자 현미경을 통해 확인하였다. 그 결과 다른 금속 이온과는 달리 백금을 전구체로 사용하였을 경우에만 큰 표면적을 가지는 평평한 구조체가 형성되었다. 또한 백금 전구체의 농도와 석출 전위가 형성되는 구조에 미치는 영향을 관찰한 결과 넓은 범위의 조건에서 큰 표면적의 백금 구조체가 형성되는 것을 확인하였다. 마지막으로 석출 속도와 표면적과의 관계를 관찰, 비교 분석하였으며 이를 통해 구조 내부에 형성되는 기공이 석출 속도와 관련이 있음을 확인하였다. 이로써, 선행연구들과 비교하여 보다 쉽게 매우 큰 표면적을 가지는 평평한 백금 구조체를 형성하였고 석출 조건에 따라 구조 내에 기공이 형성되는 정도의 차이를 표면적 측정을 통해 확인하였다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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In-situ generation of Au nanostructures by anodic dissolution followed by cathodic deposition

권수지 김종원*

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금 나노구조체는 벌크한 금과 달리 표면적이 크며 독특한 구조를 가져 물리적 및 화학적 성질이 다르다. 이는 형성된 구조에 영향을 받는 표면 증강 라만 산란법에의 기판으로 응용이 가능하여 활성을 증대시키는 금 나노구조체를 형성하는 선행 연구들이 보고되었다. 본 연구에서는 기존의 전기화학적 석출법에 변화를 주어 독특한 금 나노구조체를 형성하고 주사 전자 현미경을 통해 확인하였으며 표면 증강 라만 분광법에의 활성을 관찰하였다. 금 이온이 포함되어 있는 용액을 사용하여 구조를 형성하는 기존의 전기화학적 석출법과 달리 금 전극 표면 자체를 산화하여 금 이온을 생성한 후 그 이온을 환원시켜 구조를 형성하는 특이성을 보인다. 먼저 산화 전위 및 산화 시간에 따른 금 나노구조체의 구조는 분포도에 차이가 보인다. 이어 환원 전위를 변화하여 다양한 모양의 금 나노구조체가 형성하는 것을 관찰하였으며 환원 시간의 변화에 따라 구조의 형성 과정을 살펴보았다. 8 mM 4-아미노티오페놀을 이용하여 표면 증강 라만 산란에의 활성을 관찰한 결과 가장 극대화할 수 있는 환원 전위 조건은 -0.3 V 였다. 금 이온을 전극 표면으로부터 얻어내는 특이성을 가진 금 나노구조체 형성법을 통하여 뼈대 모양의 독특한 구조를 형성하였으며 이 구조에서 표면 증강 라만 분광 활성이 우수함을 확인하였다. 이 방법을 응용하여 다양한 금속 나노구조체를 형성할 수 있는 가능성을 제시하고 있다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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Preparation of lanthanum oxide layers by electrodeposition in organic solution

최정희 정용희*

한림대학교 화학과

Layers of lanthanum oxide were prepared on titanium by electrodeposition with an organic solution. High voltages ranging from 200 to 1000 V were employed for the deposition process. Titanium was used as anodes and cathodes. The layers were examined by scanning electron microscopy, X-ray diffraction and X-ray photoemission spectroscopy. The layers exhibited good adhesion on titanium. A preliminary result indicated that amounts of electrodeposition varied with applied voltages to some extent.

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Electrooxidation of glucose at platinum tree nanostructure electrode prepared by electrodeposition method

김다정 최수희 김종원*

충북대학교 화학과

백금은 전기촉매적 활성이 뛰어난 금속으로 다양한 분야에 응용 가능하다. 하지만 매장량의 한계로 인한 높은 비용 때문에 사용의 제한이 따른다. 따라서 적은 양의 백금으로 높은 촉매 활성을 얻기 위해 독특한 모양의 백금 나노구조체를 형성하는 연구가 진행되고 있다. 본 연구에서는 전기화학적 석출법을 이용하여 금 표면 위에 백금 나노 구조를 형성하였으며, 글루코오스 산화 반응에의 촉매 활성을 관찰하였다. 석출 전하량에 따라 형성되는 구조의 차이를 주사 전자 현미경과 전기화학적 방법을 통해 비교하였다. 형성된 구조는 석출 전하량에 따라 차이를 보이는데, 석출 전하량 0.04 C 의 백금 나노 구조의 경우 높이 500 nm 의 뾰족한 나무 구조들이 금 기판과 수직적인 구조를 이룬다. 글루코오스 산화 반응에의 촉매 활성은 형성된 백금 나노 구조에 따라 달라지며, 석출 전하량 0.04 C 로 형성된 백금 나노 나무 구조에서 가장 우수한 촉매활성이 나타났고 전하량에 따른 표면적의 변화보다 형성된 구조적 특이성이 촉매 활성에 많은 영향을 미치는 결과를 도출하였다. 전류법 반응 결과 글루코오스에 잘 감응하여 3-15 mM 의 농도 범위에서 우수한 직선성을 보이며 검정 곡선을 통해 민감도 54.7 ?AmM^{-1}cm^{-2} 를 얻었다. 또한 글루코오스 측정 시 방해작용을 하는 아스코브산에 대한 선택성도 나타남을 확인하였다. 이 결과를 통해 글루코오스 센서로서의 응용 가능성을 제시할 수 있다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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Ultrasound-assisted Polyol Synthesis of Well-dispersed Pt Nanoparticles on Titanium Nitride and Their Electrochemical Performance

박현욱 곽진수 김근오 조승익 이은직[1] 권영욱*

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In this study, we report the ultrasound-assisted polyol synthesis (UPS) of well-dispersed Pt nanoparticles (NPs) on titanium nitride (TiN) and their electrochemical performance for methanol oxidation reaction (MOR) and oxygen reduction reaction (ORR). In order to prepare Pt/TiN sample, metal precursors and TiN (20~30 nm) were dispersed in ethylene glycol and irradiated by ultrasound for 3 h. Through the structural analyses of Pt/TiN, we found that sample has uniform particle size (4~5 nm) and well-dispersed Pt NPs on TiN. Electrochemical performance of sample was investigated by rotating disk electrode (RDE) measurement. Compared with commercial Pt, Pt/TiN showed the enhanced ORR and MOR activity in acid media. In conclusion, we demonstrated that the strong metal-support interaction (SMSI) effect between Pt and TiN leads the enhanced electrocatalytic performance and durability.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

New complementary electrochromic device based on Prussian blue-Nickel oxide nanocomposite films

정영희 김종민[1] 오성훈[1] 장병용[1] 김영일[1,*]

(주)마프로 기술연구소 [1]부경대학교 화학과

Electrochromic(EC) materials are able to show the reversible optical change by an external voltage. Prussian blue(PB) and Nickel oxide(NiO) are high coloration efficiency(CE), good cyclic reversibility, low cost and anodically coloring materials. But PB can’t cover wavelength range of 400~500nm at coloring state and shows bad cyclic reversibility in 2nd redox reaction. Also, Nickel oxide shows low coloration efficiency in non-aqueous electrolyte and residue color(yellow) at bleaching state. In this study, PB-NiO nanocomposite film with highly porous structure was fabricated by mixing PB and Lithium doped NiO nanoparticles for taking advantages of both the components. It showed transmittance modulation and good coloration efficiency. PB-NiO nanocomposite film and WO3 were combined to fabricate a complementary electrochromic device, which exhibited a ΔT of roughly 30% at 660 nm and was very stable up to 1,000 cycles in Li+ electrolyte.

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발표분야: 전기화학
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Supramolecular association of enzyme on sol-gel matrix embedded gold nanoparticles supported reduced graphene oxide-cyclodextrin nanocomposite: Synergistic electrochemical biosensor

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인천대학교 화학과

Herein we present β-cyclodextrin (CD) attached reduced graphene oxide (RGO) nanosheets supported on the silicate sol-gel matrix embedded Au nanoparticles (NPs) modified electrode surface as a new affinity binding nanocomposite. Modified electrode is fabricated through the layer-by-layer drop casting followed by the immobilization of the chemically modified enzyme (HRP-ADA). This affinity system is based on the supramolecular association between the CDs and HRP-ADA is mimicking the biological avidin-biotin interactions. The cavity of the CD attached at the RGO surface (RGO-CD) functions as a macro cyclic host to form stable subramolecular inclusion complexes with enzyme conjugate. The silicate sol-gel matrix embedded Au NPs were protected by the RGO-CD nanosheets at the electrode surface and exhibits the synergistic electrocatalytic effect towards the H2O2 in the presence of 1 mM Hydroquinone when compared to the individual electrocatalytic effects of Au NPs and RGO-CD nanosheets, respectively.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual doped graphene-Fe2O3 and used as an electrochemical sensor for dopamine detection with ascorbic acid and serotonin

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전남대학교 화학과

Dual doped (N and S) graphene supported Fe2O3 (Fe2O3/NSG) have been prepared by hydrothermal method and applied for the electrochemical determination of dopamine (DA), in presence of ascorbic acid (AA) and serotonin (5HT). The Fe2O3/NSG has been characterized via Fourier transform infrared spectroscopy (IR), transmission electron microscopy (TEM) and XPS. The Fe2O3/NSG has finally been employed for the electrochemical detection of DA. The electrochemical detection of DA has verified through the cyclic voltammetry, differential pulse voltammetry and amperometric techniques in a 0.1 M phosphate buffer solution (PBS) at pH 7.4. The pH of cell solution for DA determination has been optimized as pH 7.4. The interference has also been investigated in presence of serotonin, glucose, AA, N2H4, NaCl and uric acid. The detection limit of DA has calculated as 0.039 ?M (where s/n = 3), and the linear ranges were 0.1?196 ?M at the the Fe2O3/NSG modified glassy carbon electrode (GCE).

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dopamine-functionalized graphene biosensor for dopamine determination in the presence of serotonin

주유리 **Mohammad Shamsuddin** 전승원*

전남대학교 화학과

We have synthesis of electrochemically prepared dopamine (DA) functionalized graphene and employed for the electrochemical detection of DA in presence of serotonin (5-HT). Graphene oxide-DA (GO-DA) resulted from the condensation reaction of GO and DA and the subsequent electrochemical reduction of GO-DA (ERGO-DA). The as prepared ERGO-DA was characterized via several instrumental methods. The electrochemical detection of DA has been verified through cyclic voltammetry, differential pulse voltammetry and amperometric techniques in a 0.1 M phosphate buffer saline (PBS, pH 7.4). The influence of the accumulation time and pH of the PBS at ERGO-DA modified electrode for DA oxidation has been investigated. The interference has also been performed using interfering substances such as 5-HT, glucose, ascorbic acid, H2O2, and uric acid. The detection limit and linear range of DA have been calculated as 0.04 µM and 0.5-100 µM, respectively, (where s/n=3) at the ERGO-DA modified electrode. The real sample analysis has done without any difficulty and this biosensor can be used up to 10 days.

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장소: 일산 KINTEX

발표코드: **ELEC.P-1198**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical analysis performance of boron polyanion substituted $LiFeMnPO_4$

이한솔 김민지 이영일*

울산대학교 화학과

$LiFeMnPO_4$olivine material has been taken attention as a promising new cathode material for large scale use of Li ion batteries due to its high theoretical capacity and favorable chemical components, which are abundant, inexpensive and non-toxic. The synthesized samples of boron polyanion substituted $LiFeMnPO_4$without additional carbon sources were characterized by XRD, XPS, SEM, and TEM with EELS. The electrochemical measurements of samples are also performed with half-cell. Among them, $LiFe_{0.4}Mn_{0.6}(PO_4)_{0.995}(BO_3)_{0.005}$with the best cycle performance exhibit an initial discharge capacity of 159.4 mAh g-1.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Electrocatalytic Oxygen Reduction Reaction on Polymer Functionalized Graphene with Palladium Nanoparticles

박동철 Mohammad Shamsuddin 전승원*

전남대학교 화학과

Electrochemical oxygen reduction reaction (ORR) in alkaline solution has been catalyzed by newly synthesized Poly(3,4-ethylenedioxythiophene) functionalized graphene with palladium nanoparticles (denoted as Pd/PEDOT/rGO). The structural features of catalyst are characterized by several instrumental techniques. The transmission electron microscopy (TEM) images suggest a well dispersed PdNPs onto PEDOT/rGO film. The ORR activity of Pd/PEDOT/rGO has been investigated via cyclic voltammetry (CV) and hydrodynamic voltammetry techniques in 0.1 M KOH aqueous solution. Comparative CV analysis suggests a general approach of intermolecular charge-transfer in between graphene sheet and PdNPs via PEDOT which leads to the better PdNPs dispersion and subsequently superior ORR kinetics. The results show that Pd/PEDOT/rGO has remarkable electrocatalytic activity and stability compared to Pd/rGO and state-of-the-art Pt/C. The Koutecky?Levich and Tafel analysis suggest that the proposed main path in the ORR mechanism has direct four-electron transfer process with faster transfer kinetic rate on the Pd/PEDOT/rGO.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly efficient benzylamine functionalized graphene supported palladium for electrocatalytic hydrazine oxidation

EJAZ AMMARA **Mohammad Shamsuddin** **전승원***

전남대학교 화학과

We have been synthesized an electrochemical sensor for hydrazine oxidation by using graphene functionalized by benzylamine molecules (both para and meta) and palladium (denoted as G-PxDA-Pd and G-MxDA-Pd, respectively). The as prepared material has been characterized by X-ray photon spectroscopy and transmission electron microscopy (TEM). The TEM study suggests a good dispersion of Pd nanoparticles on the surface of G-PxDA-Pd rather than G-MxDA-Pd. The material has been investigated by several electrochemical techniques including, cyclic voltammetry, differential pulse voltammetry and Chronoamperometry (CA) by using 0.05M (PBS) at pH 7.4. From these techniques this hydrazine sensor shows a good linear range of 1?10-6 M ? 7.4?10-3 M with detection limit (S/N=3) of 1.7?10-7M within fast response time of 3s. The CA experiment shows the oxidation peak current is linearly dependent on the concentration of hydrazine. The selectivity of G-PxDA-Pd towards hydrazine has been studied for a number of ions such as, Na+, Cl-, Ca+2, Mg+2, and SO4-2 and biomolecules such as glucose and ascorbic acid.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Step Synthesis of Interconnected Porous Carbon Nanosheets for Electrochemical Capacitors

윤하나* 유정준*

한국에너지기술연구원 에너지저장연구실

Activated carbons have attracted much attention for energy storage device applications such as electrochemical capacitors (ECs) and batteries since they have many important properties of relatively high electrical conductivity, chemical stability, and large specific surface area, necessary for enhancing the capacitance. Especially, 3D interconnected porous carbons with high surface area are strongly recommended as an electrode material for advanced ECs because they can facilitate ion transport within the pores by providing a smaller resistance and shorter diffusion pathways.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Glucose and hydrogen peroxide sensors based on catalytic activity of metal alloy oxide

김민영 심윤보*

부산대학교 화학과

The hydrogen peroxide and glucose sensors were constructed based on a poly(terthiopnene benzoic acid) (pTTBA) layer coated on alloy oxide. The alloy was electrochemically prepared on a glassy carbon electrode (GCE), its physical and chemical properties were characterized. The alloy oxide with a hierarchical nanostructure was electrochemically synthesized, and it characterized using SEM, XPS, electrochemistry methods. The experimental parameters for the glucose sensing were optimized in terms of pH, temperature, humidity, and interferences (acetaminophen, ascorbic acid, and dopamine). The linear calibration plots for the glucose and hydrogen preoxide analyses were obtained between 5.0uM to 16.0 mM (detection limit was 4.0 ± 1.0uM) and 1.0 uM to 16.0 mM (detection limit was 0.75 ± 0.15 uM), respectively.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solar assisted Microbial electolysis cells using p-type cuprous oxide

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건국대학교 생명공학과 [1]건국대학교 생명특성화대학 특성화학부 [2]건국대학교 특성화학부생명공학과

A solar-assisted microbial electrolysis cell (SAMEC) is a device that converts organic matters to hydrogen with solar energy to lessen the thermodynamic energy barrier. At the anode, bacteria oxidize various organic substrates generating protons and electrons. Voltage should be applied to make a microbial electrolysis cell (MEC) work. The problem is that expensive Pt cathode is needed to produce hydrogen at high rate. In this work, we used Cu_2O as a photocathode to utilize solar energy in MEC system to effectively produce hydrogen. We synthesized Cu_2O nanowire arrays and applied to an MEC. As a p-type semiconductor, Cu_2O has a favorable band structures: -0.69 V for CB and 1.51 V for VB vs NHE at pH 7.0. First we confirmed its photoeffect in 50 mM PBS solution with visible light illumination of 85 mW/cm^2. However, Cu_2O turned out to be rather unstable in that condition. To improve its stability as well as cathodic performance, we coated Cu_2O with MoS_2 film which was known to catalyze proton reduction. When -0.8 V was applied to the MoS_2-coated Cu_2O cathode under illumination, hydrogen gas was effectively generated whose rate was comparable to that of Pt. Our preliminary results show that a new MEC system with a MoS_2-modified p-type Cu_2O semiconductor cathode could be a promising material that can be practically implemented in the real world to produce hydrogen. Long term stability test and more experiments to improve SAMEC performance are in progress.

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Graphene oxide/organic ligand modified electrode for analysis of trace metal ions

박민욱 이동욱 심윤보*

부산대학교 화학과

We report simultaneous determination of heavy metal ions (HMIs, (Zn(II), Cd(II), Pb(II), Cu(II), and Hg(II)), which was performed with a disposable graphene oxide (GO)/organic ligand (OL) modified was prepared by thermal reaction and it was used as a working electrode for HMIs detection. Square wave anodic stripping voltammetry (SWASV) was performed simultaneously to analyze the HMIs by sweeping the potential between -1.4 and +0.5 V in an acetate buffer solution (pH 5.0). Analytical parameters affecting the sensor performance was optimized in term of pH, deposition time, ratio of CB:GO:OL. The calibration plot was obtained in the concentration range from 1.0 ppb to 1.0 ppm.

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Selection of Aptamers using a microfluidic channel

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부산대학교 화학과 [1]포항공과대학교(POSTECH) 화학과

SELEX is an experimental procedure that allows screening of given molecular targets by desired binding affinities from an initial random pool of oligonucleotides and oligomer. SELEX is an iterative process requiring multiple rounds of extraction and amplification that demands significant time and labor. Therefore, this study presents a novel, simple, miniature SELEX platform. The developed microsystem demonstrated fast screening of PvLDH aptamers. we report aptamer selection based on target immobilization on conducting polymer film at screen printed microchannel electrodes. PvLDH (Plasmodium vivax Lactate Dehydrogenase), a biomarker for malaria was used as a target protein in present work. At first stage PvLDH was immobilized on SPCE/p-TTBA(poly(terthiophene benzoic acid)) film by covalent bonding. Immobilized target protein and random ssDNA library interacted with PvLDH/p-TTBA/SPCE were confirmed by impedance spectroscopy. After removing unbounded ssDNA, selected aptamer was detected using amperometry spectroscopy.

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Electric double-layer capacitive slurry electrode based electrochemical flow capacitor

윤하나* 유정준*

한국에너지기술연구원 에너지저장연구실

For the practical application of the large-scale energy storage, novel technologies having major advantages of both supercapacitors and batteries are needed. It is also desirable to use cheap, environmentally friendly, and abundant materials in the new energy storage systems (ESSs). The electrochemical flow capacitors (EFCs) are highly promising for large-scale electrical energy storage because they possess several key benefits derived from both supercapacitors and flow batteries, such as the high power density, long cycle lifetime, and scalable energy capacity. In this study, we introduce an electric double-layer capacitive carbon slurry electrode based EFC and their electrochemical properties.

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발표코드: **ELEC.P-1207**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pseudocapacitive slurry electrode based electrochemical flow capacitor

윤하나* 유정준*

한국에너지기술연구원 에너지저장연구실

High energy densities of batteries are highly attractive, however, unsolved safety issues, slow charging and limited cycle lifetimes hinder their grid-scale energy storage applications. In contrast, supercapacitors have rapid response, long cycle lifetime and good safety, but they have lower energy densities than batteries. Thus, combined use of batteries and supercapacitors has been necessary for the grid energy storage. Herein, we report a pseudocapacitive flowable electrode based electrochemical flow capacitor.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Drop separation on a paper-based closed chip for microfluidics

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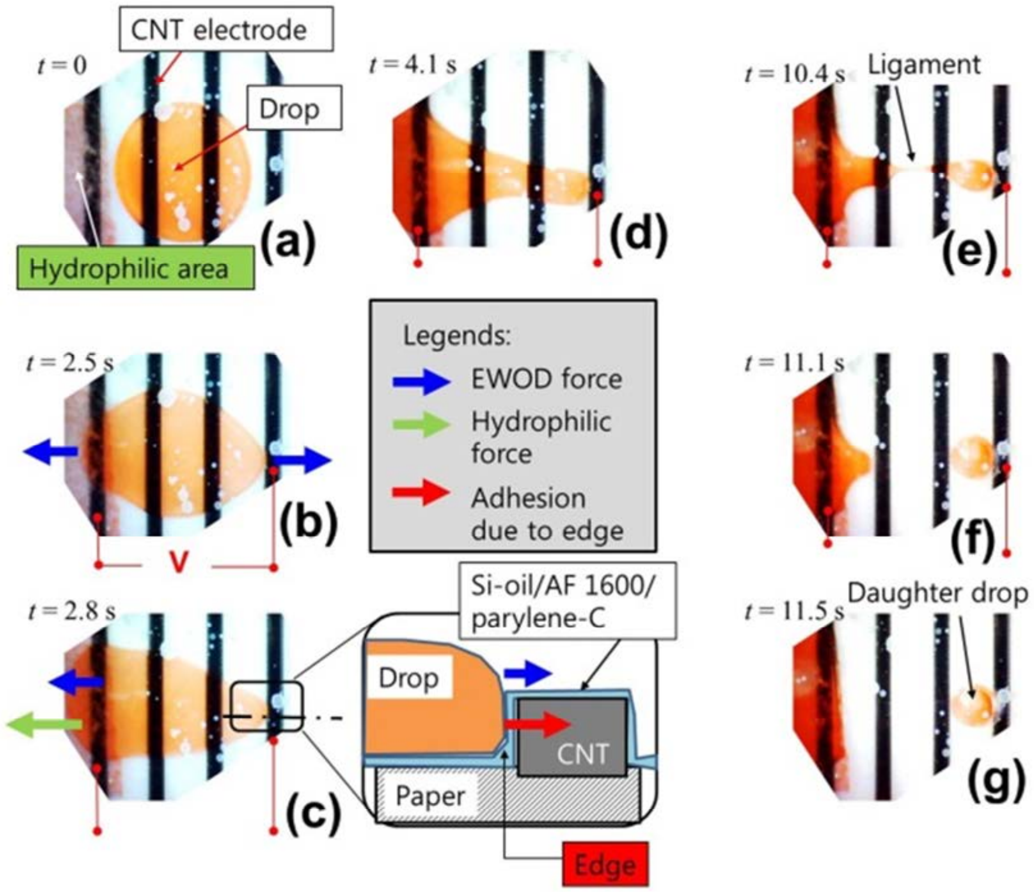
서강대학교 화학과 대학원 [1]서강대학교 화학과 [2]충남대학교 고분자공학과 [3]서강대학교 화학과 및 바이오융합과정

Drop actuation on an active paper-based closed chip for microfluidics has been studied, in which the drop was actively actuated by using electrowetting phenomenon. Unexpectedly we found the effect edge of CNT electrode on actuating force. Although it might be the undesired bump structure formed due to inkjet printing on paper overlaidly for fabrication of the flat planar chips, we found that it could provide the additional force to help splitting a drop into the fractional partitions. Furthermore the edge effect promises a good application for dispensing a drop from reservoir, resulting in all of drop actuations required for developing the complete active paper chip. In addition to the edge effect, we found that the hydrophilic surface also helps the drop separation.


CNT electrode
t = 0
Drop
Hydrophilic area
(a)
t = 2.5 s
V
(b)
t = 2.8 s
(c)
t = 4.1 s
(d)
Legends:
EWOD force
Hydrophilic force
Adhesion due to edge
Si-oil/AF 1600/ parylene-C
Drop
CNT
Paper
Edge
t = 10.4 s
Ligament
(e)
t = 11.1 s
(f)
t = 11.5 s
Daughter drop
(g)

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An Dual Amperometric/Potentiometric Microsensor for the Real-Time *in vivo* Simultaneous Measurements of NO/K$^+$

문정미 이종목 이영미*

이화여자대학교 화학나노과학과

The development of a dual microsensor for simultaneous measurements of two closely linked biological species is demonstrated. In particular, the sensor targets nitric oxide (NO)/potassium ion (K$^+$). Nitric Oxide is known to be closely related to K$^+$ in biological system. For instance, NO/cGMP (guanosine 3', 5'-cyclic monophosphate)/K$^+$ channel pathways have been reported to be involved in many biological processes including vasodilation. Due to these close linkages between NO and K$^+$, it is of great interest to analyze NO/K$^+$ concurrently.A dual microsensor possesses two microdisks: one disk is used for amperometric NO measurement and the other is used for potentiometric ion(K$^+$) measurement. Sensor performances, such as sensitivity and selectivity, are characterized and the results show the possibility for the biological application. As-prepared sensor is applied for analyzing NO and K$^+$ levels simultaneously and quantitatively in a rat brain cortex *in vivo* upon seizure activity induced by 4-aminopyridine. The basal level and concentration changes of NO and K$^+$ are considerably matched with results studied by various methods reported previously. This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (2014R1A2A2A05003769).

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Development of a selective electrochemical triple microsensor for simultaneous measurements of CO, NO, and O_2

김진후 이종목 이영미*

이화여자대학교 화학나노과학과

Carbon monoxide (CO), nitric oxide (NO) and oxygen (O_2) play important roles in regulating fundamental physiological functions. Endogenous CO and NO gases function as signaling molecules similarly to control a certain biological processes such as vasodilation and neurotransmission. In addition, the biosynthetic procedure of CO and NO is alike and enzymes in this synthetic system require O_2 and NADPH to be activated. In this study, we demonstrate the development of an amperometric CO/NO/O_2 triple microsensor which can measure these gases simultaneously. The sensor is made of a triple platinum working electrode (WE1, WE2 and WE3, with 76, 50, and 25 μm in diameter, respectively) and Ag/AgCl counter/reference electrode. The triple WE Pt disks are etched to form micropores in shape. The largest WE1 for CO sensing is modified with electrodeposition of gold. The WE2 and WE3, for NO and O_2 sensing, are electrodeposited with porous platinum layer. Silanizing solution is dispensed over each disk, lastly. Modification of three sensing disks with different surface treatments gives apparently different selectivity to each gas at WE1, WE2, and WE3. Sensor performances, such as sensitivity and selectivity, are characterized and the results show the possibility of the triple sensor for the biological applications.

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Study of fast diffusion-controlled and slow kinetic-controlled electrode reactions at porous platinum layers with different pore sizes

조윤빈 이종목 이영미*

이화여자대학교 화학나노과학과

The search for the best electrocatalyst material system is important due to the wide range of applications for electrochemical devices. Especially for sluggish reactions, such as oxygen reduction, glucose oxidation reaction, etc., loads of studies have been performed in order to develop superior electrocatalyst systems. Many researches have utilized porous structured materials in order to enhance their catalytic activity owing to their high surface area to volume ratios, uniform, controllable pore sizes, physical rigidity, chemical and thermal stability, etc. In this research, metallic platinum thin films with different porosities are electroplated on platinum disk electrode (100 μm diameter) using reverse micelle solutions with different compositions. This study examines the catalytic activity at different porous layers toward a range of electrochemical reactions from fast diffusion-controlled to slow kinetic-controlled electrode reactions: ferrocene oxidation, oxygen reduction, and glucose oxidation reaction. This work was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (2014R1A2A2A05003769).

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Synthesis and electrochemical characterization of electrospun Ag-Co_3O_4 nanomaterials

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

Electrospinning has gained much attention not only due to its diversity of the electrospinning materials but also due to its simplicity. In this study, Ag-Co_3O_4 hybrid nanomaterials were fabricated by a facile two-step procedure (electrospinning and calcination) and characterized electrochemically. The morphology and compositions of these materials were characterized by FE-SEM and EDS . For the electrochemical characterization, three-electrode cell was used with a glassy carbon electrode loaded with the synthesized Ag-Co_3O_4 as the working electrode and a saturated calomel electrode (SCE) as the reference electrode, and a coiled platinum wire as the counter electrode. Electrochemical activities of these nanomaterials were characterized by linear sweep voltammetry (LSV) and cyclic voltammetry (CV). This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (2014R1A2A2A05003769).

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Measurement of Ascorbic Acid with Single Crystalline Ruthenium Oxide Nanowires Grown on Electrospun Titanium Oxide Nanofibers

김수진 이종목 김명화[1] 이영미*

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A nonenzymatic amperometric electrochemical sensor for the detection of L-ascorbic acid (AA) is developed based on highly dense metal oxide. The aim of this study is to investigate the electrochemical activity of single crystalline ruthenium oxide nanowires grown on electrospun titanium oxide nanofibers (RuO_2NWs-TiO_2NFs) synthesized by chemical vapor deposition (CVD) for the oxidation of biological species including L-ascorbic acid (AA), 4-acetamidophenol (AP), dopamine (DA), glucose, β-nicotinamide adenine dinucleotide (NADH), and uric acid (UA). The morphology and structure of RuO_2NWs-TiO_2NFs were characterized by FE-SEM, XRD. Compared to bare glassy carbon electrode, electrochemical activities of these metal oxide materials for electrochemical oxidation of AA are characterized by linear sweep voltammetry (LSV), constant potential amperometric experiments (i-t). We also confirmed the selectivity to AA over AP, DA, glucose, NADH, and UA at their physiological levels using i-t and differential pulse voltammetry (DPV). In addition, these electrodes were applied for AA measurements in vitamin tablet samples. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2014R1A2A2A05003769).

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Electrochemical Determination of Ascorbic Acid and Uric Acid on Ruthenium Oxide Electrode

양예진 조아라 이영미* 이종목*

이화여자대학교 화학나노과학과

Uric acid (UA) and ascorbic acid (AA) are one of the most important biomolecules because their concentration in blood and urine indicate human's physical condition. For electrochemical detection of UA and AA, amperometric method was used. Ruthenium oxide film was electrodeposited on Au electrode (d=1.6 mm), which was served as a working electrode. The morphology and oxidation state of the ruthenium oxide film were characterized by field emission scanning electron microscopy (FE-SEM) and X-ray photoelectron spectroscopy (XPS). Voltammetric analysis showed different onset potential of AA and UA oxidation on ruthenium oxide. The amounts of AA and sum of AA and UA were determined by measuring the current responses at 0.2 and 0.32 V, respectively. In amperometric i-t curves the sensitivity of AA oxidation at 0.2 V and UA oxidation at 0.32 V showed 351 and 360 μA mM^{-1} cm^{-2}, respectively, with response time of 0.2 s for the linear range of zero to 1.0 mM. Sample analysis revealed that the determination of UA and AA was successful without interfering each other.

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Electrochemical Activatavation of Hollow Gold Nanoshells for Amperometric Glucose Detection

조아라 김명화[1] 이영미* 이종목*

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

In this study, we examined the change of glucose oxidation activity at hollow gold nanoshells (hAu) depending on electrochemical pre-treatment condition. Electrochemical treatments were conducted at hAu electrodes in two ways: one was the consecutive potential sweep method and the other was the potentiostatic method. These treatments were carried out in three different solutions; phosphate buffers, Tris buffers, and HEPES buffers while maintaining pH 7.4. Amperometric current responses of glucose oxidation varied with not only the way for pre-treatment also the sort of the solution for pre-treatment. We found that phosphate buffers are most appropriate solution for electrochemical activation of hAu among three kinds of solutions. At the present time enhancement of the glucose oxidation current seems to be closely related with the formation of gold oxide on the surface of hAu.

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Supportless Oxygen Reduction Electrocatalysts of Highly Porous Hollow AuPd Mesospheres

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대구대학교 화학과 [1]대구대학교 화학·응용화학과

This presentation reports the facile synthesis and characterization of highly porous hollow AuPd nanostructures. The formation of porous AuPd nanostructure is through galvanic replacement with hollow cobalt mesospheres as the templates in metal ion precursor solutions ($HAuCl_4$ and K_2PdCl_4, respectively). This approach does not require the further removal of templates and greatly simplifies the synthetic procedures. The porous AuPd nanostructures can be used as supportless electrocatalysts that exhibit enhanced catalytic activities in the oxygen reduction reaction (ORR) over commercial Pd-20/C and Pt-20/C catalysts. The compositional/structural features are characterized by scanning electron microscopy (SEM) equipped with an energy dispersive X-ray spectroscopy (EDS), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The electrocatalytic activity of the AuPd for ORR in alkaline media was investigated by rotating disk electrode (RDE) and cyclic voltammetry (CV).

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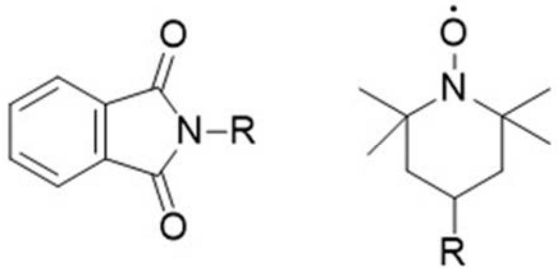
The Preparation of Phthalimide and 4-Hydroxyl-tempo Derivatives as Organic Electrolyte: Application for Redox Flow Battery

함창한 안철진*

창원대학교 화학과

Redox flow battery is a type of rechargeable flow battery that employs in different oxidation states to store chemical potential energy. To improve the energy density, we prepared phthalimide and 4-hydroxyl-tempo derivatives as organic electrolyte. In this paper, we will present the preparation of phthalimide, 4-hydroxyl-tempo derivatives and the effect of CV depending on various fuctional group.



R = -SO3Me, PhCO-, PhCH2-, Me

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Sensitive and Selective Trypsin Detection Using Redox Cycling at Bare Indium-Tin Oxide Electrodes

박선화 양해식*

부산대학교 화학과

Here, we report a simple, sensitive, and selective electrochemical method for trypsin detection that can cover a wide range of concentrations. The method is based on the proteolytic generation of an electroactive species (P) by trypsin followed by a signal-amplified electrochemical measurement of P using electrochemical?chemical (EC) or electrochemical?chemical?chemical (ECC) redox cycling. The detection is performed using bare indium-tin oxide (ITO) electrodes and does not require washing steps. P is generated by the cleavage of an amide bond between P and oligopeptide (Gly-Pro-Arg) at the C-terminal of Gly-Pro-Arg-P. In EC redox cycling, tris(2-carboxyethyl)phosphine (TCEP) is used as a reductant, whereas, in ECC redox cycling, TCEP and $Ru(NH_3)_6^{3+}$ are used as a reductant and an oxidant, respectively. Four trypsin products [4-aminophenol, 4-amino-2-chlorophenol, 4-amino-2,6-dichlorophenol, and 4-amino-1-naphthol (AN)] and their trypsin substrates are investigated to obtain a high signal-to-background ratio in ECC redox cycling. AN and its trypsin substrate produce the highest signal-to-background ratio. The detection limits obtained with ECC redox cycling involving AN (approximately 1 ng/mL and 100 ng/mL with an incubation period of 2 h and 30 min, respectively) in Tris buffer (pH 8.0) are lower than those obtained with EC redox cycling involving AN (approximately 5 ng/mL and 200 ng/mL with an incubation period of 2 h and 30 min, respectively). The interference effects of other proteases (thrombin, pepsin, papain, and lysozyme) are not significant. In trypsin detection using ECC redox cycling, the interference effects of electroactive species such as l-ascorbic acid (AA) and uric acid (UA), are also not significant. The detection limit obtained in PBS (pH 7.4) containing 5% human serum albumin, 0.1 mM AA, and 0.1 mM UA with an incubation period of 30 min is 100 ng/mL, and trypsin could be detected at concentrations within a range of 100?2000 ng/mL. This detection scheme could be applicable to the detection of other proteases.

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Manufacture of graphene oxide(GO) using microwave for glucose sensor without mediator

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단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Reduced graphene oxide (RGO) has been widely used for signal amplification in the biosensor field due to the high conductivity and large surface area. Fabrication of graphene oxide(GO) has been mainly used nitric acid, which has the disadvantage that it is time-consuming and dangerous. We used a microwave to create GO in a secure and fast time. RGO was produced graphehe oxide(GO) by electrodeposition method using the cyclic voltammetry(CV) technique of CHI 660B model. MWCNT and RGO, glucose oxidase(GOx) for good sensitivity of glucose sensor was immobilzed without mediator on the glassy carbon electrode(GCE). PEGDGE of various concentrations were applied as cross linker to bind the enzyme strongly. Surface of the fabricated electrode was confirmed using the scanning electron microscope(SEM). Electrical currents were linearly related with the concentration of glucose.

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Fabrication of Screen Printed Nickel Electrode, and Its application to glucose sensor without mediator

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단국대학교 나노바이오의과학과 [1]단국대학교 화학과

Screen printed Nickel Electrode(SPNE) on the ITO with carbon was applied to check glucose concentration without mediator. Carbon included SPNE was prepared by furnace, which temperature was 100 to 600 degree for 30 minute. The surface morphology of carbon included SPNE was examined by scanning electron microscopy (SEM). NiOOH on the carbon included SPNE was formed by cyclic voltammetry(CV) technique for 10 cycles using NaOH solution, and it was demonstrated by X-ray Photoelectron Spectroscopy (XPS). The electrical currents were measured by CV and resulting currents were linearly related with the concentration of glucose. The carbon included SPNE was prepared well by CV with NaOH and it can be applied to measure the glucose level without mediator.

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Enhancement of Electrocatalytic Activities of Long-Aged Pt Electrodes and Time Dependent Decrease of the Enhanced Electrocatalytic Activities

김종찬 양해식*

부산대학교 화학과

Pretreatment methods of long-aged Pt electrodes are commonly used to obtain increased and reproducible electrocatalytic activities prior to electroanalytical measurement. However, many pretreatment methods can cause severe surface damage. Moreover, the degree and time dependence of the increased activities have rarely been investigated systematically. This paper reports a new pretreatment method($NaBH_4$ treatment) of long-aged Pt electrodes and compares four pretreatment methods ($NaBH_4$ treatment, mechanical polishing, cathodic treatment, and anodic treatment) in terms of the degree and time dependence of the electrocatalytic activities toward oxygen reduction reaction. $NaBH_4$ treatment allows increased electrocatalytic activities comparable to those obtained after other pretreatments, without a surface damage. The high electrocatalytic activities of pretreated Pt electrodes decrease with aging in ambient air and in solution (0.1 M $HClO_4$); the activities decrease at a higher rate in air than in solution. The decrease of the electrocatalytic activities of Pt electrodes with aging is due to the increase of surface contamination.

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Phenol Detection Using Tyrosinase Based On Phenol Oxidation with Redox Cycling

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부산대학교 화학과

This paper reports sensitive phenol detection using (i) tyrosinase (Tyr)-based oxidation of phenol to catechol, combined with (ii) electrochemical-chemical-chemical (ECC) redox cycling involving $Ru(NH_3)_6^{3+}$, catechol, and tris(2-carboxyethyl)phosphine (TCEP). Phenol is converted into catechol by Tyr in the presence of dissolved O_2. Catechol then reacts with $Ru(NH_3)_6^{3+}$, generating *o*-benzoquinone and $Ru(NH_3)_6^{2+}$. *o*-Benzoquinone is reduced back to catechol by TCEP, and $Ru(NH_3)_6^{2+}$ is accumulated over the course of the incubation. When $Ru(NH_3)_6^{2+}$ is electrochemically oxidized to $Ru(NH_3)_6^{3+}$, ECC redox cycling occurs. For simple phenol detection, bare ITO electrodes are used without modifying the electrodes with Tyr. The detection limit for phenol in tap water using Tyr-based oxidation combined with ECC redox cycling is ca. 10^{-9} M, while that using only Tyr-based oxidation is ca. 10^{-7} M.

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Simple Detection of Arsenic(III) in Water Using Electrochemical-Chemical-Chemical Redox Cycling at Bare Indium-Tin Oxide Electrodes

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부산대학교 화학과

Sensitive As(III) detection in ground water is of great importance for evaluating the quality of drinking water. We report a sensitive electrochemical method for As(III) detection based on electrochemical-chemical-chemical (ECC) redox cycling involving Ru(IV) [an oxidized species of $Ru^{III}(NH_3)_5NH_2^{2+}$], As(III), and tris(3-carboxyethyl)phosphine (TCEP). Electrochemical oxidation of $Ru^{III}(NH_3)_5NH_2^{2+}$ formed from $Ru^{III}(NH_3)_6^{3+}$generates Ru(IV), which quickly oxidizes As(III). This electro-mediated oxidation of As(III) produces As(V), which is reduced back to As(III) by TCEP. Electrochemically generated Ru(IV) then reoxidizes As(III), allowing ECC redox cycling to occur at a high rate on bare indium-tin oxide (ITO) electrodes without modifying the surfaces with electrocatalytic materials. Because most interfering metal ions precipitate in a carbonate buffer, water samples are mixed with carbonate buffers prior to electrochemical measurements, rendering the effects of Cu^+, Cu^{2+}, Fe^{2+}, Fe^{3+}, and Pb^{2+} insignificant. The detection limit calculated by ECC redox cycling using a chronocoulogram is 1.2 mM, much lower than that obtained using only the electro-mediated oxidation of As(III) (90 mM).

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Facile electrochemical detection of Escherichia coli using redox cycling of the product generated by the intracellular β-?-galactosidase

FangChiewSan 양해식*

부산대학교 화학과

Various detection methods for pathogenic bacteria have been developed, most of which are based on cell culture, DNA amplification, and immunoassays. Although the methods allow highly sensitive and/or selective detection, they require long detection periods and complex detection procedures. This paper reports a facile electrochemical detection method for Escherichia coli (*E. coli*) without the use of DNA amplification or immunoassays. The detection method harnesses the intracellular β-?-galactosidase (Gal) activity of *E. coli* along with the signal amplification based on redox cycling. The Gal expression level is increased by treatment with a Gal expression-inducer (isopropyl-β-?-thiogalactopyranoside; IPTG); the enzymatic reaction of Gal is facilitated by the permeabilization treatment involving the use of chloroform and sodium dodecyl sulfate; the electrochemical signal is amplified by the electrochemical?chemical?chemical (ECC) and chemical?chemical redox cycling involving the Gal product, $Ru(NH_3)_6^{3+}$ and tris(2-carboxyethyl)phosphine. The detection limit obtained in the presence of the ECC redox cycling, with a total detection period of only 4.5 h, is ca. 1 colony forming unit (CFU)/mL, indicating that ECC redox cycling allows for a sensitive detection.

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Nanodielectric Properties of 16-MHDA self-assembled monolayers

Wang Wenxiu 손용근*

성균관대학교 화학과

Many researchers have tried various chemicals and fabrication methods to produce nanoscale dielectrics on a substrate for the nanoelectronics. The fabrication of an alkylsilanes molecular dielectric using a method of producing self-assembled molecules on heavily doped n+-Si substrates has been reported, but it requires strict and harsh conditions. Thus, it is necessary to develop a new molecules system to fabricate the self-assembled monolayers (SAMs) dielectrics under an easily-controlled and mild condition. Herein, we report a facile and novel method capable of producing the nanodielectrics layer for the electronics. A new type of potential organic nanodielectric was constructed by only using self-assembled 16-mercaptohexadecanoic (16-MHDA) molecular layers. The formation of the SAMs on the gold substrate was performed under mild conditions using only an ethanol solution. As a result, we found that when the number of assembled layers increased to 6, the tunneling effect could be avoided and a large capacitance of 251 nF?cm-2 at 105 Hz could be obtained.This is the first known and reported article that alkanethiols SAMs can be used to make nanodielectric. Our new facile method to fabricate the nanoscale dielectric with strong dielectric property SAMs is expected to allow future industrial mass production of molecular electronics.This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy(No. 2010501010002B)

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MnO_2 nanostructure modified by proton irradiation for energy storage applications

장현석 이원길 유국현*

동국대학교 화학과

The pseudo capacitive materials, MnO_2 is a promising electrode material because of its high theoretical specific capacitance, abundant resources, low-cost, and eco-friendliness. But the poor conductivity and less electron transport properties of MnO_2 limited their applications. Among the several ways to improve the properties of MnO_2, we focused on the high power proton irradiation. This irradiation can modify the electronic properties and surface states of material. So using this method, we researched about electronic properties of the proton irradiated MnO_2 by fabricating electrodes for super capacitor and checked the modifications of MnO_2 nanostructure.

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Inverse Opal SnO_2 based Photoelectrochemical Water Splitting

윤건 강순형*

전남대학교 화학교육과

Nowadays, the exploration of new photoelectrode architectures to improve the light-harvesting and charge-collection properties of photoelectrochemical cells and related devices has been regarded as a challenging work. Here, we demonstrate the synthesis of the inverse opal SnO2 and Sb doped SnO2 film for photoelectrochemical water splitting was prepared by the spin-coating method. Using 350 nm polystyrene beads, we synthesized the SnO2 and Sb doped SnO2 inverse opal structure showing the photonic crystal effect. These results were confirmed using Field-emission scanning electron microscopy, X-ray diffraction and ultraviolet-visible spectrophotometer. Upon this template, the TiO2 layer with various thicknesses was deposited by atomic layer deposition. Herein, it is expected that an optimal TiO2 layer takes part in a role as a photoactive material and demonstrates the effect of electric field. Based on these results, SnO2 and Sb doped SnO2 inverse opal film as well as TiO2/SnO2 and TiO2/Sb doped SnO2 inverse opal films as a photoelectrode were applied to photoelectrochemical water splitting to identify their unique properties and evaluated exploring the photocurrent-voltage measurement.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Simultaneously carbohydrate separation and detection by using electrochemical potential modulated microchannel

HOSSAINMOHAMMADMOZAMMAL 심윤보*

부산대학교 화학과

Rapid analysis and low concentration separation of carbohydrate performed using electrochemical potential modulated microchannel (EPMM) device. The separation effect was evaluated by LSV and amperometry techniques. Under optimized conditions, an efficient separation achieved based upon their molecular size / charge-to-mass ratio, glycosidic linkages and also their physical properties (dipole moments) varied with the strength of the AC field. The proposed system perfectly separated eight carbohydrate compounds within 170 s with good reproducibility. The lowest detection limits obtained by electrochemical sensing. Reproducible response was observed during multiple injections of samples with a RSD of

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Smartphone-based Colorimetry for Paper-based Pool Water Quality Sensor

오성훈 장병용[*]

부경대학교 화학과

Until now, Various means to check the quality of water , for example chemical experimental method and Paper-based test paper that can easily purchase, is developed. But, Chemical experimental method is too complicated and difficult to use in everyday life and Paper-based test paper is incorrect because of this method's detector is naked eye. If we use Smartphone as a detector and processing unit, this problem can be overcome. So we developed an application that can check the Pool Water quality (PoolScan). We expect to apply this methodology to another test paper.

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Amperometric immunosensor for the detection of cancer biomarker based on sandwich approach

HUSSAIN KHALIL 심윤보*

부산대학교 화학과

Mammalian cancer cell biomarker (HIF 1α) was detected using an amperometric immunosensor combined with hydrazine labeled bioconjugate. The sensor probe was fabricated by immobilizing Primary anti body onto a layer composed of gold nano particles (AuNPs) and a conducting polymer (TTBA). The bioconjugate composed of hydrazine, secondary anti body and AuNPs where hydrazine was used as redox indicator. Morphology and performance were investigated using SEM, XPS, EIS and cyclic voltammetry. The calibration plot at optimized experimental conditions showed a linear range of 25?350 pM/mL. The reliability of the immunosensor was evaluated in different kind of cancer cells which demonstrated an excellent selectivity and sensitivity.

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NADH detection in biological samples based on polyethyleneimine / graphene oxide modified biosensor

AKHTARMAHMOODHASSAN 심윤보*

부산대학교 화학과

A robust amperometric sensor for β-nicotinamide adenine dinucleotide (NADH) detection was fabricated using the polyethylenimine (PEI)/graphene oxide (GO) layer. The probe (GO/PEI) reveals a catalytic property to the NADH oxidation that brought new capability for highly sensitive electrochemical detection of NADH at the low oxidation potential. Surface characterization revealed that negatively charged GO acted as nanofillers in the positive polymer matrix. Cyclic voltammetery (CV), amperometery and electrochemical impedance spectroscopy (EIS) were performed to confirm the electrochemical activity of the sensor surface. The sensor showed the excellent selectivity to NADH in L-ascorbic acid, uric acid, catechol and dopamine containing solution with well separated potentials. The dynamic range of NADH was determined to be 0.12 to 2.6 mM. The reliability of the sensor was evaluated with human blood serum sample.

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Structural Studies of the Oxygen Evolution Reaction by the FeOOH Catalysts at Neutral pH

남기민* <u>박기상</u>

목포대학교 화학과

Collecting and storing solar energy in chemical bonds, as nature accomplishes through photosynthesis, is a highly desirable approach to solving the energy challenge. This solar to fuels conversion requires proton coupled multielectron oxidation of water to oxygen with the release of four protons and their subsequent reduction to hydrogen. An appropriate oxygen evolution reaction (OER) catalyst can help electron transfers for evolution of oxygen under low overpotentials. We present that the synthesis, characterization, and phase transition of FeOOH nanorods. The FeOOH catalysts exhibited phase dependent OER activity at neutral pH. Our studies raise promising possibilities for designing effective OER electrocatalysts.

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BiVO4 Photoanodes with Oxygen Evolution Catalysts for Solar Water Splitting

남기민* 곽지선

목포대학교 화학과

Photocatalysis is a light-driven chemical process over the surface of a semiconductor that can produce hydrogen from water. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary co-catalyst 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 catalysts. To investigate the effect of catalyst on BiVO4 (band gap: 2.4 eV), a layered structure was prepared using Mn, Co, and Fe based catalysts. The synthesis and characterization of the semiconductor electrodes and the effect of co-catalyst layers on the photoelectrochemical performance are discussed in detail.

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Electrodeposited WO3 Film on Various Metal Substrates and Its Morphological Effect for Photoelectrochemical Water Splitting

강순형

전남대학교 화학교육과

Metal oxides such as TiO_2, WO_3, ZnO, SnO_2 etc. have widely investigated because of low cost, environmental friendliness, and the application to various energy related devices. In particular, WO_3 having the energetic band gap of about 2.8 eV has the absorption of more visible light, the suitable position of conduction band to transfer the photogenerated electrons to the substrate, and the stable photoresponse in the strong acidic condition. Herein, we prepared the WO_3 film by electrodeposition that provides the clean and reproducible technique. That is, a compact structured WO_3 film with a thickness of 780 nm was prepared by facile electrodeposition at a constant potential of -0.47 V versus saturated Ag/AgCl electrode. For a nanoporous structured WO_3 film, polystyrene (PS) beads with a size of 320 nm were used as the template, and the electrodeposition was performed under the same experimental conditions by varying the reaction time from 1 to 3 min to adjust the thickness of the depositing layer. The PS beads were completely removed from the template by the calcination at 450 °C for 3 h under air, affording inverse opal WO_3 films with a pore size of 300 nm. For the inverse opal WO_3 film with a thickness of 790 nm prepared by electrodeposition for 1 min, the highest photocurrent density (1.75 mA/cm2 at 1.5 V versus sat. Ag/AgCl) was achieved, followed by compact WO_3, inverse opal WO_3 (2 min), and inverse opal WO_3 (3 min) films with photocurrent densities of 1.2, 0.74, and 0.35 mA/cm2, respectively. The further discussion on the morphological and crystalline properties of the prepared WO_3 film was confirmed by a field emission scanning electron microscope and X-ray diffraction.

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Effect of Ti addition as NiO formation inhibitor in Ni rich cathode materials for Li-ion batteries

NURPEISSOVA ARAILYM 김성수*

충남대학교 에너지과학기술대학원

Among high capacity cathodes, LiNi0.8Co0.15Al0.05O2 has a high capacity and stable electrochemical performance, although it suffers from degradation upon cycling and aging as a result of the formation of inactive NiO on the surface edges. In this study, the role of Ti, which partially replaces Ni in the transition metal layer that is in particular intended to surface region not in bulk of LiNi0.8Co0.15Al0.05O2, is investigated on the electrochemical performance and interfacial phenomena using transmission electron microscopy coupled with energy-dispersive X-ray spectroscopy, electron energy loss spectroscopy, and X- ray diffraction analyses before and after electrochemical cycling. As a result, formation of NiO inactive phase is inhibited for the Ti-doped LiNi0.8Co0.15Al0.05O2, so that the electrode could deliver higher capacity upon cycling test. Further electrochemical impedance analysis is performed to understand the interfacial behavior of Ti-doped LiNi0.8Co0.15Al0.05O2.

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Electrocatalytic Oxidation of Formic Acid in an Alkaline Solution with Graphene-oxide-supported Ag and Pd Alloy Nanoparticles

설희진 전승원[1,*]

한양대학교 공동기기원 [1]전남대학교 화학과

The electrocatalytic activities of metal-decorated graphene oxide (GO) catalysts were investigated. Electrochemically reduced GO-S-(CH2)4-S-Pd [ERGO-S-(CH2)4-S-Pd] and GO-S-(CH2)4-S-PdAg alloy [ERGO-S-(CH2)4-S-PdAg] were obtained through the electrochemical reduction of GO-S-(CH2)4-S-Pd and GO-S-(CH2)4-S-PdAg in a pH 5 PBS solution. It was demonstrated that the application of ERGO-S-(CH2)4-S-Pd and ERGO-S-(CH2)4-S-PdAg used in a modified GCE improves the electrocatalytic oxidation of formic acid. The addition of an Ag nanoparticle with a carbon chain-Pd in the electrode provides an electrode with very interesting properties for the electrocatalytic oxidation of formic acid. The ERGO-S-(CH2)4-S-Pd and ERGO-S-(CH2)4-S-PdAg were characterized via X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). ERGO-S-(CH2)4-S-Pd and ERGO-S-(CH2)4-S-PdAg can be employed for the electrocatalytic oxidation of formic acid. The electrochemical behaviors of this electrode were investigated using cyclic voltammetry (CV), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS).Keywords: Silver nanoparticles; palladium nanoparticles; alloy; electrocatalytic oxidation; formic acid; graphene

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An Efficient Current Collector for Hematite-based Photoelectrochemical Water Splitting

김광현 이정엽[1] 장지현*

울산과학기술대학교(UNIST) 친환경 에너지 공학부 [1]UNIST Chemistry

?-Fe_2O_3, a widely used photoanode in photoelectrochemical water splitting, has some restrictions that need to be overcome such as short carrier lifetime and poor light absorption near the band edge etc. We addressed these issues by utilizing an efficient patterned current collector that serves as a direct transport medium of photogenerated electrons with a shorter pathway, and a light scattering layer to enhance light absorption. The improved properties were confirmed by the analysis of an electrochemical impedance spectroscopy, optical properties, and photoelectrochemical properties.

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Observation of electrocatalytic amplification of platinum signle nanoparticle collision on palladium ultramicroelectrodes

신창환 권성중*

건국대학교 화학과

Detection of single nanoparticle (NP) collision is being researched by electrocatalytic amplification method. One system for this consists of Pt NP, Au ultramicroelectrode(UME), and hydrazine oxidation reaction. When Pt NPs are collided on Au UME, increasing current response is observed via hydrazine oxidation. In order to make biosensor-device from this concept, it is important that the flexibility of metal substrate is obtained. So, alternative metal was found. It is the metal palladium (Pd) which is employed for the electrode. The substituted Pd UME has wide potential range available which can be applied for detection of NP adsorption. In case of detection of Pt single nanoparticle collision using Au UME, the electrode is applied by near 0 V (vs. Ag/AgCl). On the other hand, available potential of Pd UME is applied by 0.1 ~ -0.2 V for that; the signal is observed without changing shape.

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Observation of Single Iridium Oxide (IrOx) Nanoparticle Collisions by Electrocatalytic Amplification using Copper (Cu) Ultramicroelectrode

최용수 권성중*

건국대학교 화학과

Recently, the observation of the electrocatalytic behavior of individual nanoparticles(NPs) such as Pt or Iridium oxide(IrOx) by electrochemical amplification method has been reported1-4. The amplified current is due to the single nanoparticle collision at the ultramicroelectrode (UME). The IrOx NP has blip type collision current response and is well known as a good electrocatalyst for water oxidation and is known to be better than Pt3. Therefore, catalytic reaction by the IrOx NP is shown on the Pt UME in a designed potential (0.8 V vs. Ag/AgCl) and results in a detectable amplified current transient. However, the bare Pt UME had poor reproducibility and was inconvenient to use without surface pre-treatment. So, we need to find out other metal electrodes have been investigated for reproducible data analysis and convenient use. Also, the adhesion coefficient between NP and the new UME was studied for better understanding of the single NP collision system.

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Highly graphitized nitrogen-doped hollow core mesoporous shell carbon: synergistic bifunctional catalyst for oxygen reduction in an alkaline electrolyte

송민영 유종성* 양대수[1] 박현열[1] SINGHKIRANPAL[1]

대구경북과학기술원(DGIST) 에너지시스템공학과 [1]대구경북과학기술원(DGIST) 에너지시스템공학

There are many studies portraying the role of iron (Fe) and nitrogen (N)-doped carbon as an electrocatalyst. Even though the presence of N is undeniably needed for the efficient catalysis, but the presence and role of Fe are still debated. To clearly understand the role of Fe in a electrocatalyst, we report the synthesis of N-doped hollow core mesoporous shell carbon (N-HCMSC), prepared by a simple nanocasting of Fe phthalocyanine (FePc), a single precursor of for carbon, N and Fe into silica with solid core mesoporous shell (SCMS), followed by pyrolysis and HF/NaOH washing to selectively remove silica template and/or Fe. From various analysis techniques it is confirmed that N is successfully doped into the HCMSC structure. Interestingly, it is found that presence of Fe in N-HCMSC (FePc) leads to the efficient graphitization of N-HCMSC structure. The role of Fe for the electrocatalytic reaction is then studied through catalytic reduction of oxygen. The ORR performance of graphitized N-HCMSC (FePc) show that it hold the potential to be an efficient bi-functional electrocatalyst.

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Observation of Iridium Oxide Nanoparticle Collision at Millimeter-Sized Electrode by Drop-Coating Method

주진우 권성중*

건국대학교 화학과

In recent days, The nanoparticles(NPs) with various size, shape and material can be synthesized in interest. Noble metal NPs are studied to be used as catalysts for reaction in fuel cells or solar cells. Studies about catalytic ability of NP are enabled by the Electrocatalytic Amplification(EA method) developed by A. J. Bard. In EA method, dia. 10 ~ 25 μm ultramicroelectrode(UME) was necessary to reduce background current and noise. In this study, we tried to observe the catalytic activity of NP with millimeter-sized electrode. Some of collisions of NP aggregates were observed with Au deposited Si wafer. Then by means of drop-coating method, reproducible amperometric signals were detected. The sigmoidal relationship between concentrations of NPs and frequencies of collisions was fitted. The result can be explained as constant number of aggregates was formed above certain concentration of NP. The integrated areas of peaks also were saturated by limitation of hopping. With this analysis, catalytic ability of NP can be studied with millimeter-sized electrode.

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단입자 실험을 통한 LCO 단입자의 전기화학적 특성평가

Evaluation of electrochemical properties of LCO particles by single particle mesurement

임성현 Yuto Yamada[1] Kiyoshi Kanamura[1] 김성수[*]

충남대학교 에너지과학기술대학원 [1]Department of Applied chemistry Tokyo Metroplitan University

통상적인 양극 활물질의 특성평가는 활물질로 전극을 제작하여 셀의 특성평가를 통해 이루어진다. 그러나 전극 제작과정에서 첨가되는 바인더, 도전재, 집전체 등이 충전, 방전과정에서 전기 화학적 특성에 영향을 주게 되어 순수한 입자 본연의 성질을 관찰 하는 데에 방해요소로 작용한다. 따라서 본 연구에서는 입자 고유의 전기화학적 특성을 알아보기 위해서 micro-electrode 를 이용하여 입자의 충전과 방전을 진행하는 단입자 실험을 통해 LCO 단일입자의 전기화학적 특성 평가를 진행하였다. 실험은 LCO 단일입자에 Pt-glass 미세전극을 직접 접촉시킨 후에 nA 수준의 미세한 전류로 충전과 방전실험을 진행하였고 tafel plot 을 이용하여 교환전류 및 전하이동저항을 관찰하였다.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Role of iron in preparation and oxygen reduction reaction activity of nitrogen-doped carbon

양대수 송민영 박현열 유종성*

대구경북과학기술원(DGIST) 에너지시스템공학과

Fuel cells are regarded as the most promising renewable energy conversion devices due to their high energy efficiency along with negligible pollutant emission.Requirements for obtaining efficient N-doped electrocatalysts include a high electrical conductivity, large surface area and suitable pore structure for efficient mass transfer during the ORR process.Ordered mesoporous carbon (OMC) possesses excellent surface properties such as large surface area and pore volume, tuneable pore size and structural uniformity. It has been sought that presence of Fe-N in carbon network helps enhancing oxygen reduction reaction (ORR) activity of the carbon. In this study, N-doped platelet ordered mesoporous carbon is prepared using Fe-phthalocyanine as a single precursor for nitrogen, iron and carbon sources. We show that physical presence of Fe is not necessary to enhance the ORR activity of N-doped carbon, although Fe is required to create more active sites and to increase the electrical conductivity in the carbon framework.

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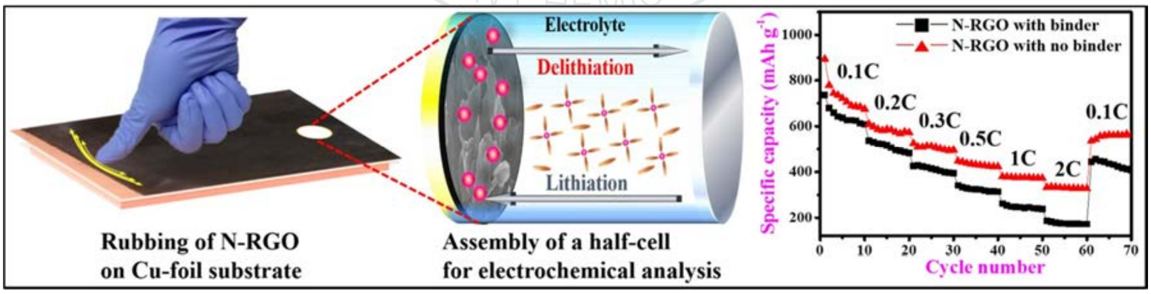
Simple approach to advanced binder-free nitrogen-doped graphene electrode for lithium batteries

박현열 양대수 송민영 유종성*

대구경북과학기술원(DGIST) 에너지시스템공학과

A simple binder-free synthesis approach of just rubbing nitrogen-doped reduced graphene oxide (N-RGO) powder on mechanically grinded Cu-foil substrate with rough surface is proposed for lithium ion battery (LIB). The nitrogen content of N-RGO is found to be 2.1 wt %. The binder-free N-RGO electrode shows excellent reversible capacity of 551 mA h g^{-1} as compared to 433 mA h g^{-1} of binder-added N-RGO electrode at a current density of 50 mA g^{-1} after 100 cycles. The process is not only highly reproducible and successful, but also results in high LIB performance, proposing ease scaling-up of such electrode for commercial application.



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Iodine-treated heteroatom-doped carbon: conductivity driven electrocatalytic activity

SINGHKIRANPAL **송민영[1] 유종성[1,*]**

대구경북과학기술원(DGIST) 에너지시스템공학 [1]대구경북과학기술원(DGIST) 에너지시스템공학과

A high conductivity and surface area are the most highly desired properties of an electrocatalyst. However,simultaneously obtaining a high conductivity and high surface area has been found to be challenging and one property can only be achieved by sacrificing other. Herein, wer eport a novel technique to synthesize highly conductive and microporous N and S-doped carbon from polyaniline (PANI) via a simple, template-free hydrothermal method followed by carbonization in the presence of iodine. The iodine treatment removes a large amount of the attached oxygen atoms and other heteroatoms and, as a consequence, increases the carbon content. Thus, the iodine treatment decreases the doping of catalytically active heteroatoms, which is unfavourable for the ORR, but at thesame time, significantly increases the electrical conductivity, which is beneficial for the ORR. Inparticular, iodine-treated carbonized PANI (CPANI) shows an exceptionally high conductivity i.e., about 3 times that of untreated CPANI. Iodine treatment is also found to enhance the micropore surface area of the PANI during carbonization without using a harmful activating agent or a hard template. An electrocatalytic study indicates that the activity of the iodine-treated sample is considerably higher than that of an untreated sample. This remarkable upsurge in activity is mainly attributed to the large increase in the conductivity and surface area of the iodine-treated sample. The ORR activity is discussed in terms of the heteroatom content, surface area and conductivity of the carbon. This convenient, innovative approach can offer new possibilities for the design of future highly efficient fuel cell electrocatalysts.

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발표코드: **ELEC.P-1246**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and electrochemical characterization of flexible thin film supercapacitor with long-term thermal stability

유정준

한국에너지기술연구원 에너지저장연구실

Electronic products have been asked to be small, light, safe, eco-friendly and even flexible. Supercapacitors (called electrochemical double-layer capacitor) are one of the great candidates of the next generation rechargeable energy storage devices for the portable electronic devices. Here, we have proposed a new scalable fabrication approach for making a flexible thin film supercapacitor that achieved high areal capacitance and high temperature-long term stability. The total thickness of the packaged prototype device was ~ 0.37 mm. This unique film-type supercapacitor could be applicable for commercial subminiature electronic devices.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A New Class Electroactive Fe and P-Functionalized Graphene for Oxygen Reduction

Fatemeh Razmjooei **SINGHKIRANPAL 유종성**[1,*]

대구경북과학기술원(DGIST) 에너지시스템공학 [1]대구경북과학기술원(DGIST) 에너지시스템공학과

While metal and nitrogen-containing carbon, where metal and nitrogen act as a catalytic center, has aroused a great interest as an efficient catalyst towards oxygen reduction reaction (ORR), no combination of metal with other heteroatom-containing carbon has received much attention. In the present work, we report the synthesis and the electrochemical properties of a new class electroactive iron and phosphorous-functionalized graphene (GPFe), which provides renewed insights into ORR catalysis. GPFe catalyst havebeen synthesized by simply pyrolyzing graphene oxide (GO) with phytic acid (PA) and iron (II) chloride(FeCl2.4H2O) as C, P, and Fe sources, respectively. (GPFe) catalyst shows remarkable electrocatalytic activity in terms of onset potential and limiting current density compared to that of its metal-freecounterpart (GP) in alkaline medium and illustrates much enhanced activity in acidic medium as well. Introduction of Fe causes remarkable synergistic effects on P-doped reduced graphene oxide by increasing surface area, enhancing P doping level due to the interaction between Fe and P and generating electrochemically active Fe-P species. In addition, it is found that PA, used as a P precursor, acts as aporogen at high temperature, which helps to increase the surface area of pristine reduced graphene oxide(RGO). We propose this study surely will provide renewed insights into ORR catalysts.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Au(111) 표면에 BTB 분자를 이용한 2차원 분자 네트워크 형성

이재성 이충균*

충남대학교 화학과

본 연구에서는 Au(111) 표면 위에 BTB 분자를 이용하여 2 차원 분자 네트워크를 형성시켜 STM 을 통해 관찰하였다. Au(111) 위에서 BTB 분자의 거동을 이해하기위해 비가역 흡착되는 용매를변화시켜 관찰하였고 흡착용매가 알코올인 경우, 알코올의 탄소사슬이 길어지게 되면 Pore 를 지니는구조로 변화하는 것을 관찰하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

탐구 요소별 과학 글쓰기를 활용한 과학 수업이 고등학생의 과학 탐구 능력과 과학에 대한 태도 및 과학 학업 성취에 미치는 영향

김경임* 조선화

경북대학교 과학교육학과

본 연구는 탐구 요소별 과학 글쓰기를 활용한 수업이 고등학생들의 과학 탐구 능력과 과학에 대한 태도 및 과학 과목 학업 성취에 미치는 영향을 알아보는 것이다. 탐구 요소별 과학 글쓰기를 활용한 과학 수업을 개발하기 위해 Park(2013)이 제시한 탐구 요소별 과학 글쓰기 수업 모형을 화학Ⅰ 내용에 적용하여 총 13 개 주제에 대해 26 차시 수업으로 개발하였으며, 약 4 개월에 걸쳐 실험 집단에 실시하였다. 비교 집단에는 같은 화학Ⅰ 내용에 대해 전통적 수업 방식으로 수업하였다. 본 연구를 위해 고등학교 2 학년 남학생 63 명을 실험 집단 30 명과 비교 집단 33 명으로 나누었으며, 두 집단의 사전, 사후 과학 탐구 능력과 과학에 대한 태도 및 과학 학업 성취를 비교 분석한 결과, 탐구 요소별 과학 글쓰기를 활용한 수업을 실시한 실험 집단에서 과학 탐구 능력(p

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

초중등 예비교사의 대기 관련 환경 문제 이해도와 확신도

한재영* **백성혜**[1]

충북대학교 사범대학 화학교육과 [1]*한국교원대학교 화학교육과*

지구의 대기와 관련된 환경 문제는 현재와 미래 인류의 삶에 직접 영향을 미치므로 세계의 모든 사람이 관심을 가지고 대처해야 하는 심각한 문제이다. 이러한 문제에 대처하는 데에는 환경 교육을 담당하는 초중등 교사가 매우 중요한 역할을 한다. 따라서 초중등 교사는 대기 관련 환경 문제의 원인과 해결 방안에 대해 올바른 지식을 가지고 미래 세대를 교육해야 한다. 이 연구에서는 초중등 예비교사가 대기 관련 환경 문제에 대해 얼마나 이해하고 있으며 자신의 생각에 어느 정도 확신하고 있는지 조사하였다. 검사 도구는 대기 환경 문제 진단 평가(Arslan 등, 2012)를 사용하였고, 3 개 교육대학과 4 개 사범대학에 재학하고 있는 예비교사 392 명을 대상으로 조사하였다. 검사 도구는 지구 온난화, 온실효과, 오존층, 산성비에 대해 13 개 내용을 3 단계로 질문한다. 조사 결과 예비교사의 내용 이해도는 질문 내용에 따라 21%에서 95%까지 다양하게 나타났다. 그리고 자신의 응답에 대한 확신 정도는 평균 61%에 그치고 있었다. 교육대학과 사범대학에서 예비교사에 대한 환경교육을 좀 더 강화할 필요가 있다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

2009 개정 초등학교 과학 교과서의 이독성 분석

강석진

전주교육대학교 과학교육과

이 연구에서는 2009 개정 과학교육과정에 의거하여 개발된 초등학교 3 학년 1 학기 과학 교과서의 이독성을 어휘와 문장 수준에서 분석하였다. 어휘 수준의 분석에서는 어휘를 난이도에 따라 1-4 등급으로 분류하고, 등급별 빈도를 비교하였다. 문장 수준의 분석에서는 문장을 단문과 복문/중문으로 분류한 뒤, 종류별 빈도를 비교하였다. 또한 문장의 평균 길이, 즉 한 문장에 포함된 어휘의 수도 계산하여 비교하였다. 연구 결과, 2009 개정 과학 교과서는 2007 개정 과학 교과서에 비해 어휘의 종류와 빈도가 증가한 것으로 나타났다. 2009 개정 과학 교과서에서는 2007 개정 과학 교과서에 비해 복문/중문의 비율이 소폭 감소하였으나, 문장의 평균 길이는 비슷하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

과학관 활용 수업을 위한 중등 예비과학교사의 교수 설계에서 나타나는 특징

양찬호 노태희*

서울대학교 화학교육과

이 연구에서는 사례연구를 통해 과학관 활용 수업을 위한 중등 예비과학교사의 교수 설계에서 나타나는 특징을 분석하였다. 서울 소재 사범대학의 예비과학교사 3 명이 연구에 참여하였으며, 국립과천과학관을 활용한 수업을 계획 및 실행하였다. 예비교사들이 제작한 모든 교수학습 자료를 수집하였고, 수업을 관찰하면서 수업 장면을 촬영 및 녹음하였으며, 교수 실행 전후에 반구조화된 면담을 실시하였다. 예비교사의 과학관을 활용한 교수 설계의 특징을 분석하기 위해 DeWitt & Osborne (2007)의 박물관 학습 수행 전략 틀을 예비과학교사의 맥락에 맞게 수정하여 사용하였다.

연구 결과, 예비교사들은 교수 설계 과정에서 과학관 수업을 서로 연계된 방문 전, 중, 후 활동으로 구성하는 '구조 제공하기', 방문 후 활동을 통해 방문 중 학습을 강화시키는 '학습 경험 강화', 과학관 학습을 학생 개인의 경험과 연결시키는 '개인적 관련성' 측면을 비교적 적절히 고려하는 것으로 나타났다. 그러나 방문 전 활동을 통한 '낯설음 감소시키기', 소집단 활동을 통한 '공동의 산출물 만들기', 다양한 상호작용을 촉진시킬 수 있는 수업을 구성하고 진행하는 '사회적 상호작용', 학생들이 자신의 학습을 직접 선택하거나 스스로 결정하도록 하는 '선택과 조절' 측면에 대한 인식과 실행 지식은 부족하였다. 한편, 예비교사들은 교수 계획 과정에서 주제 및 전시물을 선정하거나, 전시물을 학교 교육과정과 연계하여 활용하는 데 어려움을 느끼는 것으로 나타났다. 또한, 교수 실행 과정에서는 전시물이 작동하지 않아 당황하거나 학생들의 질문에 대한 대처, 시간 조절, 토의 진행, 흥미 유발 등의 측면에서 어려움을 겪었다.

이러한 결과는 예비교사 교육과정에서 과학관 학습에 대한 전문성 향상의 기회를 충분히

제공하지 않는다면, 향후 현직에 나간 예비교사들이 과학관 학습을 효과적으로 실행하기 어려울 것임을 의미한다. 그러나 기존 예비교사교육에서는 과학관을 활용한 교수 설계를 체계적으로 경험하기 어려운 실정이므로, 과학관 학습에 대한 예비교사교육 프로그램을 마련하여 제공할 필요가 있다. 특히, 과학관을 활용한 교수 설계는 교육 실습을 통해서도 경험하기 어려우므로, 대학에서의 예비교사교육에서 과학관 학습을 계획 및 시연하고 반성적으로 평가할 수 있는 기회를 제공해야 할 것이다. 이에 예비교사들의 인식 및 실행 지식이 부족한 것으로 드러난 측면이나 교수 설계 과정에서 겪은 어려움에 대한 연구 결과를 바탕으로 예비교사의 과학관 학습 관련 전문성을 향상시키기 위한 교육 방안을 제안하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

성격 특성과 과학에 관련된 태도가 화학Ⅰ 학업 성취에 미치는 영향(The Effects of Personality Traits and Science-related Attitudes on ChemistryⅠ Academic Achievement)

조선화* 김경임

경북대학교 과학교육학과

본 연구의 목적은 성격 특성과 과학에 관련된 태도가 고등학교 화학Ⅰ 학업 성취에 미치는 영향에 대해 살펴보고자 하는 것이다. 본 연구에서는 3 가지 검사 도구를 사용하였는데, 성격 특성을 측정하기 위한 BFI(Big-Five Inventory), 과학에 대한 태도를 측정하기 위한 TOSRA(Test of Science-Related Attitudes), 그리고 송영욱과 김범기(2010)에 의해 개발된 과학적 태도 검사지이다. 고등학교 2 학년 학생 170 명으로부터 자료를 수집하였으며, 학생들의 성격 특성과 과학에 관련된 태도, 그리고 화학Ⅰ 학업 성취와의 관계를 살펴보기 위해 다중 회귀분석(Multiple regression analyses)을 사용하여 분석하였다. 성격 특성 중 성실성이 화학Ⅰ 학업 성취에 통계적으로 유의미한 영향을 미쳤으며(p

일시: 2015년 4월 15~17일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **EDEC.P-1254**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

과학적 용어 연상 및 나열을 활용한 가설 설정 과정의 수업 전략 효과

강순희* 정솔

이화여자대학교 과학교육과

본 연구에서는 서울시 소재 사범대학에 다니는 예비 교사들을 대상으로 한 탐구화학 실험 수업에 적용할 수 있는 가설설정 기법을 강조한 교수 전략을 개발하였다. 학생들이 한 학기 동안 창의적 사고력과 비판적 사고력을 향상시키는 측면으로 개발된 교수 전략에 따른 총 10 개의 실험을 경험한 후, 그 교수 전략이 학생들의 창의적 사고력과 비판적 사고력에 미치는 효과를 알아보고자 하였다. 본 연구의 한 학기 동안의 수업 처치가 끝난 후, 가설설정 기법을 적용한 실험 교수 전략을 경험한 학생들의 창의적 사고력이 통계적으로 유의미하게 향상되었다(p.05).

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2009 개정 교육 과정 화학 II 교과서에 포함된 탐구 활동 분석: 8가지 과학 실천을 중심으로

최애란[*] 전영[1]

이화여자대학교 과학교육과 [1]이화여자대학교 화학교육학과

본 연구에서는 2009 개정 과학 교육과정에 따른 고등학교 화학Ⅱ 교과서 4 종에 제시된 173 개의 탐구 활동을 Next Generation Science Standards (NRC, 2013)에서 제시한 8 가지 과학 실천 즉, '질문하고 문제 규정하기' '모형 개발하고 사용하기' '조사 계획하고 수행하기' '자료 분석하고 해석하기' '수학 및 전산적 사고하기' '설명 구성하기' '증거에 입각하여 논의하기' '정보를 얻고 평가하고 소통하기'를 기준으로 분석하였다. 분석 결과 III 단원 '화학 평형'에 가장 많은 과학 실천이 포함되어 있었고 다음으로 I 단원 '다양한 모습의 물질'에 많은 과학 실천이 포함되어 있었으며 V 단원 '인류 복지와 화학' 에 가장 적은 과학 실천이 포함되어 있었다. 또한 '자료 분석하고 해석하기'와 '설명 구성하기'의 과학 실천에 편중되어 있고, '모형 개발하고 사용하기'와 '정보를 얻고, 평가하고, 소통하기'의 실천은 거의 포함되어 있지 않았다. 본 연구의 결과는 향후 과학 탐구 활동 개발시 고려해야 할 여러 가지 시사점을 제공한다.

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Research on establishing content standards for the recognition of senior secondary school qualifications between Korea and New Zealand: Chemistry curriculum comparative analysis

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사회가 글로벌화됨에 따라 국가 간의 교류가 활발해지고 있으며 국가 간 경계를 넘어 자신의 목표와 진로에 따라 학업을 진행할 국가를 선택하는 학생들이 증가하고 있다. 현재 세계적으로 고등학교까지 이수한 학교와 대학을 진학하는 나라가 다른 경우가 많아지고 있으며, 특히 뉴질랜드의 경우 국제 유학생 중 한국 학생의 비중은 매우 큰 편이다. 이에 뉴질랜드에서는 자국의 학력자격 인증제도(NCEA, National Certificate Education Achievement)를 시행하기 위해 교과별로 상세한 자격 규준을 설정하고 이를 바탕으로 타국과의 학력자격 상호 인증 제도를 시행하고 있으며, 2014 년부터 한국과 뉴질랜드의 고등학교 교육과정에 대한 상호인증을 통해 양국에서 고등학교 과정을 이수한 학생들이 학력자격을 인정받기 위한 제도적 장치를 설정하려 하고 있다. 이를 위한 기초 연구로 본 연구에서는 화학 과목을 중점으로 한국과 뉴질랜드의 학력자격 상호인증을 위한 교육과정을 비교하고 고등학교 졸업에 필요한 화학과 내용기준을 분석하였다. 연구 내용은 한국과 뉴질랜드의 교육과정 내용기준, NECA 평가기준, 교과서 내용진술 등을 참조하여 양국의 고등학교 졸업에 필요한 공통 학력기준을 설정하였다. 연구 방법은 NZQA(New Zealand Qualification Authority)에에서 설정한 화학과 교육과정 내용진술 및 뉴질랜드 NCEA 성취기준을 참조하여 고등학교에서 이수하는 화학과 교과내용을 우리나라 화학Ⅰ, 화학Ⅱ 과목과 비교하여 분석하였다. 여기서 NZQA 에서 설정한 화학과 교육과정 Level 8 은 NCEA 성취기준 Level 3 에, Level 7 은 NCEA 성취기준 Level 2 에, Level 6 은 NCEA 성취기준 Level 1 에 상응한다는 것을 전제하였다. 연구 결과 우리 주변의 화학, 원자구조와 주기율표, 분자의 구조와 극성, 화학 결합, 유기화학과 탄화수소, 반응속도, 화학평형, 산과 염기, 산화와 환원 등의 영역에서는 한국과 뉴질랜드 양국 간에 상당한 연계가 발견되었다. 우리나라 화학Ⅰ, Ⅱ의

대부분의 교육과정 내용요소가 뉴질랜드 교육과정의 level 7~8 에 해당되었으며, 2009 개정 화학과 교육과정에서 축소된 유기화학 등 일부 영역은 뉴질랜드의 level 6 에 해당하였다. 특징적으로 뉴질랜드의 화학과 교육과정의 경우 과학 탐구 관련 교육과정을 별도로 중요하게 다루고 있으나 우리나라의 경우 화학Ⅰ,Ⅱ의 전 영역과 관련되고 특정 교육과정과 관련된 것은 아니었다. 또한 분광학 등의 경우에는 뉴질랜드에서는 다루고 있지만 한국의 화학 교육과정에서는 관련 내용을 발견하기 어려웠다. 이에 뉴질랜드와 우리나라의 고등학교 화학 교육과정은 많은 부분에서 상당히 유사하지만, 각 국에서 전혀 다루지 않는 부분도 나타나므로 한국-뉴질랜드 간의 고등학교 학력자격 인정 규준을 설정하기 위해서는 양국의 교육과정에서 차이가 나는 부분에 대해 학력자격 인정 범위를 설정을 위한 추가적인 연구가 필요할 것이다.

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2009 교육과정의 중학교 과학 교과서에 반영된 사회정서학습(SEL) 요소 분석

신선희 박현주[1,*]

조선대학교 과학교육학과 [1]조선대학교 과학교육학부

사회정서학습(Social Emotional Learning, SEL)은 또래, 교사, 가족 등의 타인과의 긍정적 관계를 촉진하는데 초점을 둔 개인간 발달을 반영하는 (1)사회적 측면과 정서 또는 감정 그리고 개인의 정서와 연결된 인지 또는 사고와 관련된 자기인식 및 자기지식의 증진에 초점을 둔 (2)정서적 측면이 있다. 그리고 (3)학습적 측면은 사회적 및 정서적 영역에서의 성장과 적응이 수업, 연습, 피드백을 통해 가르치고 학습될 수 있음을 의미한다. 즉 사회정서를 교과 학습에 포함시킴으로써 개인 간 및 개인 내 발달의 목적을 달성하기 위해 구체적인 수업활동, 수업지도안, 교육과정을 적용할 수 있음을 나타낸다. 본 연구는 과학 교과와 사회정서학습의 관련성을 2009 교육과정의 중학교 과학교과서에 포함된 사회정서학습 요소를 분석함으로써, 사회정서학습의 과학 교과 적용성 및 활용성에 대한 시사점을 제공하였다.

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소집단을 활용한 융합 수업 모델의 개발 및 적용-고등학교 화학Ⅰ 수업을 중심으로-

서재현 우애자[1,*]

와부고등학교 교사 [1]이화여자대학교 과학교육과

본 연구는 ‘융합 인재 교육’, ‘핵심 역량 기반’과 관련된 과학 교육의 목표를 성취하기 위한 노력의 하나로서 화학Ⅰ 교과 중심의 소집단 활용 융합 프로그램을 인문계열형과 자연계열형으로 나누어 개발하고, 이를 적용한 후 학생들에게 나타난 과학에 대한 정의적 태도 변화, 과학 탐구 능력 변화, 창의적 인성 변화, 수업 적용 후 프로그램에 대한 인식을 정량적인 분석과 함께 일부 정성적인 분석을 통해 알아본 것이다. 연구는 일반계 고등학교 2 학년 학생으로 인문계열 79 명, 자연계열 45 명을 대상으로 하였으며, 정규 교육과정 내에서 실천할 수 있는 수업 전략을 활용하여 전체 수업 68 차시 중 개발된 프로그램 23 차시를 투입한 것이다. 연구 결과 과학에 대한 정의적 영역 중 ‘태도’ 영역과 과학 탐구 능력은 인문계열 학생과 자연계열 학생 모두 통계적으로 유의미하게 향상되었고, 창의적 인성의 경우 인문계열 학생에게 통계적으로 유의미한 향상 효과가 나타났다(p

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2009 개정 교육과정에 의한 융합형 과학이 학생들의 과학의 본성과 STS에 대한 이해, 과학 관련 정의적 영역에 미치는 영향

김민환 양찬호 노태희*

서울대학교 화학교육과

이 연구에서는 2009 개정 교육과정에 의한 융합형 과학이 고등학교 1 학년 학생들의 과학의 본성과 STS 에 대한 이해, 과학에 대한 흥미와 포부에 미친 영향을 조사하였다. 서울특별시의 8 개 지역구에서 한 학교씩 총 8 개 고등학교를 선정하였으며, 학교당 한 학급을 무선표집하여 고등학교 1 학년 학생 214 명(남학생 127 명, 여학생 87 명)이 연구에 참여하였다. 연구 참여 학생들은 2014 학년도에 2009 개정 교육과정에 의한 융합형 과학을 이수하였다. 과학 수업이 시작되기 전인 2014 년 3 월 초와 과학을 이수한 후인 2014 년 12 월 말에 각각 동일한 검사지를 사용하여 검사를 실시하였다.
융합형 과학 이수 전후 학생들의 과학의 본성에 대한 이해 검사 점수에 대한 대응표본 t-검증 결과, 과학 이수 후 과학의 본성 검사의 평균 점수가 이수 전보다 약간 낮았으나, 통계적으로 유의미한 차이는 없었다. 그러나 과학의 본성에 대한 이해 검사의 하위영역별 점수의 대응표본 t-검증 결과, 과학 지식의 임시성과 상상력의 사용 영역에서 과학 이수 후의 검사 점수가 이수 전보다 통계적으로 유의미하게 낮았다. 과학 이수 전후 학생들의 STS 에 대한 이해 검사의 각 문항에 대한 범주별 응답 빈도를 $\chi 2$ 검증한 결과, 통계적으로 유의미한 차이가 있는 문항은 없었다. 과학 이수 전후 학생들의 과학에 대한 흥미와 과학에 대한 포부 검사 점수의 대응표본 t-검증 결과, 과학 이수 후 과학에 대한 흥미 검사의 평균 점수가 과학 이수 전보다 약간 낮았으나 통계적으로 유의미한 차이는 없었다. 또한, 과학 이수 후 과학에 대한 포부 검사의 평균 점수가 과학 이수 전보다 약간 높았지만 통계적으로 유의미한 차이는 없었다. 이상의 결과를 종합하면 융합형 과학의 이수가 고등학생들의

과학의 본성에 대한 이해와 STS 에 대한 이해, 과학에 대한 흥미나 포부를 실질적으로 향상시키지 못하였다고 할 수 있다.

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2009 개정 과학교육과정에 따른 고등학교 화학 교과서 탐구활동 분석

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내용 과학에서 탐구는 주요한 부분으로 많은 과학 교육 연구자들이 어떻게 학생들이 탐구 수업을 통하여 학습하는지 또한 교사들은 어떻게 탐구 수업을 하는지 연구해오고 있다. 미국연구회 NRC(National Research Council)는 탐구에 대하여 과학 지식의 구성 과정의 다양성과 비형식성을 암시하기 위한 용어로써 공학적 실행(practices framework)을 제안하고 과학자들의 이와 같은 생성과정을 이해하는 것이 과학에 대한 이해의 기초가 된다고 주장하였다. 또한, NRC 는 여러 과학 분야에서 행해지는 과학자들의 실천적 특성을 과학교육에 적용할 수 있는 8 가지 형태(질문하고 문제 규정하기, 모형 개발하고 사용하기, 조사 계획하고 수행하기, 자료를 분석하고 해석하기, 수학 및 전산적 사고 이용하기, 수학 및 전산적 사고 이용하기, 설명 구성하고 문제 해결 고안하기, 증거에 입각하여 논의하기, 정보를 얻고, 평가하고, 소통하기)로 제시하였다. 본 연구에서는 2009 개정 과학 교육과정에 따른 고등학교 화학 교과서에 제시된 탐구활동을 공학적 실행(engineering practices) 개념을 이용하여 분석한다. 이에 학생들에게 제공되는 탐구 활동의 목적과 과학적 실천과의 연관성을 논의하고자 한다.

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중, 고등학교 실험실 안전의 향상에 관한 대안

김현영

경북대학교 일반대학원 과학교육학과

중,고등학교에서 실험의 중요성은 이미 여러차례 강조 되어 왔다. 실험이 그만큼 중요함에도 불구하고대부분 학교에서는 실험의 안전에 관한 관심은 부족하다. 그로인해 대학교, 사회로 진출해서도 안전에 대한 불감증으로 인해 사고가 발생한다. 그런 사고를 예방하기 위해서는 중, 고등학교에서 실험을 할때부터 안전에 관한 인식을 가지고 실험에 참여해야 한다. 교사와 학생, 학교 차원에서 실험실 안전 향상에 관해 어떤 조치를 취할수 있는지에 대해서 알아볼 것이다.

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모델링을 강조한 논의 기반 일반화학실험에서 학생들의 모델링에 대한 인지과정 탐색

이동원* 남정희 강여은[1]

부산대학교 화학교육과 [1]부산대학교 교육대학원

이 연구는 모델링을 강조한 논의 기반 일반화학실험에서 수행하는 모델링에서 나타나는 학생들의 인지과정에 대한 탐색을 통해 논의에 바탕을 둔 교수 전략이 모델링에 어떠한 영향을 미치는지와 변화의 이유를 알아보는 것을 목적으로 하였다. 이를 위해 일반화학을 수강하는 사범대학 화학교육과 1 학년 학생 21 명을 대상으로 모델링을 강조한 논의 기반 일반화학실험 여섯 개 활동을 1 학기 동안 적용하였다. 모델링에서 나타나는 학생들의 인지과정을 탐색하기 위해 학생 인터뷰 자료를 수집하였다. 모델링 수행에서 나타나는 인지과정의 분석 결과, 효과적인 모델의 요소에 대해 학생들은 시각적 표현, 설득력 있는 설명의 제공, 수사학적 구조의 측면에서 응답하였다. 모델링 과정에서 사용한 전략에 대해서 학생들은 모델링 수행 전과 수행과정의 두 가지 측면에서 응답하였다. 모델링 수행 전에는 실험 보고서를 작성하는 과정에서 중요한 키워드 등을 미리 정리해 두거나 개요를 따로 작성하고 실제 모델링 수행 과정에서는 다양한 자료를 이용, 자료를 재구성하여 제시, 핵심개념에 대한 정의와 설명을 제시, 수사학적 구조를 고려, 메타인지를 이용하는 전략을 사용하였다. 모델링 과정에서에서 겪는 어려움에 대한 학생들의 응답은 모델링 전략의 부재, 이해 부족의 두 가지 범주로 나눌 수 있었으며, 이러한 어려움의 해소에 대한 학생들의 응답은 모델링 전략의 부재와 내용 이해 부족으로 나타나는 어려움을 해소하기 위해 어떻게 모델링 전략을 습득하고 내용을 이해하는지로 구분되었다. 학생들은 피드백 단계, 모델링 경험, 실험 보고서에 대한 평가, 자신이 이전에 작성한 모델, 참고문헌을 통해 전략을 습득하며, 내용에 대한 이해는 수업 단계에서 나타나는 논의 과정과 실험 보고서 작성 과정을 통해 이루어졌다. 이러한 결과로부터 모델링을 교수학습에 이용할 때 논의에 기반을

둔 학습전략이 정신 모델을 검증하고 수정하여 표현된 모델로 구현하는 과정에 도움을 주고 과학 개념과 더불어 메타모델링 지식의 이해를 도와 학생들의 모델링 발달에 영향을 줌을 보여 주었다.

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예비 화학교사의 탐구지도 경험에 관한 질적 연구: 탐구의 인식과 실천 사이의 딜레마 해소 과정을 중심으로

백종호

서울대학교 과학교육과(화학전공)

오랜 기간 동안 과학교육 분야에서 탐구는 과학 학습의 핵심적인 목표이자 수단으로 자리매김해왔다. 그러나 탐구의 중요성에 대하여 많은 연구에서 동의하는 것과 달리, 교육의 맥락에서 탐구의 역할과 기능, 실행방안에 대한 논의는 여전히 분분하다. 본 연구에서는 예비 화학교사의 탐구 지도 경험을 살펴봄으로써, 교육 상황에서 탐구를 통한 교수학습이 실제로 작동하는가에 관하여 비판적으로 검토하고자 했다. 이를 위해 다음의 연구 질문에 답을 하고자 했다. 첫째, 예비 화학교사의 과학 탐구에 대한 인식은 어떻게 나타나는가? 둘째, 예비 화학교사의 과학 탐구에 대한 인식과 실천 사이의 갈등은 어떻게 나타나는가? 셋째, 예비 화학교사는 과학 탐구 지도 과정에서 발생한 갈등을 어떻게 해소하는가? 위의 문제에 대하여 3 명의 예비 화학교사들의 탐구지도 준비와 수업, 평가의 과정을 2 인의 연구자가 추적하였다. 연구 결과에 의하면 예비 화학교사들은 탐구를 학습자의 자율적인 흥미와 관심에 따라 스스로 문제를 해결하는 일종의 '주체-화' 과정으로 인식하고 있으며, 충분한 과학 지식과 연역적인 절차를 담보로 하는 '과학적인 방법'이 기반이 되어야 한다고 주장하는 것으로 나타났다. 그러나 예비교사들의 탐구 인식은 실제의 교육 상황에서 원래 의미한대로 실현되기 어렵기 때문에 이상화(idealization)되며, 실천과의 부정합으로 인한 딜레마가 발생했다. 인식과 실천에서 나타난 딜레마의 양상은 크게 '발산하는 탐구와 수렴하는 과학', '흥미 중심의 탐구와 학습 중심의 탐구', '학습 주체로서의 학생과 부족한 지식인으로서의 학생'으로 구분할 수 있었다. 예비교사들은 학생이 온전한 주체가 되어 능동적으로 탐구를 수행하는데 여전히 의구심을 갖고 있으며, 결국 탐구는 교사의 기대와 목적에 따라 주어진 장의 결론에 수렴하는 '교수 행위'일 수밖에 없음을 언급하였다.

따라서 본 연구 결과를 토대로 탐구를 제대로 인식하고 실천하기 위한 학문적·제도적 정비와 더불어, 교사는 과학 지식에 완전한 전능자가 아니라 학생과 함께 새로운 것에 과감히 도전할 수 있는 학습자라는 개방적 인식 변혁을 제안하였다.

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초등 과학 수업에서 스토리텔링을 이용한 전략의 효과

강석진

전주교육대학교 과학교육과

이 연구에서는 초등학교 과학 수업에서 스토리텔링을 이용한 전략의 효과를 학생들의 학업 성취도와 학습 태도 측면에서 조사하였다. 1 개 초등학교의 5 학년 2 개 학급 43 명의 학생들을 처치 집단과 통제 집단으로 배치하였다. 사전 검사로 학업 성취도 검사, 과학에 대한 태도 검사, 과학 수업에 대한 태도 검사를 실시하였다. 처치 집단에는 스토리텔링을 이용한 전략에 따라 수업 지도안을 개발하고 10 차시 동안 수업 처치를 실시하였고, 통제 집단에는 교과서와 지도서에 기반하여 과학 수업을 실시하였다. 사후 검사로 학업 성취도 검사, 과학에 대한 태도 검사, 과학 수업에 대한 태도 검사를 실시하고, 2 개월 후 학업 성취도 파지 검사를 실시하였다. 연구 결과, 학업 성취도와 과학 및 과학 수업에 대한 태도 측면에서 처치 집단과 통제 집단 사이에 유의미한 차이는 나타나지 않았다. 그러나 학업 성취도 파지 검사의 경우, 통제 집단과 달리 처치 집단 학생들의 점수가 오히려 상승하였다.

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한국과 미국 과학 및 화학 교과서의 실험안전 영역 비교

이재환

경북대학교 과학교육학과

실험실 안전사고의 주된 원인은 학생 부주의에 의한것으로 작은 사고도 큰 부상을 일으킬 수 있다. 사고는 예방할 수 있고 이것은 학생과 교사 모두 안전에 대한 의식과 태도가 강화되었을 때 이루어 질 수 있다. 학생과 교사 사이의 의사소통의 도구이자 교수 학습의 기본인 교과서에는 이러한 안전에 관한 내용이 충실히 반영될 필요가 있다. 따라서 본 연구자는 한국과 미국의 중학교 과학 및 고등학교 교과서에 제시된 실험 안전에 관한 내용을 비교하여 좀 더 실용적으로 활용할 수 있는 안전 교재를 개발하는데 기초자료를 제공하자고 한다.

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Effects of water on the CO_2 absorption properties of $NaNO_3$-MgO absorbent

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In the triple temperature design of carbon capture and sequestration technology under development, the absorbent operating in the mid-temperature range (200-500°C) is very important. Presently, MgO, with the help of a promoter $NaNO_3$, is the only known material that satisfies the thermodynamic requirements for this purpose. From the literature data and our own experience, it appears that the CO2absorption behavior of MgO-$NaNO_3$ absorbent depends on the presence of water. Therefore, in this study, we have investigated the effects of water on the CO_2 absorption characteristics of MgO-$NaNO_3$ absorbent. We prepared three different samples and measured their CO2absorption properties: Sample A is a MgO-$NaNO_3$ absorbent prepared in the conventional method by mixing MgO and $NaNO_3$ followed by a heat treatment, sample B is derived from sample A by exposing it to a controlled amount of water vapor, and sample C is obtained by heating a mixture of $Mg(OH)_2$ and $NaNO_3$ under a controlled manner to control the amount of water in the sample. Depending on the presence of water and the method to introduce water, the absorbents showed different CO_2 absorption behaviors. Especially, while sample B shows almost the same behaviors as sample B both in kinetics and thermodynamics, sample C shows enhanced absorption kinetics and capacity than sample A. Details of the data and their explanations will be presented in the poster.

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Analysis of CO_2 absorption behavior of chemically modified MgO

조승익 김강영 곽진수 홍다영[1] 안영인 권영욱[*]

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Magnesium oxide with promoter $NaNO_3$ is one of the intermediate-temperature (temperatures ranging from between 200~400℃) solid CO_2 absorbents. In order to enhance its performance, it is important that we understand CO_2 absorption process of MgO absorbents and the role of promoter. We postulate that both CO_2 and MgO are dissolved in $NaNO_3$ and react to form $MgCO_3$. So, our group has been investigating various aspects of CO_2 absorption on MgO and related materials. We have developed an improved preparation method for the MgO absorbent. The absorbents were synthesized by precipitation and ball-milling method of MgO and $NaNO_3$. We also checked the effect of Ni and Zn doping in MgO on the CO_2 absorption and desorption. Substitution of Ni in MgO is relatively easy without change of lattice energy because NiO and MgO have similar lattice structures, lattice energies, and the sizes of cations. Solid-solution between MgO and ZnO was also synthesized well. By doping MgO with Ni and Zn, the CO_2 absorption capacity was generally lower than that of pure MgO. We expected that Ni and Zn in MgO hindered the absorbent to react with CO_2 (or absorb CO_2 or form $MgCO_3$). Therefore, we anticipate that doping effect helps to identify the CO_2 absorption mechanism of MgO in molten $NaNO_3$.

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Effect of Metal Carbonate Salts on the CO2 Absorption on NaNO3-promoted MgO Absorbent

김강영 곽진수 조승익 홍다영[1] 안영인 권영욱[*]

성균관대학교 화학과 [1]성균관대학교 자연과학부 화학과

Many researchers have studied CO2 absorption behavior by MgO absorbent in the presence of metal carbonates. Most of them focused on the ability of metal carbonates as an agent to increase CO2 absorption capacity of MgO absorbent. We report here the rate of CO2 absorption of MgO absorbent is enhanced by the addition of carbonates. We prepared MgO samples mixed with varied amounts of alkali or alkaline earth carbonates and measured their CO2 absorption kinetics. The absorption kinetics showed variations depending on the nature and the amount of carbonate. A small amount of SrCO3 appears to enhance the kinetics most efficiently. Plausible mechanisms based on the observation will be discussed.

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Controlling the spatial distribution of quantum dots in polymer nanofiber for dye-sensitized solar cells

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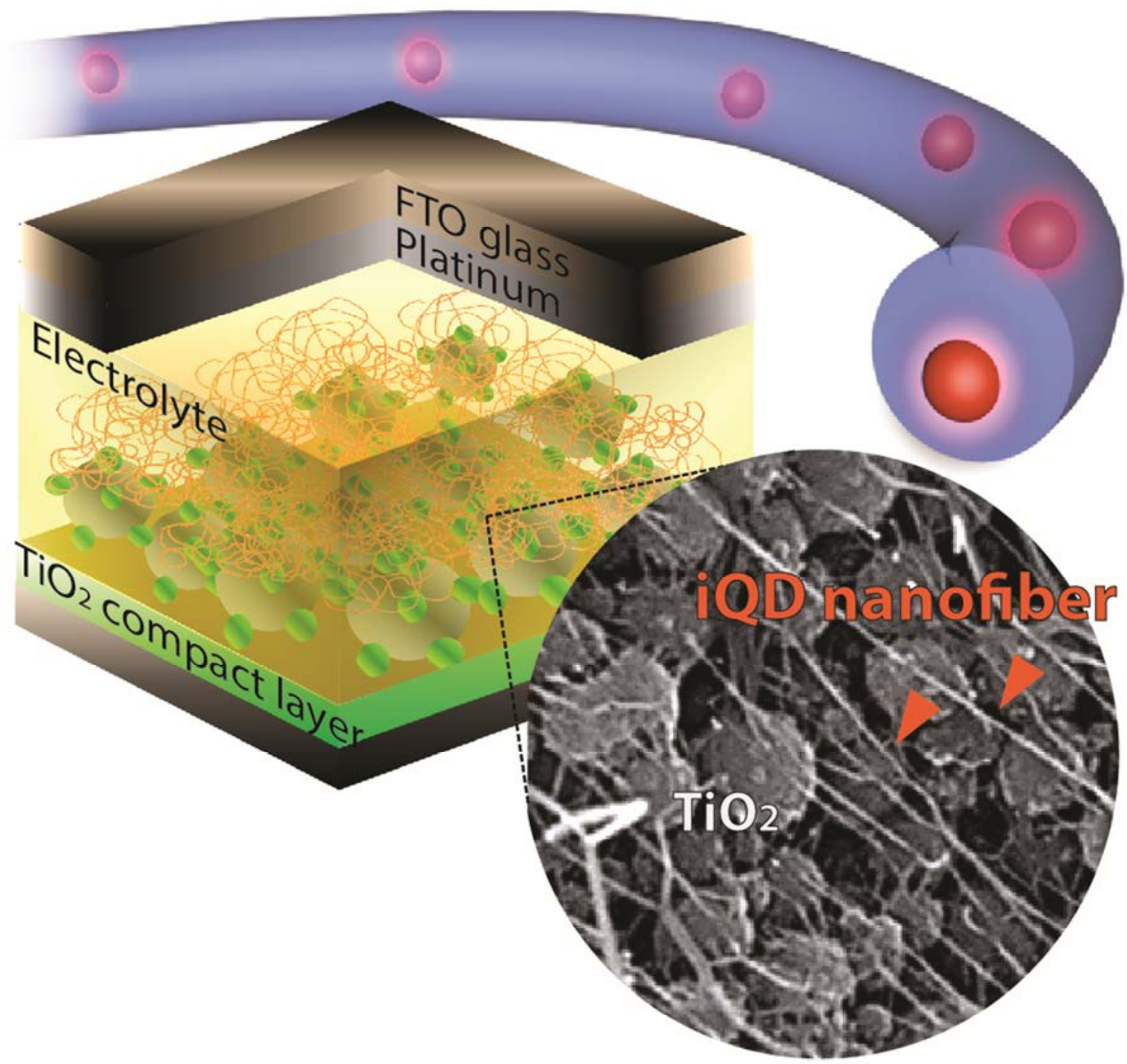
연세대학교 화학과

An approach to inter-dot or inter-molecule spacing control of functional moieties in solid-state devices has long been sought in both fundamental and technological field. In this study, we present a new strategy for controlling the distance between QDs based on one-dimensional spatial confinement in polymer nanofiber template. This reliable technique allows for isolating QDs with sufficient distance in thick film and retaining their monomeric characters, such as distinct spectrum from aggregates (ca. 30 nm shift) and monoexponential photoluminescence decay, which indicates the suppressed inter-dot interactions. We successfully developed light-harvesting devices by incorporating QDs in the nanofiber as an auxiliary light-harvester and improved the performance of devices from 5.9 to 7.4 % due to its additional absorption and efficient energy transfer. This strategy offers a viable pathway to control the arrangements of various functional moieties in solid-state devices.


FTO glass
Platinum
Electrolyte
TiO2 compact layer
iQD nanofiber
TiO2

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparison of CO_2absorption properties of MgO promoted by $NaNO_3$and $NaNO_2$

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성균관대학교 화학과 [1]성균관대학교 자연과학부 화학과

MgO is well known as an intermediate-temperature CO_2 absorbent because its carbonate decomposition temperature is lower than other alkaline metal oxide. Its CO_2 absorption kinetic is very slow because its lattice enthalpy is so high. $NaNO_3$ is used as a promoter in order to enhance CO_2 absorption capacity of MgO. MgO can absorb about 75% of CO_2 with $NaNO_3$. But $NaNO_3$ has several problems to use a promoter of CO_2 absorption. It can be decomposed into noxious material and the velocity of CO_2 absorption of MgO with $NaNO_3$ is not fast enough. So we wanted to find another promoter which can compensate a defect of $NaNO_3$ and have similar performance for CO_2 absorption promoter with $NaNO_3$. We chose $NaNO_2$ because it has similar chemical and physical property with $NaNO_3$. MgO showed high performance for CO_2 absorption with $NaNO_2$ and the absorption velocity of MgO is higher than using $NaNO_3$. However, $NaNO_2$ decompose at high temperature so we try to complement on this point. We expect that $NaNO_2$ can be a good promoter compare to $NaNO_3$.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

자동차 냄새 유발물질의 분석

장대익

(재)울산산업진흥테크노파크 정밀화학소재기술연구소

추후입력

일시: 2015년 4월 15~17일(수~금) 3일간
장소: 일산 KINTEX
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Reductive Dechlorination of Chlorinated Organic Compounds Using Nickel/Palladium(Ni/Pd) Nanoparticles Produced by Pulsed Laser Ablation in Liquid(PLAL)

정현진 최명룡*

경상대학교 화학과

Nickel nanoparticles exhibit useful optical or electrical functions as well as catalytic actions. 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 nickel nanoparticles in methanol. The morphological and optical properties of nickel nanoparticles were characterized by X-ray diffraction, field emission - scanning electronic microscope, energy dispersive spectrometer and high resolution - transmission electron microscope. Synthesized nickel/palladium bimetallic nanoparticles were applied to dechlorinate chlorinated organic compounds under various conditions. Rapid dechlorination of chlorinated organic compounds suggests that nickel nanoparticles can be used for remediation of chlorinated organic compounds in the environment.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Reductive Dechlorination of 4,4'-DDT and Its intermediates using Fe/C/Pd Nanoparticles Produced by Pulsed Laser Ablation in Liquid

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경상대학교 화학과

Persistent organic pollutants have concerned public due to their toxicity, bioaccumulation and persistency in the environment and human health. Bimetallic catalysts have recently appeared significant effect for the remediation of groundwater and sediment contaminated with chlorinated organic compounds. Fe/C/Pd bimetallic nanoparticles (NPs) were synthesized by a two-step method. Firstly, Fe nanoparticles were produced by a pulsed Nd:YAG laser (1064nm, 10Hz, 7ns) ablating onto an Fe plate immersed in methanol with a reducing agent, ascorbic acid. Then, the bimetallic NPs were prepared through mixing $PdCl_2$ with as-prepared Fe NPs under sonication at an ambient temperature. The morphological and optical properties of Fe/C/Pd catalysts via PLAL were characterized by transmission electron microscopy, X-ray diffraction, and Ultraviolet-visible spectroscopy. Fe/C/Pd catalysts were used for the dechlorination of 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (4,4'-DDT), 1,1-Dichloro-2,2-bis(4-chlorophenyl) ethane (4,4′-DDD), 1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene (4,4′-DDE), 2-Chloro-1,1-bis(4-chlorophenyl)-ethene (4,4′-DDMU) under various conditions. The products of dechlorination reactions were analyzed by gas chromatography. According to this study, Fe/C/Pd catalysts could potentially be employed to degrade rapidly 4,4’-DDT and its intermediates in the contaminated environment.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of morphologically different TiO2 nanoparticles by sol gel method and their photocatalytic applications

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한국기초과학지원연구원 하이테크소재연구부 [1]한국기초과학지원연구원 부산센터 [2]한국교통대학교 교양학부 - 화학

TiO2 nano materials are highly photo-sensitive, efficient photo-catalyst, strong oxidizing agent, and are easily available, highly stable, nontoxic. They are generally obtained through hydrothermal, solvothermal, sol-gel and electro-deposition process.Three different TiO2 nanoparticles in the present study were obtained following sol-gel process. The samples morphology was significantly varied by modifying the calcination or drying process, concentration of Ti precursor reagent, reaction time period, acid quantity, reaction temperature. Scanning Electron Microscopy, Tunneling Electron Microscopy and X-ray diffraction results show samples had diverse morphology, with the anatase phase. The photocatalytic activities of the Titanium dioxide nanoparticles (TiO2 NP) samples were evaluated by measuring the degradation of methyl orange and rhodamine B and compared the efficiency of three different TiO2 NP. The photocatalytic activity was followed using UV-Vis and Fluorescence spectroscopy. The photocatalytic degradation of the organic pollutants activity was achieved efficiently with the TiO2 nanoparticles samples prepared using higher concentration of precursor, due to their higher surface area, smaller size.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel self-assembled bimetallic structure of Bi/Fe^0 : The oxidative and reductive degradation of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)

이충섭 장윤석*

포항공과대학교(POSTECH) 환경공학부

A novel self-assembled bimetallic zero-valent bismuth/iron (Bi/Fe^0) composite was synthesized, characterized, and used successfully to remove hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) from wastewater. To assess the oxidative and reductive reactivities of Bi/Fe^0 nanoparticles (NPs), RDX degradation experiments were conducted in either ambient or anaerobic conditions, respectively. The best RDX degradation was achieved using 4%-Bi/Fe^0 (atomic ratio) NPs. In ambient conditions, concentrations of Fe^{2+} ions and H_2O_2 were lower in the Bi/Fe^0 solution than in the Fe^0 solution; this difference indicates that most Fe^{2+} ions and H_2O_2 reacted to produce hydroxyl radicals and superoxide radical anions, thereby resulting in the remarkable degradation of RDX. In anaerobic conditions, the presence of Bi increased the electron generation rate from the surfaces of the Bi/Fe^0 NPs. This increase was responsible for the excellent reductive degradation of RDX. Based on Density Functional Theory (DFT) calculations, the adsorption of water was endothermic on Fe^0 NPs and exothermic on Bi/Fe^0 NPs. Therefore, only the dissociation reactions of H_2O in the Bi/Fe^0 system were spontaneous, and these reactions resulted in the prominent reactivity of the Bi/Fe^0 NPs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A comprehensive strategy for Aroclor 1248 removal using nano-bio remediation

이충섭 장윤석*

포항공과대학교(POSTECH) 환경공학부

The existence of Aroclor 1248 in soils and sediments is an important environmental concern due to its persistence, health risks and high concentration. The co-existence of various PCB congeners from Aroclor 1248 in contaminated site is a challenge of remediation. The PCB can be anaerobically dechlorinated by many PCB dehalorespiring cultures collected from sediments. Recently, new catalysts, such as: nanoscale zero-valent iron (nZVI) or bimetallic based nZVI (Pd/nFe and Ni/nFe) have been developed for the degradation of halogenated pollutants. To integrating the advantages of both chemical and biological treatments, the anaerobic dechlorination of Aroclor 1248 was promoted using bimetallic Pd/nFe and the oxidative degradation of dechlorination metabolites was performed by *Burkholderia xenovorans* LB400 in our research. According to chlorine measurement, 89.3% chlorine was removed from PCB mixture. Investigating removal efficiency of 32 PCB congeners (62.5% total PCB in Aroclor 1248) showed that 99% Tri-CB was dechlorinated while percentage of tetra-, penta- and hexa- and higher CB were reduced 92%, 84% and 28%, respectively. Biphenyl was found as the main intermediate of the PCB dechlorination using bimetallic nanoparticles and was rapidly biodegraded by B.xenovorans LB400. Benzoic acid and cis-cis muconic acid, metabolites in were detected by HPLC. The decreased toxicity of PCB after nano-bio hybrid treatment was evaluated via less TEQ value (from 33.8×10^{-5} to 9.5×10^{-5}), low cytotoxicity towards *E.coli.* Reactive oxygen species (ROS) level in the Aroclor 1248 sample before treatment was higher 2.4 times and 5.7 times in comparison to samples after treatment and control, respectively. Gluthathione peroxidase activity increased from 0.3 mU in control without any treatments to 9.4 mU and 2.6 mU in samples before and after treatment.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reduction kinetics of divalent mercury by Fe(II) using natural and synthetic Fe(III) oxides

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Mercury contamination of groundwater, where mercury undergoes various abiotic and biotic transformations, presents a significant threat to wildlife and humans. As reduction of Hg(II) to Hg(0) reduces its toxicity and increases its mobility, the understanding of Hg redox transformation in subsurface environments is critical for predicting groundwater quality. In this study, we investigated the reduction kinetics of Hg(II) in the presence of natural iron-bearing minerals and synthetic iron oxides (magnetite and hematite) in Pipes-buffered artificial groundwater of pH 6.8. The mineralogical properties of natural and synthetic iron oxides were determined by X-ray diffraction (XRD) and extended X-ray absorption fine structure (EXAFS), and the surface areas of minerals were determined by Brunauer-Emmett-Teller (BET) analysis. Abiotic reduction experiments were conducted to measure rates of Hg(II) reduction and to determine the effect of iron oxide surface area, using natural and synthetic iron oxides suspended in Pipes-buffered artificial groundwater spiked with 2.5 mM of $FeCl_2 \cdot 4H_2O$ and 50 nM of $HgCl_2$. The experimental results showed higher rates of Hg(II) reduction with increasing surface area and Fe(II) content of iron oxide, indicating that the oxidation of adsorbed Fe(II) to Fe(III) is involved in Hg(II) reduction. In the comparison of natural and synthetic iron oxides, Hg(II) reduction was significantly slower for natural iron-bearing minerals than for synthetic Fe(III) oxides: Hg(II) reduction by iron oxides is likely to be less efficient in natural sediments.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Risk Assessment of PCDD/Fs and DL-PCBs in Animal Food

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) and polychlorinated biphenyls (PCBs) are concerned compounds among 12 persistence organic pollutants of the Stockholm convention. These compounds can increase the risk of cancer and cause damage to immune system. The number of 17 PCDD/Fs has TEF (toxic equivalence factor) for calculation of TEQ value. Among the total 209 PCBs, only 12 PCBs congeners which have dioxin-like toxicity are classified as DL-PCBs. The amount of intake and exposure from animal food groups has simultaneously increased through economic development. Animal food samples (78 food, total 502 samples) collected in six cities have been analyzed for a range of dioxins (29 congeners; PCDD/Fs 17 congeners and dioxin-like PCBs 12 congeners) using the isotope dilution method in HRGC/HRMS. For the test method validation, certified reference materials were analyzed. Based on the measured dioxins levels, average daily dietary intake estimates of dioxins were calculated. For risk assessment of PCDD/Fs and DL-PCBs, the data of daily intake from Korea National Health and Nutrition Examination Survey (2008~2010) are considered. The range of detected PCDD/Fs and DL-PCBs (the total sum of PCDD/Fs and DL-PCBs) levels were 0.0000 ? 0.5050 pg WHO05-TEQ/g weight, low fat milk and duck egg, respectively. PCDFs, penta-PCBs and hexa-PCBs in congeners were mainly detected when converted into TEQ (toxicity equivalents). As a result of estimated daily intake and TEQ value, total amount of PCDD/Fs and DL-PCBs exposure to Korea general population was 0.05 pg-TEQ/kg bw/day. On account of Korean TDI (tolerable daily intake) is 4 pg-TEQ/kg bw/day, compared to TDI, daily intake of dioxins via fish ingestion was 1.3%.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Time Trend of Dechlorane compounds and Polybromianated Diphenyl Ethers (PBDEs) in the Korean General Population

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

Dechlorane compounds, including Dechlorane Plus (DP), mirex, Dechlorane (Dec) 602, 603 and 604, were measured in 61 serum samples collected from a Korean urban area (Seoul) in 2013. Dechlorane Plus and Dec 602 were dominant in most samples whereas Dec 604 was not detected in any samples. The median value of DP was 0.75 ng/g lipid, comparable with the levels observed in Europe, but lower than that observed in China. Statistically significant correlations among Dechlorane compounds were observed. The average anti-isomer fractional abundance (fanti) was 0.75 and negative correlation between fanti and DP concentrations in serum samples was observed. Polybrominated diphenyl ethers (PBDEs) were also measured for comparison with Dechlorane compounds and BDE-153 was the most abundant congener with the median value of 1.43 ng/g lipid. A time trend of Dechlorane compounds was investigated in 6 pooled serum samples to cover the period from 2006 to 2013. A distinct trend of Dechlorane compounds was not observed, while PBDEs were steadily decreasing with time.

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발표코드: **ENVR.P-1280**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Risk Assessment of Hexabromocyclododecane (HBCD) in Fish and Shellfish

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

The levels and distributional characteristics of hexabromocyclododecane (HBCD) diastereoisomers have largely been reported for fish and certain shellfish. In this study, we investigated the concentration of HBCD in fish and shellfish, which were highly consumed by general population of Korea. 8 fish species and 12 shellfish species were chosen based on National Health and Nutrition Examination Survey and all samples were purchased from traditional fish market located in 5 major cities (Seoul, Daejeon, Gwangju, Busan, and Jeju). Fish and shellfish containing entrails showed high concentration of HBCD, compared to the other shellfish without entrails. The following order of ∑2HBCD (α- and γ-HBCD, ng/g-ww) was observed: herring > halibut > mackerel > gray mullet > catfish > anchovy > pacific saury and oyster > mussel > scallop > white clam > cockle > manila clam > abalone > east asian white clam > pen shell > conch > whelk > river snails for fish and shellfish, respectively. However, considering the daily intake of fish and shellfish, the results indicated the importance of daily intake of those foodstuffs (g/day). In general, mackerel, anchovy, oyster, and manila clam were highly consumed and ∑2HBCD was about 0.12, 0.055, 0.040, 0.028, and 0.018 ng/kg-bw/day. Quantitative analysis of HBCD diastereoisomers was performed with isotope-dilution method and HPLC/ESI(-)/MS/MS.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

The exposure assessment of new POPs in multimedia and development of monitoring technology for POPs alternatives

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

Brominated flame retardants (BFRs) and perfluorinated compounds (PFCs) which have been registered as new persistent organic pollutants (POPs) in Stockholm Convention are considered hazardous substances for human health. These are mainly present in everyday life in the form of daily supplies and the indoor environment rather than the special circumstances occurred in the industrial area. Although the substances are closely related to daily life, there are no researches that the basic information and assessment techniques about integrated human exposure for new POPs and alternate materials. The object of this research was to develop emission assessment techniques, exposure assessment techniques and ecological toxicity assessment. Ultimately, the methods will be applied to develop the integrated human exposure assessment model. On the basis of this research, we are able to reduce the effect of the substances on human body and environment by suggesting reduction and management methods of emission, exposure of new POPs and alternate material and contribute the national strategy for Stockholm Convention.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hexabromocyclododecane (HBCD) Diastereoisomers in meat from Korean markets

신은수 장윤석[*]

포항공과대학교(POSTECH) 환경공학부

Hexabromocyclododecane (HBCD) is a brominated flame retardant used in polystyrene foams in thermal solution and electrical equipment. The HBCD commercial mixture consists mainly of γ-HBCD (70%) and two other diastereoisomers in lower amounts: β- and α-HBCD 16% and 13% respectively. HBCD has recently been adopted for addition to Annex A of Stockholm convention. The presence of HBCD in wide range of matrices, its suspected toxic effects and continuous massive use may indicate a public health concern. One of the many sources of human exposure to HBCD is through diet. Similar to other POPs it is expected that consumption of fish and meat are two important pathways of human oral exposure. However, in this research the HBCD concentration in meat samples were investigated due to higher consumption in Korean population in comparison with fish product. Little information is available regarding HBCD level in meat and to our knowledge this is the first study to determine the HBCD diastereoisomers in meat samples in Korea. In this study, a total of 59 meat samples were collected from local market and department stores of 5 cities in Korea. Concentrations of HBCD diastereoisomers were determined by liquid chromatography?tandem mass spectrometry (LC?ESI-MS/MS). α-HBCD was the predominant diastereoisomer in 90% of the meat samples. It has to be noted that the diastromeric distribution of HBCD can change due to bioisomerization and biotransformation in biological materials. The concentration was higher in pork (139 pg/g ww) than beef (110 pg/g ww), however, the difference was not significant. Levels of HBCD diastereoisomers found in Korean meat samples were relatively low in comparison with food samples from other countries.

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Long range transportation and bioaccumulation of selected persistent organic pollutants (POPs) candidates

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In 2001, UNEP ratified the Stockholm Convention on Persistent Organic Pollutants (Stockholm Convention) to phase out twelve numbers of toxic, persistent, long-range transporting, and bioaccumulative chemicals, named persistent organic pollutants (POPs). According to phasing out of POPs, their alternatives have been developed and used to replace POPs. Some of alternatives have similar chemical structure and physicochemical property with small modification. Monitoring in polar region, like Antarctica, gives direct evidence of POP candidate to be POP. In this study, we analyzed emerging POPs, including HBCDs, PCNs, and DPs, and existing POPs in tissues of skua and penguin from King George Island, Antarctica. HBCDs were detected in all samples with levels from 1.67 to 713.03 ng/g-lipid. In penguins, total concentration of PCNs were 0.69 ? 2.07 ng/g-lipid, while those in south polar and brow skua were 7.41 ? 174.53 ng/g-lipid. Dechloranes were detected in all samples and the concentrations were 0.60 ? 1.30 ng/g-lipid in penguins, and 6.57 ? 47.39 ng/g-lipid in skuas. Despite of limited number of samples, we detected HBCDs and Dechloranes in the skua and penguin samples from Barton peninsula in King George Island. Beside we found that BMF between skua and penguin is high enough compared to existing POPs. This study gives an evidence that PCNs and Dechlorane.s fulfill 3 of 4 criteria of POPs, which is persistency and ability to long-range transport and bio-accumulate. As POPs source of POPs in skua tissue is unclear, further studies are required to evaluate TMF of POPs candidates.

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Role of Flavin and Fe(II) in Mercury (II) Reduction by Shewanella oneidensis MR-1

QASIM GHULAM HUSSAIN 한승희*

광주과학기술원(GIST) 환경공학과

Shewanella oneidensis MR-1 has been shown to reduce inorganic divalent mercury, Hg (II), in anoxic environments under low Hg(II) concentrations (

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Accelerated oxidation of elemental mercury in ice compared to aqueous phase

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Mercury is of environmental concern in polar ecosystems due to its potent toxicity and biomagnification property. Once deposited on ice surface through mercury depletion events (MDEs), the chemical reaction between Hg(0) and organic ligands in the ice is likely to oxidize Hg(0), thus increasing the bioavailable fraction of Hg. Nevertheless, the reactions and fate of Hg(0) in the ice are not well understood. To determine whether Hg(0) oxidation is accelerated in ice compared with water, we compared the extent of Hg(0) oxidation in ice (at -20 °C, pH 8) to that in aqueous phase (at 25 °C, pH 8) spiked with 50 nM Hg(0). The results showed that within 1 hour, approximately 40% of Hg(0) was oxidized to Hg(II) in the ice, compared with 20% in the aqueous phase. Decrease of pH from 4 to 2 also increased Hg(0) oxidation from 50 to 80% in ice, whereas the effect of pH was less significant in water (10% at pH 4 and 25% at pH 2). The increased Hg(0) oxidation rate in the ice might be caused by the freeze-concentration effect of reactants in the ice grain boundaries. Further acceleration would be contributed from a change of pH during the freezing processes. The Hg(0) oxidation rates were additionally determined: 1) with seawater and lake-water ice mimics; and 2) in the presence of dissolved organic matter. The overall results imply that high levels of methylmercury commonly found in the polar ecosystem could be related to the accelerated rate of Hg(0) oxidation in ice.

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Recovery of ITO from Waste Electrical and Electronic Equipment using chemical and electrochemical methods

최동철 손용근*

성균관대학교 화학과

As we understood, tremendous amount of Indium, the rare material, has been used in flat panel LCD industries. Global indium resource is quite limited e.g. the world's reserve is merely 16,000 tons while the current annual consumption is about 1,400 tons. The current indium consumption rate will make in reservoir exhausted by the year of 2025. Therefore, recycling of indium has become a very important issue these days. Discarding LCD panel will lead us to meet a serious environmental pollution and resource wasting. To combat the depletion of indium and tin resources recycling of the elements from waste electrical and electronic equipment (WEEE) has become important. In this study we suggested a new recycling technology which can separate ITO from the LCD panel. The ITO was recovered in two different ways which were lift-off and low current electrolysis methods. We have tried to recover ITO from the TFT-LCD scrap for resource recycling purpose. ITO was successfully recovered by using the two different methods. XPS, EDX, XRD, SEM and ICP were done for this sample.This work was supported the Energy & Resource Recycling of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy (No.2010501010002B)

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A potential pathway of natural Cr(VI) contaminations: $Cr(OH)_3(s)$ oxidation mediated by surface catalyzed Mn(II) oxidation

남궁선이 이기현*

연세대학교 지구시스템과학과

This study examined the feasibility of $Cr(OH)_3(s)$ oxidation by the product of surface catalyzed Mn(II) oxidation as a potential pathway of natural Cr(VI) contaminations without any anthropogenic sources. Batch experiments were conducted with 1.0 g/L $Cr(OH)_3(s)$ and/or 50 μM Mn(II) in 50 mM $NaNO_3$ electrolytes at pH 7 ? 9 under oxic or anoxic conditions. The solution pH was adjusted with 10 or 50 mM buffer (MOPS for pH 7 and 8, CHES for pH 9). The results showed that homogeneous Mn(II) oxidation by dissolved O_2 (DO) in the absence of $Cr(OH)_3(s)$ was not observed at pH ≤ 8.0 for 50 days, whereas dissolved Mn(II) at pH 9.0 was completely removed within 8 days and precipitated as hausmannite (Mn_3O_4). When $Cr(OH)_3(s)$ was present, this solid was oxidized and released substantial amounts of Cr(VI) soon after dissolved Mn(II) was added into the suspension at pH ≥ 8.0 under oxic conditions. In addition, the extent of Cr(VI) formation increased with increasing pH and initial Mn(II) concentrations. The results suggest that $Cr(OH)_3(s)$ was effectively oxidized by a newly formed Mn oxide as a result of surface catalyzed Mn(II) oxidation, and the rate and extent of $Cr(OH)_3(s)$ oxidation was likely controlled by those of surface catalyzed Mn(II) oxidation. The product of surface catalyzed Mn(II) oxidation was verified by the XANES analysis of the residual solids after the reaction between 1.0 g/L $Cr(OH)_3(s)$ and 204 μM Mn(II) at pH 9.0 for 22 d, which is analogous to birnessite. This study evokes the potential environmental hazard of sparingly soluble $Cr(OH)_3(s)$ that can be a source of Cr(VI) in the presence of dissolved Mn(II).

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Preliminary results of the formation of diverse Mn oxides under varying conditions

남궁선이 이기현*

연세대학교 지구시스템과학과

Mn oxides play an important role in the environment by controlling the fate and transport of various contaminants. More than 30 different types of natural Mn oxides exist in various geological settings with different structure and/or commonly with mixed valence of structural Mn, consequently having a unique physicochemical property and reactivity. However, the geochemical processes controlling the diversity of Mn oxide formation and phase transformation have not been clearly understood yet. The primary goal of this study is to understand geochemical processes controlling the formation of diverse Mn oxides. Formation and phase transformation of various Mn oxides were examined in the absence or the presence of solid substrate ($Cr(OH)_3(s)$ or birnessite), and during the solid-solid interactions between various Mn oxides and $Cr(OH)_3(s)$. Hausmannite (Mn_3O_4) was formed from homogeneous Mn(II) oxidation ($[Mn(II)]_0$ = 50 ? 994 μM) at pH 9.0 open to the atmosphere. By contrast, surface catalyzed Mn(II) oxidation in the presence of 1.0 g/L $Cr(OH)_3(s)$ otherwise under the same conditions produced mixed valence Mn oxides analogous to birnessite. In addition, feitknechtite (β-MnOOH) was produced from birnessite with heterogeneous Mn(II) reaction under anoxic conditions. When 1.0 g/L each of $Cr(OH)_3(s)$ and birnessite were reacted at pH 7.0 ? 9.0 open to the atmosphere, a secondary Mn oxide was formed at all pHs after the solid-solid interaction. The XRD patterns of the residual solids suggested the formation of feitkenechtite. It is likely that the secondary Mn oxide formation substantially affect the extent of redox reactions between the two solids. These results suggest that the factors controlling the formation and phase transformation of various Mn oxides should be clearly elucidated to understand the fate and transport of various contaminants in the environment.

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Effects pH on the reductive removal of Cr(VI) using zero-valent magnesium (ZVMg)

박재선 이기현*

연세대학교 지구시스템과학과

We investigated the effect of initial pH (pH_i) on Cr(VI) reduction mediated by ZVMg particles in aqueous solution. In this study, 18.1 μM Cr(VI) was reacted with 500 mg/L ZVMg particles in 10 mM NaCl electrolyte at the pH_i 2.0 ? 6.8 without additional effort to control the pH. During the reaction, the pHi increased and reached a plateau at 10.1 ± 0.3 within 240 min in every case. At $pH_i < 4$, the rate of Cr(VI) reduction substantially increased with decreasing pH_i. By contrast, the effect of pH_i was negligible on the rate and extent of Cr(VI) reduction at $pH \geq 4$. For example, at pH_i 2.0 Cr(VI) concentration decreased below the detection limit (30 μg/L) within 20 minutes, but > 540 min at higher pHs. Results from SEM and XPS analyses clearly revealed that Cr(VI) was reduced and precipitated as Cr-(oxy)hydroxide on the surface of ZVMg particles. The link between pH and ZVMg-mediated Cr(VI) reduction suggest that the proton is likely the dominant oxidant of ZVMg at $pH < 4$, but has negligible effect on the oxidative-dissolution of ZVMg dissolution and subsequently Cr(VI) reduction at $pH \geq 4$. In addition, H? would be a significant reductant of Cr(VI) under acidic condition because [H?] would increase with increasing [H+]. The rate and extent of Cr(VI) reduction observed in this study suggests that ZVMg can reduce Cr(VI) effectively under the experimental conditions employed in this study.

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Reductive removal of chromate mediated by zero-valent magnesium under neutral pH conditions

박재선 이기현*

연세대학교 지구시스템과학과

Recently, Zero-valent magnesium (ZVMg) has been tested as a powerful reductant especially of organic contaminants due to the several advantages for remediation of environmental contaminants. This study examined the reduction of 5 ? 100 μM $[Cr(VI)]_0$ in the presence of 50 mg/L ($[Mg^0]_0$ = 2.06 mM) ZVMg particles at pH 7 buffered with 50 mM Na-MOPS. The reduction of Cr(VI) was completed within 60 min with $[Cr(VI)]_0$ = 4.9 or 9.6 μM but substantially retarded at > 120 min with higher $[Cr(VI)]_0$ (49.9 or 96.9 μM) likely due to the rapid dissolution and the surface passivation of ZVMg in water. The effect of dissolved oxygen was negligible on the rate and extent of Cr(VI) reduction. Experimental results indicated that Cr(VI) was reduced not directly by ZVMg but by reactive intermediates produced from water reduction by ZVMg. In addition, the observed rates of Cr(VI) reduction appeared to follow an order below unity (0.19) with respect to $[Cr(VI)]_0$. These results imply that ZVMg-mediated Cr(VI) reduction likely occurred via an alternative mechanism to the direct surface mediated reduction typically observed for other zero-valent metals. At pH 7 with 10 μM Cr(VI), ZVMg would reduce it more rapidly than common iron-based solid reductants such as ZVI or green rusts, when normalized to the surface area. Consequently, ZVMg may be an effective and powerful reductant that can be applicable to the reductive treatment of various inorganic contaminants.

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Effect of microenvironment on heavy metal sorption in soil

박재선 이기현*

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Microenvironment (micropore or micro-size soil particles) of soil is one of the most important properties that affect the retention of contaminants and the efficiency of soil treatment processes. However, the research of microenvironment in soil has not been explored well. In this study, the effect of micro-size clay and micropore on heavy metal sorption/desorption in soil were examined. Illite and kaolinite were chosen as micro-size (< 63 μm) clay and Pb, Cu, Cr(VI) were used as heavy metal contaminants. Bulk soil samples were prepared with a mixture of commercial sand, illite, and kaolinite at varying proportions. The surface area and micropore volume of each clay, sand, and soil mixtures were calculated by the BET (Brunauer-Emmett-Teller) method and t-plot method from N_2 adsorption and desorption isotherm. Sorption isotherm experiments were conducted 1 g/L of solid (sand, illite or kaolinite) for Pb and Cu, and 5 g/L for Cr(VI) in 10 mM $NaNO_3$ at pH 6.0 ± 0.1. The results showed that the surface area and micropore volume of soil mixtures increased in proportion to the ratio of clay to sand. Sorption isotherm results showed that Pb and Cu were sorbed most to illite followed by kaolinite and sand in decreasing order when normalized to mass. Cr(VI), by contrast, was sorbed more to kaolinite than to illite. It is interesting that sand exhibited the highest sorption affinity when normalized to surface area. In addition, the extent of sorbed Cr(VI) was lower than that of Pb or Cu toward the solid samples examined in the study. The results of this study suggest that soil microenvironment would play a dominant role on the fate and transport of heavy metal contaminants.

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Recovery of nitrogen and phosphorus by struvite crystallization from wastewater

정지현 최현철*

전남대학교 화학과

Nitrogen (N) and phosphorus (P) are the indispensable elements for all living organisms. They play an irreplaceable role in the breeding, growth, and development of organisms. However, pollution problems related to the N and P discharge of wastewater commonly include eutrophication and dissolved oxygen depletion in water bodies as well as toxicity to the aquatic life. Therefore, the removal of N and P from wastewater is an important priority for maintaining water quality and alleviating environmental pressure. Various chemical and biological processes have been developed for N and P removal, such as metal precipitation, biological nutrient removal processes, enhanced biological phosphorus removal processes, and the struvite crystallization process. Among these processes, the struvite crystallization process is an ideal technique because it can simultaneously remove and recover P and N from wastewater. Precipitation of struvite is affected by several factors, such as pH, concentrations of Mg^{2+}, PO_4^{3-}, and NH_4^+, and presence of other interfering ions, such as calcium (Ca^{2+}). The objective of this study is to investigate removal and recovery of PO_4^{3-} and NH_4^+ ions as struvite from livestock wastewater. Effects of the molar ratio $[Mg^{2+}]$:$[NH_4^+]$:$[PO_4^{3-}]$ and pH were investigated.

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폐추진제 재활용 - AP 정제 공정 개발

심용호* 이승현 하상욱 유동진[1] 유은실[1] 장혜리[1]

(주)제이제이프로테크 [1]전북대학교 공과대학,에너지저장/변환공학과 대학원

심용호 1, 하상욱 1, 이승현 1, 유은실 2, 장혜리 2, 유동진 2 주)제이제이프로테크 1, 전북대학교 에너지저장/변환공학과 대학원 2 키워드 : 재활용, 과염소산암모늄수명이 완료된 폐추진기관의 재활용 연구는 전 세계적으로 관심을 갖는 분야이다. 폐추진기관의 주성분은 polybutadien binder 와 산화가연제인 ammonium perchlorate (AP)로 구성되어 있다. AP 가 70% 이상 함유되어 있으므로 재활용 시킬 경우 경제적 의미가 크다. Binder 에서의 AP 분리 자체에 대해서는 많은 연구가 이루어져 있는 바, 이번 연구과제는 분리된 AP 의 순도를 높이는데 초점을 맞췄다. Binder 에서의 분리는 공정상에서 안정적으로 이루어지지만 기대하는 것 만큼의 고순도의 회수공정이 아니다. 상업화를 생각한다면 순도가 결정적인 요소이기에, 경제적 고부가가치를 달성하지 못하고 있는 현실이다. 이번 연구는 분리공정을 거쳐서 얻어진 AP 의 순도를 고순도로 정제하는 공정개발 연구이다. AP 는 국내에서의 생산이 없으며 전량 수입에 의존하는 물질이므로, 이번 공정개발 연구를 통해서 고순도의 AP 를 얻게 되었고, 국내 자체공급은 물론, 향후 수출을 통해, 국가적 차원에서 큰 경제적 이득을 얻을 수 있을 것이다.

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미생물 세포의 외막과 산화전극이 이루는 계면에서 일어나는 전하 전달 경로의 이해

최찬수

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미생물 연료전지(MFC)에 수반된 세포외 전자전달(EET)을 깊히 이해하기 위해서 마커스 이론을 성공적으로 응용할 수 있었다. 산화환원 결합 폴리머 막 전극들을 박테리아 외막을 모방하기 위해서 제작하였다. 순환전압 전류 실험을 산화환원 물질 주입 폴리머 막 전극에 대해서 NADH, acetate 및 flavin 용액에서 수행하였는데 NADH 의 산화반응은 세포막 결합 훌라빈 모노 누클레오타이드를 산화환원 촉매로 하는 시뮬레이션 결과로 미생물 박테리아의 EET 모델링을 잘 설명하였다. NADH 가 촉매 산화할 때 아세테이트의 첨가시 $FMNH_2$ 의 산화 봉우리는 전류가 증가함과 동시에 음의 전위 쪽으로 이동하였다. 이는 NADH 에 의하여 $FMNH_2$ 의 농도 증가를 일으키고 이는 네른스트 식에서 환원형의 농도의 증가로 평형전위가 음으로 이동하는 현상으로 잘 설명할 수 있었다. 다만 아세테이트가 NAD^+와 반응하여 직접 NADH 를 생성하는 연계 반응이 균일계에서 일어날 수 있는냐를 증명하여야 할 것이다. 그러나 실 박테리아 세포질에서는 아세테이트를 출발로하는 TCA 회로를 통한 NADH 는 충분히 공급이 될 수 있다는 점이 매우 흥미롭다. 박테리아 세포막에 결합되어 있는 FMN 의 제 1 산화환원 $E_{1/2}$ 은 NHE 기준으로 -0.27 V 에서 발견되는데 NADH 와 아세테이트가 녹아있는 용액에서 FMN 주입 나피온 막 전극에도 같은 위치에서 일어났다. 전자전달에 대한 마커스 이론에 따라 NADH 와 c-Cyt 공여체-수용체 쌍의 반응 깁스 에너지가 NADH 와 FMN 쌍의 그것보다 더 방출에너지적이기 때문에 전자의 그것이 후자의 그것보다 더 유리했다. 그럼에도 불구하고 세포막 결합 MFN 의 산화환원 봉우리들이 실제로는 CV 상에 나타났다. 그러므로 전하전달 속도에 대한 거리 효과가 반응 깁스 에너지 효과를 압도하는 것을 알 수 있었다. 박테리아 미생물과 산화전극 사이의 계면에서

EET 경로는 세포 외막(OM) 단백질에 결합된 FMN←NADH(세포질)을 경유하여 FMNH$_2$ 를 생성하고 이로부터 산화전극으로 터널링에 의하여 일어나는 것이 가능하다는 결론에 이를 수 있었다. 이 EET 의 메커니즘적 이해는 미생물 연료전지, 폐수의 생물학적 재생 및 오염 침적물의 처리 등의 최적화에 매우 중요하다.

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Evaluation of the consumer exposure to two isothiazolinone biocides, 5-chloro-2-methylisothiazol-3(2H)-one (CMI) and 2-methylisothiazol-3(2H)-one (MI), in a liquid air freshener

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There exist public concerns about wide-spread use of isothoazolinone biocides added to various consumer products such as air fresheners, personal hygene products, perfumes, and deodorants.Two most-widely used isothiazolinones,5-chloro-2-methylisothiazol-3(2H)-one(CMI) and 2-methylisothiazol-3(2H)-one(MI),are suspected to undergo chemical transformation under ambient use conditions. However, there are only limited studies about their reactivity and the rate and pathways of transformation.Hydrolysis at pH 4, 7, and 9 and photolysis testsusing a 50 W three wavelengths compact fluorescent lampwere performed to evaluate their stability in liquid products.Hydrolysis and phototransformation rate constants were not quantifiable except for the hydrolysis of CMI at pH 9 with the rate constant of 0.032 day-1.To better understand human exposure to MI and CMI while using consumer products, we evaluated vaporization of MI and CMI from a selected air freshener. Specifically, the mass transfer rate constant for evaporation was evaluated in a custom-made chamber. Whereas evaporation of MI was almost negligible for 7 days, significant amount of CMI evaporated with the evaporation mass transfer coefficient of 0.0071 cm day-1 for the same test period likely due to higher Henry’s law constant. Because the volume of air freshener decreases over time due to evaporation of water, concentration of MI in the product showed noticeable increase whereas concentration of CMI remained constant due to evaporation.Exposure assessment was also conducted using an exposure scenario and measured rate constants in this study.