

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PLEN-1**

발표분야: 기초강연

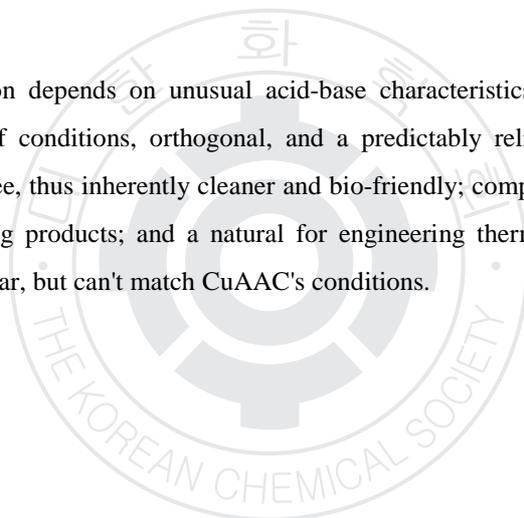
발표종류: 특별강연, 발표일시: 목 13:30, 좌장: 김병문

Click2—another near-perfect click reaction

K. Barry Sharpless

The Scripps Research Institute

This sulfate-linking reaction depends on unusual acid-base characteristics. Like CuAAC, it is ultra-reliable within its range of conditions, orthogonal, and a predictably reliable chemical linker. Unlike CuAAC, Click2 is metal free, thus inherently cleaner and bio-friendly; compatible with several acid-base catalysts; better at purifying products; and a natural for engineering thermoplastic polymers. Click2's linked groups are less polar, but can't match CuAAC's conditions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **AWARD-1**

발표분야: 기념강연

발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 미정

Novel Functional Polymer Nanostructure Systems: Synthesis, Fabrication, Structure and Properties

이문호

포항공과대학교 화학과

A series of well-defined brush, star, and block copolymer systems bearing various functional moieties (biomolecules, mesogens, and charge-trapping molecules, and so on) were newly synthesized. All the polymer were found to be thermally stable up to high temperatures (200-500 °C), providing a process and utilization windows. They often self-assembled and formed various unique nanostructures, depending on the chemical architecture and regularity as well as the thermal-annealing, solvent-annealing or their combinations. Such self-assembly nanostructures and their orientation were successfully analyzed in detail using synchrotron grazing incidence X-ray scattering and reflectivity; the determined nanostructures were understood with considering favorable interactions of the polymer backbones and functional moieties. The phase and surface characteristics in the self-assembled nanostructures can be well controlled. In particular, biomolecule-containing brush polymer self-assemblies were successfully controlled to always provide biomolecule rich surface over various processes, which are essential to demonstrate excellent biocompatibilities, anti-adherence of bacteria, anti-adsorption of proteins, and drug deliveries. Moreover, some other interesting nanostructure systems demonstrated ultra-low dielectric constant, programmable digital volatile and nonvolatile memories or liquid crystal controllability, which are highly demanded for advanced microelectronics and flat panel displays.

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장소: 창원CECO

발표코드: **POLY1-6**

발표분야: Current Trends in Biomedical Polymers

발표종류: 분과기념강연, 발표일시: 목 11:30, 좌장: 강영중

Photofunctional Nanodevices for Biomedical Application

장우동

연세대학교 화학과

Photodynamic therapy (PDT) has attracting interests as less invasive treatment for solid tumors. Recently, we have reported ionic dendrimer porphyrin (DP) and dendrimer phthalocyanine (DPc) as an efficient photosensitizer for PDT. The charged ionic surface can form polyion complex micelles by means of electrostatic interaction with oppositely charged block copolymer. The large dendritic wedges can effectively prevent the aggregates formation of core porphyrin or phthalocyanine unit even in highly concentrated micellar core. In this symposium, I would like to report recent results about the design of multifunctional nano-devices for the combination cancer therapy and diagnosis. A polymer-metal complex micelles (PMCMs) were formed by coordination interaction of CDDP with DPc and poly(ethylene glycol)-block-poly(L-aspartic acid) (PEG-PLAn; molecular weight of PEG segment = 12,000 g/mol; polymerization degrees of aspartic acid segment $n = 68, 96$). PMCMs have great potentials as a biomedical nano-device for combination therapy as evidenced by the sustained release of CDDP from PMCMs under physiological saline conditions and the generation of singlet oxygen under light irradiation. LbL nano-capsules also have been prepared for the anticancer drug delivery as well as PDT. Under light irradiation, the LbL nano-capsules exhibited strong photoinduced toxicity and controlled release of anticancer drug. The detailed aspect will be reported in the symposium.

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장소: 창원CECO

발표코드: **POLY1-1**

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 09:15, 좌장: 이연

Multilayer Nano-platforms for Biomedical Applications

홍진기

중앙대학교 화학신소재공학부

Recent developments in biomaterials for tissue engineering, novel cell culture techniques, and newly discovered chemicals as a replacement of the growth factors have opened new area toward the engineered technique of biomedical applications, for use in both research and clinical applications. Ideal bio-platform must be biocompatible that is to say, they should show both proper surface stability for the promotion of cell attachment and functions with drug delivery. However, plenty of challenges are still in progress, as the reason for the high compatibility of polymer film in cell culture environment and precisely controlled functional release of their drugs. To fulfill satisfactory of these requirements, attention has turned recently to not only introduce new materials but also developing nano-size controlled film structure of drug-delivery platforms as such films can enhance the specific functions including stimuli cell-differentiation, -expansion, fighting infection and promoting wound-healing. Much effort has been devoted to controlling drug release via manipulating the degradation or dissolution of the films. Layer-by-layer (LbL) self-assembly technic has been developed and used to prepared biocompatible multilayer films and polyelectrolyte capsules for drug delivery. Certain drug molecules, such as active proteins, cytokine, growth factors, enzymes, nucleic acids, and DNA, have been immobilized into nano-sized multilayer films. The advantages of LbL multilayer films as drug delivery systems include the variation of candidate materials, also drug molecules itself can use as either functional drugs or components of the film, and easy to combine to additional functions due to their evenly distributed structure. Furthermore sustained drug release is possible through controlling the film physical & chemical properties, in addition multilayer films have the potential to protect drug molecules from losing their biological functions, and the film preparation process is simple and can be automated. The drug release behavior of polyelectrolyte multilayer films depends on the permeability, the disassembly or erosion of the multilayer structure, and other experimental variables. In this presentation, we prepared the cell friendly platform by take full

advantages of LbL assembly with evenly distributed drug loading by nano-sized layer assembly. The platforms are prepared by various materials including not only synthetic-, natural-polymers but also functional materials such as growth factors, cytokines which are resulting different film degradation profiles. In addition, we also introduced the functional objects into multilayer film, such as block copolymer micelle as a drug container, nanotubes for enhanced mechanical strength. The structures including functional objects could be very useful in achieving additional functions for various cell studies. These results lay a cornerstone for future studies to achieve the multi-functional platforms including programmed loading/release of drugs for therapeutic purposes.



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장소: 창원CECO

발표코드: **POLY1-2**

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 이연

Effect of the Hydrated Viscoelastic Factor of the Polymer Surfaces on the Cellular Responses

서지훈

Tokyo Medical and Dental University

In this presentation, the effect of the hydrated viscoelastic factor of the polymer surfaces on the cellular responses such as adhesion morphology, responding time, and differentiation, etc. will be introduced. Various factors governing cellular responses to artificial materials have been studied in recent decades. Even though it has been clarified that the magnitude of a cellular response, such as adhering density or proliferation rate, is strongly dependent on the protein density on the material surface, the critical factors that affect the cell functions are yet to be studied extensively. One of the traditional factors explaining biological responses, i.e., surface free energy represented by surface wettability, was primarily applied to discuss the one of the cellular responses, i.e. morphology of adhering fibroblasts in this study. However, it was confirmed that the surface free energy could not explain the morphology of adhering fibroblasts, but could only be related to the amount of protein adsorption and the extent of cell adhesion, such as projected cell area. Instead, the hydrated viscoelastic factor of polymer surfaces was confirmed as an important factor that influences the morphology of adhering fibroblasts on the polymer surfaces. This result suggests a novel concept, namely that hydrated viscoelastic factor should be considered when discussing the cellular responses on the polymer surfaces, as distinct from the traditional concept of surface free energy.

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장소: 창원CECO

발표코드: **POLY1-3**

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 10:05, 좌장: 이연

New polysaccharide-based thermogelling polymers for biomedical applications

허강무

충남대학교 고분자공학과

Over the past few years, thermogelling polymers that undergo a thermo-responsive sol/gel transition in aqueous media have been extensively studied for various biomedical applications, especially for drug delivery and injectable tissue engineering. These polymers have several advantages compared to other polymer hydrogel systems, and offer the opportunity to perform a less invasive surgical procedure. These polymers can be loaded with pharmaceutical agents or cells by a simple mixing procedure in a solution state, and injected into the target site where they form hydrogel depots and serve as carrier matrices for localized drug delivery or cell growth. Several synthetic polymers are known to show such thermoresponsive sol/gel transition behavior. Copolymers of poly(ethylene oxide) and poly(propylene oxide) (known as poloxamer), and copolymers of N-isopropylacrylamide have been widely studied as commercially available thermo-sensitive synthetic polymers. They could demonstrate excellent thermo-sensitive properties, but their clinical applications have been limited due to their lack of biodegradability, biocompatibility and physical stability. Therefore, there has been a continuing need to develop a new biodegradable thermogelling system with enhanced biocompatibility and physical stability. In this study, new thermo-responsive polymers were synthesized by N-acylation of glycol chitosan and evaluated as thermogelling systems. Their physico-chemical and thermo-responsive properties were characterized in terms of degradation, cytotoxicity, rheological properties, and in vitro and in vivo gel formation, and evaluated for several biomedical applications.

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장소: 창원CECO

발표코드: **POLY1-4**

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 김태일

Molecularly Self-assembled Nucleic Acid Nanoparticles for the Delivery of RNAi Therapeutics

이혁진

이화여자대학교 약학대학

Nanoparticles are useful for delivering therapeutics into cells. However, size, shape, surface chemistry and the presentation of targeting ligands on the surface of nanoparticles can affect circulation half-life and biodistribution, cell specific internalization, excretion, toxicity, and efficacy. A variety of materials have been explored for delivering small interfering RNAs (siRNAs) - a therapeutic agent that suppresses the expression of targeted genes. However, conventional delivery nanoparticles such as liposomes and polymeric systems are heterogeneous in size, composition and surface chemistry, and this can lead to suboptimal performance, lack of tissue specificity and potential toxicity. Here, we show that self-assembled DNA tetrahedral nanoparticles with a well-defined size can deliver siRNAs into cells and silence target genes in tumours.

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발표코드: POLY1-5

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 11:05, 좌장: 김태일

Engineered Nanomaterials for Enhanced Antitumor and Antiviral Effect

임용택

충남대학교 분석과학기술대학원 분석과학기술학과

The design and chemical synthesis of multifunctional nanomaterials have been providing potential applications in biomedical fields such as molecular imaging and drug delivery. Recently, bio-derived and/or synthetic nanostructured materials capable of modulating the immune system have been also issues of interest in immunology-related nanomedicine fields. In this talk, the recent research results on the development of nanostructured materials for enhanced immunity would be presented. In the first part, we have designed and synthesized an immunomodulatory hybrid nanoconjugates (HNC) system based on polymer nanocomposites containing quantum dots (QDs; as imaging tracers) that are decorated with CpG ODNs (as a TLR9 ligand) and STAT3 siRNAs (as an immunosuppressive gene silencer). These HNC efficiently targeted immune cells, induced TLR activation, and silenced immunosuppressive genes. Simultaneous in vivo delivery of STAT3 siRNA and CpG ODN to dendritic cells (DCs) in the tumor microenvironment induced both the inhibition of STAT3 and activation of DCs by CpG ODNs, and synergistically elicited anti-tumor effects. By using NIR-emitting QDs, the migration of in vivo DCs to lymph nodes was also tracked by real-time NIR fluorescence imaging. In the second part, we focus on the development of a nanodelivery system for the effective mucus delivery of a viral antigen that can induce strong mucosal immunity without additional immunostimulatory adjuvant materials, such as alum, emulsion, and cationic lipid. To accomplish this goal, we designed and synthesized a mucosal vaccine delivery system based on biosynthetic mucoadhesive polymer nanomicelles. We have also tested the adjuvant function of nanomicelles in the presence of an influenza A viral antigen, that is, the inactivated virus of influenza A/PuertoRico/ 8/34 (PR8;H1N1). Intranasal immunization with PR8 in the presence of nanomicelles induced high levels of functional antibodies and IFN- γ producing cells, suggesting that our

nanomicelle system could function as an effective adjuvant for inducing both humoral and cellular immune responses.



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장소: 창원CECO

발표코드: **POLY1-1**

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 박수영

NMR Investigation of Properties of Electrochemical Materials and Fuel Cell Reactions

한옥희

한국기초과학지원연구원 대구센터, 충남대학교 분석과학기술대학원, 경북대학교 화학과

Nuclear magnetic resonance (NMR) spectroscopic techniques can provide abundant information on a given system. In this presentation, our NMR investigation on electrochemical systems such as fuel cells (FCs) and batteries will be introduced as an example. For a FC system, electronic, chemical, and structural changes of FC constituents during each FC assembly such as mixing catalysts with ionomers and hot-pressing for membrane-electrode-assembly can be detected by NMR. Proton conduction and water mobility through polymer electrolyte membranes can be observed by different MR techniques. In addition, in situ observation of direct alcohol fuel cells (DAFCs) by NMR spectroscopy to detect the functional difference of anode catalysts such as Pt and PtRu, and the analyses of the anode exhaust of DAFC for quantitative correlation of the amount of electrical current generated to the quantities of each chemical product are possible. If time permits, the Li⁺ ion mobility comparison of battery electrode materials will be briefly discussed.

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장소: 창원CECO

발표코드: **POLY1-2**

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 박수영

크로마토그래피 법을 이용한 고분자 분석

유진숙

(주)LG화학기술연구원 CRD 연구소

산업적으로 널리 사용되는 합성 고분자는 용도에 따라 다양한 분자량과 조성 분포를 갖는다. 따라서 정확한 물성을 이해하기 위해서는 합성 고분자가 가지는 분포를 정확히 분석할 수 있어야 한다. HPLC (high performance liquid chromatography)는 고분자의 분포를 측정할 수 있는 유일한 방법이며 분자 크기나 조성에 따라 분리도 할 수 있는 유용한 분석 방법이다. 본 발표에서는 HPLC의 원리와 특징, 그리고 방법 별로 고분자 분석에 적용한 사례를 보고자 한다.

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장소: 창원CECO

발표코드: **POLY1-3**

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 박수영

Two-Dimensional Correlation Spectroscopy in Polymeric Materials Characterization

정영미

강원대학교 화학과

Vibrational spectroscopy plays an important role in polymer study. In addition, two-dimensional correlation spectroscopy (2DCOS) provides better understanding of development of novel polymeric materials and their applications. 2DCOS is now a well-established technique for interpreting spectral data sets obtained during the measurement of spectra with an external perturbation that provides considerable utility and benefit in various polymer studies. In this presentation, some of the exciting contributions of 2DCOS to polymer study will be introduced.

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장소: 창원CECO

발표코드: **POLY1-4**

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 정영미

Micellar structures of amphiphilic block copolymers in the selective solvents

박수영

경북대학교 고분자공학과

Micellar structures of amphiphilic block copolymers in the selective solvents were studied using small angle X-ray and neutron scatterings and generalized indirect Fourier transformation (GIFT) method. Vesicular, cylindrical, and spherical micelles were controlled by the composition of the block copolymer and the solvent selectivity. The systematic screen of the solvent selectivity was performed by changing the mixing ratio of the two selective solvents and the solvent temperature. As the selectivity of solvent increased, the shape of the micelle was changed from sphere, to cylinder, and finally to vesicle. The mixing ratio and the temperature of solution could be parameterized into a Flory interaction parameter, χ . The discontinuous change of the solvent selectivity during heating was demonstrated at T_{ni} with PS-b-LCP and nematic liquid crystal solvent, 5CB.

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장소: 창원CECO

발표코드: **POLY1-5**

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 정영미

Characterization of Nanoscale Materials Using Small Angle Neutron Scattering

김태환

한국원자력연구원 중성자과학연구부

Small angle neutron scattering (SANS) techniques have been a very powerful tool to study nanoscale (1-100's nm) bulk structures in various materials such as polymer, self-assembled materials, nano-porous materials, magnetic materials, metal and ceramics. Furthermore, SANS is the most popular instrument among cold neutron instruments. Therefore, in 2010, two SANS instruments (18m and 40m SANS) with fairly good performance were constructed at HANARO cold neutron research facility and have been opened to external users. Once it has been commissioned in 2010, two SANS instruments are providing great opportunities as a key instrument for nanoscale materials research in Korea. In this talk, the characterization of the nanoscale materials using SANS techniques will be briefly introduced with a few examples including polymers.

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장소: 창원CECO

발표코드: POLY1-6

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 정영미

FEL Applications on Nanostructured Materials

신태주

포항가속기연구소 빔라인부

4 세대 가속기인 X-선 자유전자레이저(XFEL)는 고휘도의 전자빔 번치를 발생시키는 전자총, 이를 가속시키는 전자가속기, 전자빔 번치가 사행운동을 하면서 방사광을 발생시키는 여러 쌍의 영구자석으로 이루어진 언들레이터, 방사광을 실험장치까지 유도하여 실험을 하는 빔라인으로 구성되며 생성되는 단일 펄스를 기준으로 할 때 3 세대 방사광에 비하여 약 100 억 배 이상의 밝기를 가진다. 자유전자레이저(XFEL)는 거의 100%에 달하는 결맞음 특성, 펨토초 단위의 펄스폭, 매우 낮은 빔 퍼짐성 등의 특성을 가지고 있어, 기존의 3 세대 방사광원을 이용하여 수행하기 어려운 다양한 실험이 가능할 것으로 기대된다. 본 발표에서는 현재 진행중인 포항가속기연구소의 XFEL 사업을 소개하고, 고분자재료 및 생명, 화학, 환경, 의학, 에너지재료 등의 다양한 분야에서의 응용성에 대해 논하고자 한다.

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장소: 창원CECO

발표코드: POLY1-7

발표분야: Recent Trends in Characterization of Polymers

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 정영미

Introduction to Wyatt Technology's advanced Laser Light Scattering photometers(Multiangle static and Dynamic Light Scattering) with Size Exclusion Chromatography and Flow-field flow Fractionation system

김낙현

인성크로마텍(주) 기술영업부

1. SEC-MALS:

Not all macromolecules behave alike. Polymer samples may have a different conformation than molecular standards or exhibited unexpected column interactions. As an absolute technique for determining molar mass and rms radius R_g in solution, MALS overcomes the limitations of column calibration. Multiangle Static Light Scattering (MALS) measures molar mass directly, independent of elution time.

DAWN HELEOS : the most sensitive MALS available. Includes 18 angular detectors to determine molar masses from 200 Da to 1 GDa and radii from 10-500 nm., heated /cooled option(-15C -- 150C), and High Temperature options (to 210C), miniDAWN, Optilab T-rEX, ViscoStar II and WyattQELS.

2. FFF-MALS:

Field Flow Fractionation (FFF) is a versatile separation technique that overcomes many of the limitations of analytical SEC. Combine with MALS and/or DLS for absolute molar mass and size distributions of macromolecules and nanoparticles.

Available in two formats, Asymmetric flow field-flow Fractionation(AF4) and Hollow fiber flow field flow Fractionation(HF5) provide numerous advantages over other separation techniques.: 1nm to 1 > um. Eclipse DUALTEC and Eclipse AF4 systems.

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장소: 창원CECO

발표코드: IND1-1

발표분야: Recent Trends in Graphene/Carbon Nanotube-Based Materials

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 이준승

Nanocarbon Hybrid Materials for Flexible Electronics

이건용

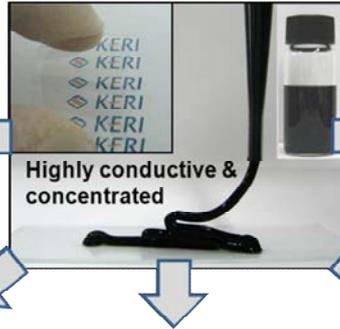
한국전기연구원 나노융합기술연구센터

나노카본소재는 미래 flexible 또는 soft electronics 에 매우 적합한 고유연성, 고전도성 등 우수한 전기전자 특성을 보이는 재료로서 향후 출현하게 될 유연디스플레이, 유연태양전지의 핵심소재가 될 것으로 판단된다. 유연전극 개발을 위해서는 고분자 기판에 적합한 소재 유연성과 높은 광전기적 특성, 인쇄전자공정과 같은 프린팅 적합성, 저온공정성 등이 요구된다. CNT 를 기반으로하는 투명전도성 필름 형성에 있어 각 재료간의 계면을 적절히 조절함으로써 응용분야에 적합한 최적의 코팅막을 형성시킬 수 있으며, 향후 투명전도성 필름의 다양한 응용분야에 적용을 위한 지속적인 연구가 필요하다. 화학적 박리 그래핀은 화학증기증착법에 의해 제조된 그래핀에 비해 전기전도도는 우수하지 않지만 산화과정에서 형성되는 관능기를 활용할 경우 다양한 나노소재와의 하이브리드가 용이하고 대량 생산 및 대면적 적용이 용이하고 용액공정에 의한 직접 패터닝이 가능하기 때문에 이를 활용하여 전기전자소자의 성능향상에 획기적으로 기여할 수 있을 것으로 기대된다. 이를 위해서는 그래핀의 원자구조에 대한 정확한 이해와 용액공정을 위한 용액내 분산문제, 산화그래핀의 효과적인 환원, 박막형성기술, 하이브리드 기술 등에 대한 지속적인 연구가 필요하다. CNT/그래핀을 기반으로하는 투명전극 및 유연전극 응용기술은 계면공학과 인쇄전자기술을 활용해 다양한 유연소자분야에 적용을 위한 지속적인 연구가 필요하다. 본 강의에서는 탄소나노튜브(CNT)와 고분자계 바인더를 조합하여 기판 접착성과 내구성을 동시에 갖는 투명박막 및 용액공정에 의한 ITO 대체용 투명전극 제조기술과, 화학적 박리 그래핀을 이용한 인쇄전자용 전도성 잉크, 에너지저장소자용 전도성 페이스트 등 나노카본소재를 응용한 각종 유연 전기전자소자에 대한 연구결과를 소개하고자 한다.

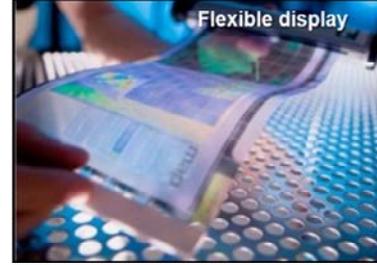
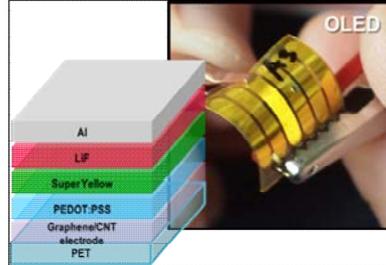
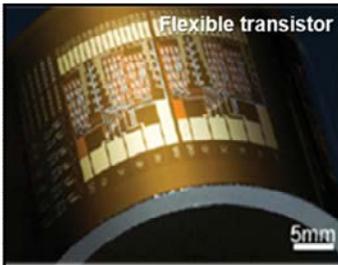
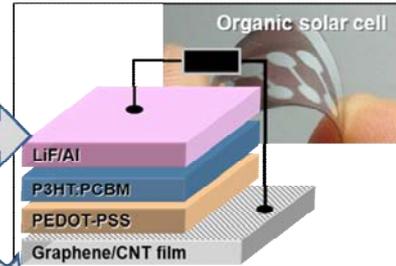
➤ Touch panel



➤ NC Ink or Paste



➤ Flexible OPVs



➤ Flexible display and transistors



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND1-2

발표분야: Recent Trends in Graphene/Carbon Nanotube-Based Materials

발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 이준승

Hybrid Nanosheets of Reduced Graphene Oxide and Transition Metal Dichalcogenides

신현석

울산과학기술대학교(UNIST) 에너지공학부

The rapid progress in graphene research has led to intensive exploration of novel 2D materials. In particular, transition metal chalcogenides, with their layered structures, have received significant attention because they offer many opportunities for fundamental and technological research in a variety of fields, including catalysis, energy storage, sensing, and electronic devices. In this talk, I demonstrate how to prepare various transition metal chalcogenides/reduced graphene oxide (rGO) composites by a simple hydrothermal method, for instance, VS₄/rGO and WS₂/rGO. In particular, an interesting thing is that VS₄ was selectively synthesized on graphitic layer such as rGO. In the same experimental condition without rGO, only VS₂ was synthesized. Furthermore, I introduce that VS₄/rGO and WS₂/rGO can be promising functional materials for Li storage and hydrogen evolution, respectively.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND1-3

발표분야: Recent Trends in Graphene/Carbon Nanotube-Based Materials

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 이건웅

Chemistry in the production of graphene nanoplatelets and their catalytic applications

박성진

인하대학교 화학과

During the last half decade, chemically modified graphene (CMG) has been studied in the wide range of applications, such as polymer composites, energy-related materials, sensors, 'paper'-like materials, field-effect transistors (FET), inks, actuators, and biomedical applications due to its excellent electrical, mechanical, and thermal properties. Chemical modification of graphene oxide, which is generated from graphite oxide, which is produced by simple oxidation of graphite, has been a promising route to achieve mass production of CMG platelets via their colloidal suspensions. Graphene oxide contains a range of reactive oxygen functional groups, which renders it a good candidate for use in the aforementioned applications (among others) through chemical functionalizations. In this presentation, I will discuss my recent research activities on the fundamental chemistry of graphite oxide, as well as novel applications based on CMGs. Topics will include the chemical structure of CMGs as well as catalytic applications.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND1-4

발표분야: Recent Trends in Graphene/Carbon Nanotube-Based Materials

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 이건웅

Synthesis of metallic nanoparticle supported on N-doped graphene oxide and their catalytic ability to hydrogenation

SINGHAJAIKUMARRAMKIRPAL 김동표*

포항공과대학교 화학공학과

The implementation of sustainable hydrogen production and subsequent hydrogen conversion to energy is called hydrogen economy. Hydrogen gas is generally formed by liquid fuel (alkane) oxidation at high temperature and pressure but we have also limited fuel. In commercial carbonyl group hydrogenation reaction is performing by the using hydrogen gas and Pd/C catalyst at high temperature and pressure. Unfortunately, its physical properties make the transport and handling of hydrogen gas difficult. To overcome this, formic acid can be used as material for the storage of hydrogen, because of it is a liquid at room temperature contains ~4.38 percent hydrogen and also biomass material. However, the state of art methods for production of hydrogen gas from formic acid and used this hydrogen for catalytic hydrogenation of biomass material at low temperature and low pressure. Here we described an efficient aqueous-phase formic acid dehydrogenation and hydrogenation for biofuel up gradation, which is facilitated by the stable metallic nanoparticle supported N-doped graphene oxide catalyst. Excellent catalytic results were achieved. This would make the selective hydrogenation of carbonyl compound at very low temperature.



Figure 1: Schematic presentation for biofuel upgrade by using catalyst road.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-1

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김용암

The Unique Properties of Carbon Nano Composite Fibers for Energy Applications

양갑승

전남대학교 고분자 섬유 시스템공학과

Electrospinning is unique and productive process for preparation of the organic nano-size fibers providing the properties of large specific surface area and good connectivities at relatively low volume fraction which are applicable to filters and enthalpy wheel. Blend solution can be easily spun to develop the functional properties of the composite fibers. The phase behavior of the blend solutions is controlling factor of the precursor fiber structure and that follows the determination of the morphological structure of the carbonized fibers. The morphological structure of the carbonized fibers derives the unique pore structure and related electrical conductivity. The carbonized nano-fibers generated large specific surface area form the shallow open pores on the nano-size fibers. The ultramicropores with specific functionalities introduced not only the larger adsorption amount and but also the adsorbent selectivity. The electrical conductivity was also dependent on the morphological structure and components; as pitch, silicone oxide, graphene, carbon nanotube; in the carbonized fibers. The high specific surface area from the ultramicropores and high electrical conductivity introduced elevations of power and energy densities of the electrical double layer capacitor (EDLC) and the introductions of the polar functional group gave further increases in the specific capacitance from the Faraday effect.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-2

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김용암

국내 탄소소재 연구개발 현황

안계혁

한국탄소융합기술원 연구개발본부

그동안 국내의 탄소소재 연구는 탄소나노튜브와 그래핀 위주의 나노탄소소재 연구가 주류를 이루었으나, 근래에 국가의 대형 연구사업에 힘입어 탄소섬유가 국내에 양산되기 시작하면서 탄소산업이 국내에 급부상하고 있다. 본 발표에서는 현재 국가의 대형 연구사업으로 추진되고 있는 WPM, 미래선도사업, 탄소밸리구축사업 등 탄소소재에 관련된 연구사례를 소개하고자 한다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-3

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김용암

리튬 이차전지용 음극소재 기술 개발동향

이상의

지에스에너지 전지소재연구소

리튬이차전지는 노트북, 휴대폰, 전동공구 등 소형 전자기기용 시장이 지속적으로 확대되고, 전기 자동차를 중심으로 한 새로운 중대형 시장이 급속히 팽창할 것으로 예상된다. 이뿐만 아니라 조만간 스마트 그리드, 신재생 에너지 분야에서도 새로운 수요가 창출된다면 향후 10년 이내에 전 세계 리튬이차전지 시장 규모는 1,000억 달러 수준으로 성장하여, 장기적으로는 반도체와 디스플레이 산업을 능가하는 규모로 성장해 나갈 것으로 전망되고 있다. 리튬이차전지는 성격이 매우 다른 네 가지 핵심재료인 음극, 양극, 분리막, 전해질로 구성되어 있다. 음극은 대표적인 환원 특성을 지니는 탄소이며, 양극은 산화물인 금속산화물로 그 태생부터 판이하게 다르다. 음극과 양극은 고분자 분리막으로 격리되어 있으며, 용매와 염으로 구성된 전해질이 음양극과 분리막을 적시고 있다. 이처럼 이질적인 네 가지 핵심재료는 서로의 약점을 보완하고, 때로는 시너지 효과를 내면서 리튬이차전지의 대표적 성능인 에너지, 출력, 수명, 안정성을 좌우한다. 어느 하나가 부족하게 되면 그 균형이 무너지면서 곧바로 성능 부족으로 이어진다. 성능을 향상시키기 위한 목적과 더불어 이차전지 산업의 국가적 경쟁력을 높이기 위해서도 이들 네 가지 핵심소재의 균형 잡힌 성장은 중요하다고 할 수 있다. 이처럼 시장의 폭발적인 확대가 예상되고 있는 현시점에서 네 가지 핵심소재의 균형 성장이 요구되고 있지만 현실은 그렇지 않다. 2010년도 지식경제부 로드맵에 따르면 네 가지 핵심 소재 중 양극재와 전해질의 국산화율은 벌써 80%를 넘어섰고, 분리막도 국산화의 교두보를 마련하였으므로 지속적인 수치의 증가만이 남아 있을 뿐이다. 그러나 음극재만이 유일하게 국산화율 제로라는 명에서 벗어나지 못하고 있다. 리튬이차전지 시장점유율 세계 1 위라는 위상은 음극재에게만 유독 프리미엄으로 듣고 있지 않다. 본 발표를 통해 음극재라는 業의 본질을 파악하여 음극재의

국산화를 이뤄내고 더 나아가서 우리나라의 리튬이차전지 경쟁력을 높이는데 도움이 되고자 한다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-4

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 김용암

Effects of thermal treatment on the structural and capacitive properties of polyphenylsilane-derived porous carbon nanofibers

김보혜* 양갑승¹

대구대학교 과학교육학부 ¹전남대학교 고분자 섬유 시스템공학과

Organic-inorganic hybrid composite carbon nanofibers (CCNFs) are prepared by one-step electrospinning and subsequent thermal treatment using polyphenylsilane (PPS) as an inorganic precursor. We investigate the structural properties and electrochemical behavior of these CCNF materials when applied as supercapacitor electrodes as a function of the carbonization temperature ranging from 800 to 1000 °C. The introduction of PPS induces thermal stability for the organic-inorganic hybrid CCNFs via the incorporation of a porous structure with stabilized functional structures such as silicon oxynitride (SiO_xN_y) and silicon oxycarbide (SiO_xC_y). This phenomenon is attributed to the synergistic effect of both the double-layer capacitance and the pseudo-capacitive effect induced by the porous carbon layer and the some surface functionalities), thereby providing high charge capacity, power and energy density.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-5

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 김보혜

Substitutionally Boron-Doped Single-Layer Graphene

김용암

전남대학교 고분자섬유시스템공학과

The introduction of foreign atoms into the hexagonal network of a monolayer network of sp_2 -hybridized carbon atoms, such as nitrogen, has been the hottest topic as an effective tool to tailor the intrinsic properties of graphene. Here we, for the first time, report that boron atoms are substitutionally present within graphene because boron is the neighboring to carbon atom in the periodic table. The amount of the substitutional boron atoms in graphite was ca. 0.22 atomic % from X-ray photoelectron spectroscopy whereas the boron atoms were substitutionally and spatially distributed in a single layer graphene with a distance of 4.76 nm from Raman spectroscopy. We envisage that boron atom is a powerful route to engineer the physical and chemical properties of graphene.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-6

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 김보혜

Catalysts for the Oxygen Reduction Reaction

심준호

대구대학교 화학·응용화학과

Nanostructured noble metals with unique physical and chemical properties have received considerable interest in the recent years, not only for their fundamental scientific interest, but also for their specific applications. Among the many different approaches to nanomaterials synthesis, controlling the size, composition, shape and architecture are important key parameters in determining, revealing and enhancing their functions and potential applications. Platinum and platinum-based catalysts have been used extensively in a variety of fields, such as fuel cells and nonenzymatic sensors, etc. However, the high cost of catalysts caused by the exclusive use of platinum catalysts in the fuel cells is one of the major impediments to the popularization of these research areas. Over the past two decades, considerable research efforts have been focused on the exploration of less expensive, more abundant non-platinum catalysts that can offer acceptable performance. This talk will focus on our efforts to develop non-platinum catalytic materials in the electrocatalysis of the oxygen reduction, and hydrogen peroxide, known as an intermediate of oxygen reduction reaction, reduction/oxidation which is important in the field of fuel cells and biosensors. In addition, we introduce hierarchically driven metal dioxide nanowires directly on a platinum/carbon fiber microwire, which allows a simple fabrication of the amperometric sensor. The nanostructured electrodes show a favorable electronic property desired for sensing of hydrogen peroxide and NADH oxidation without having the enzymes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND2-7

발표분야: Recent Trends in Carbon Fiber-Based Materials

발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 김보혜

Nanocarbon-Polymer Nanocomposites and Application: Use of Individually Dispersed and Functionalized CNTs and Graphene

정용채

한국과학기술연구원(KIST) 탄소융합소재연구센터

Nanocarbon (CNT, Graphene, Fullerene etc.)-based materials have attracted much attention due to their significant role in the development of new advanced materials. In spite of many advantages such as the high mechanical, electrical, and thermal properties of nanocarbons, their homogeneous dispersion in a polymer matrix has been a problem in obtaining high performance nanocomposites because of strong interfacial interactions between nanocarbons. The choice and control of tailored functionalization sites due to chemical modification of CNTs or graphenes are important to achieve high performance properties in the polymer nanocomposites. There have been several reports on the functionalization of nanocarbons including defect functionalization, covalent functionalization and noncovalent functionalization. In this talk, the effective preparation methods of Nanocarbons-polymer nanocomposites are focused with some applications for polymer actuators. Acknowledgments: This work was supported by the KIST Institutional Program (2Z03870 and 2E23640).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR1-1**

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김철

Chemical Tools and Tactics to Study the Role of Metal-Associated Proteins in Alzheimer's Disease

일미희

울산과학기술대학교(UNIST) 나노생명화학공학부

Neurodegenerative disorders impose an enormous financial and emotional burden on patients, their families, and communities. More than 24 million people worldwide have Alzheimer's disease (AD), a devastating and fatal neurodegenerative disease that remains poorly treated due to an incomplete grasp on the disease etiology. A key neuropathological hallmark of AD is amyloid- β ($A\beta$) plaques in the brain. The mechanisms driving formation of these protein aggregates and their causal link to dementia are still unclear. An additional observation in the AD brain is the accumulation of metal ions, which has been proposed to be associated with $A\beta$ aggregates and neuronal death, yet relatively little is known, further sustaining the controversy surrounding this aspect of the disease. Even through a large body of continuously reported literature regarding metal ions and $A\beta$ species, direct connection of metal- $A\beta$ interaction with AD onset and development has been neglected in this field due to lack of appropriate tools and/or tactics. Therefore, we have developed chemical tools and/or tactics that are capable of specifically targeting metal-associated $A\beta$ species and modulating their interaction and reactivity. Using our chemical reagents, we have been able to regulate metal-induced $A\beta$ aggregation and neurotoxicity in vitro and in living cells. Here, our rational structure-based design principle and recent findings for chemical tools and tactics for investigating metal- $A\beta$ chemistry and biology in AD and/or potential therapeutic agents for AD will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR1-2

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김철

Reactivity comparison of nickel(II)-superoxo and nickel(III)-peroxo complexes

조재홍

대구경북과학기술원(DGIST) 신물질과학

Mononuclear metal-dioxygen adducts, such as metal-superoxo and -peroxo species, are generated as key intermediates in the catalytic cycles of dioxygen activation by heme and non-heme metalloenzymes. We have shown recently that the geometric and electronic structure of the Ni-O₂ core in [Ni(O₂)(n-TMC)]⁺ (n = 12 and 14) varies depending on the ring size of the supporting TMC ligands. In this study, mononuclear Ni(II)-superoxo and Ni(III)-peroxo complexes bearing a common macrocyclic TMC ligand, such as [Ni^{II}(O₂)(13-TMC)]⁺ and [Ni^{III}(O₂)(13-TMC)]⁺, were synthesized in the reactions of [Ni^{II}(13-TMC)(CH₃CN)]²⁺ and H₂O₂ in the presence of tetramethylammonium hydroxide (TMAH) and triethylamine (TEA), respectively. The Ni(II)-superoxo and Ni(III)-peroxo complexes bearing the common 13-TMC ligand were successfully characterized by various spectroscopic methods, X-ray crystallography, and DFT calculations. Based on the combined experimental and theoretical studies, we conclude that the superoxo ligand in [Ni^{II}(13-TMC)(O₂)]⁺ is bound in an end-on fashion to the nickel(II) center, whereas the peroxo ligand in [Ni^{III}(13-TMC)(O₂)]⁺ is bound in a side-on fashion to the nickel(III) center. Reactivity studies performed with the Ni(II)-superoxo and Ni(III)-peroxo complexes toward organic substrates reveal that the former possesses an electrophilic character, whereas the latter is an active oxidant in nucleophilic reaction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR1-3**

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 김철

How does iron coordination affect the function of zinc finger proteins?

이승재

전북대학교 화학과

Zinc finger proteins use zinc as a structural co-factor to function, typically by binding to nucleic acids with sequence specificity. Although zinc is typically thought to be the physiologically relevant metal ion for zinc finger protein function there is evidence that other metal ions, including iron, may replace zinc under certain conditions. Studies on iron binding to two zinc finger proteins, Tristetraprolin (TTP) and ZIF-268 will be presented. TTP has two zinc binding domains each of which is composed of three cysteine residues and one histidine residue (Cys3His) that bind zinc. TTP is an RNA binding protein that regulates inflammatory response. Peptides corresponding to the zinc binding domains were prepared and their metal binding and RNA binding properties in the presence of iron were determined using a combination of UV-visible spectroscopy and Fluorescence Anisotropy. These studies demonstrated that both ferric and ferrous iron can substitute for zinc in TTP and still remain functional: i.e. bind to RNA with sequence selectivity and specificity. We then developed a spectroscopic assay to measure the oxidative susceptibility of the iron substituted TTP peptides and determined that iron substitution increases the rate of oxidation of the peptides compared to zinc. ZIF-268 is a classical zinc finger protein that contains three zinc-binding domains of the form Cys2His2. A peptide corresponding to the zinc-binding domain of ZIF-268 was prepared and its metal and DNA binding properties determined. As with TTP, iron can substitute for zinc in ZIF-268 and the protein retains functional. These results as well as studies on the oxidative susceptibility of iron substituted ZIF-268 will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR1-4

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 김진홍

Late-Stage Fluorination for Positron Emission Tomography (PET)

이은성 Jacob M. Hooker¹ Tobias Ritter^{2,*}

포항공대 화학과 ¹Athinoula A.Martinou Center for Biomedical Imaging, Massachusetts General Hospital and Harvard Medical School, Charlestown, MA 02129, United States ²Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138, United States

Positron emission tomography (PET) is a non-invasive and powerful imaging technique to probe biological processes in vivo and requires synthesis of PET tracers which contain positron-emitting isotopes, such as ¹¹C, ¹³N, ¹⁵O, and ¹⁸F. Among them, the ¹⁸F isotope is used most widely in clinical PET applications due to its longer half-life of 110 minutes, which allows synthesis and distribution of radiotracers for PET imaging. However, C-F bond formation is challenging, especially with ¹⁸F. Here we present practical late-stage fluorination reactions with high-specific activity ¹⁸F fluoride to make aryl and alkenyl fluorides from organometallic palladium and nickel complexes. The late-stage fluorination reactions enable the synthesis of conventionally unavailable positron emission tomography (PET) tracers for anticipated applications in pharmaceutical development as well as pre-clinical and clinical PET imaging.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR1-5

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 김진홍

Responsive Multi-Domain Free-Standing Films of Gold Nanoparticles Assembled by DNA-Directed Layer-by-Layer Approach

박소정* Zaki G. Estephan¹ Zhaoxia Qian¹ Daeyeon Lee¹ John C. Crocker¹

이화여자대학교 화학나노과학 ¹University of Pennsylvania, USA

Responsive free standing films of gold nanoparticles are fabricated by a new approach combining the programmable DNA-directed self-assembly and the layer-by-layer (LbL) thin film fabrication technique. This approach allows for the assembly of multi-domain nanoparticle films with each domain possessing distinct properties in response to external stimuli, which is essential for the formation of dynamic nanostructures. Large area free standing films of DNA-modified gold particles are fabricated by the selective melting of a sacrificial nanoparticle domain, taking advantage of the unique sharp melting transition of DNA-modified gold nanoparticles. Furthermore, we show that released multi-domain films can be designed to further split into multiple intact daughter films in a precisely controlled manner, demonstrating that this new approach provides a powerful means to fabricate free standing nanoparticle films that are capable of programmable shape transformation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR1-6

발표분야: Symposium for Young Inorganic Chemists

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 김진홍

Morphology Control of Porous Materials for Selective Adsorption and Size-selective Separation: Key Components for Bio-refinery Processes

유원철

한양대학교 응용화학과

For the production of fuels and chemicals, plant biomass is the only sustainable resource which can substitute the use of petroleum sources. In this respect, lignocellulose decomposition to monomeric sugars, control of the isomerization and catalysis of sugars and biomass derivatives, and energy-efficient selective separations have challenged the commercial realization of processes that can generate liquid fuels and chemicals. Porous materials with various sizes from sub-nanometer to several tens of nanometer and compositions have been used as a sorbent, separation membrane, catalyst as well as a template for hierarchical/multifunctional materials. For advanced applications of porous materials, the morphology control (implying surface texture, size and shape as well as growth mechanism) of porous materials is desired. In this seminar, various approaches to control the morphologies of porous materials (carbon, silica, zeolite, titania etc.) will be introduced. Surfactant-induced re-assembly via micelle formation with dissolved species was used to understand and create the extra porosities on the silica and zeolite (MFI) materials. Confined syntheses of zeolite and titania materials using hard templates (carbon and silica) were applied to control the morphology. In addition, a nanocasting method for fabricating mesoporous carbon materials from a silica template was carried out. The designed porous materials were implemented for their intrinsic applications such as selective adsorption and size selective separation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR2-1

발표분야: Bioinorganic Chemistry: Recent Trends and Outlooks

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이석중

Low-valent Nickel Chemistry; Transformation of Small Molecules

이윤호

KAIST 화학과

There has been a surge of interest in the chemistry of low-valent, redox-active complexes of the mid-to-late first row transition metals in recent years. This interest has been in part motivated by a desire to generate species that feature uncommon metal-to-ligand multiply bonded species such as oxo, imide, carbyne and nitride via partial or complete group transfer. Particular study of such species will be presented to show their respective roles in small-molecule transformations that include, carbon dioxide transformation for CODH chemistry and CO reduction as a key step for Fisher-Tropsch synthesis. To test the validity of hypotheses concerning nickel's direct role in the stepwise reduction of CO₂ and CO, nickel model systems are needed. Such systems can test the chemical compatibility of nickel with various proposed intermediates, and the reactivity patterns of such species. A square planar (PNP)Ni-L scaffold (PNP = N[2-P(CHMe₂)-4-methylphenyl]₂) where the L site is occupied by ligands such as CO, OCHO, CO₂ and COOR will be described. The systems accommodating terminally bound CO in the three formal oxidation states (nickel(0), +1, and +2) and their reactivity toward CO₂ will be illustrated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR2-2

발표분야: Bioinorganic Chemistry: Recent Trends and Outlooks

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이석중

Photochemical Reduction of Proton and Nicotinamide Cofactor Using Metal Complexes/Nanoparticles

김진홍

이화여자대학교 화학·나노과학과

As fossil fuels are gradually decreasing, the replacement of fossil fuels by sustainable energies is greatly required. To avoid the negative environmental impact of greenhouse gases, hydrogen has attracted increasing attention as an alternative energy resource. An organometallic rhodium complex has been frequently employed as an efficient catalyst for hydride transfer during chemical and electrochemical formation of NADH to selectively reduce NAD⁺. Several electrochemical NADH regeneration systems have been reported using Rh catalysts to study electron transfer phenomena. Here, we present a novel, simple system that employs only Pt nanoparticles (PtNPs) for the efficient photochemical generation of NADH. This system first demonstrated that PtNPs can be used in the visible light-driven photogeneration of NADH without an additional chromophore in the presence of a sacrificial electron donor, and can directly perform the catalysis of the NAD⁺ reduction in the absence of another homogeneous heavy-metal catalyst in aqueous media. A visible light-driven photocatalytic system for the generation of NADH from aqueous protons was examined using molecular cobaloxime catalyst. Introduction of an electron-donating or electron-withdrawing substituent in the para position of the pyridine changed the rate constant and affected the conversion efficiency. In addition, the reduction of CO₂ was carried out in the presence of formate dehydrogenase using the NADH photochemically generated using cobaloxime. Bulk electrolysis of NAD⁺ carried out with a Rh catalyst in the absence and presence of platinum nanoparticles (PtNPs) generates enzymatically active 1,4-NADH. An efficient catalyst for the selective decomposition of formic acid in aqueous solution yielded hydrogen and carbon dioxide.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR2-3

발표분야: Bioinorganic Chemistry: Recent Trends and Outlooks

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 이석중

Mimicking Active Sites of O₂ Activating Metalloenzymes for Mechanistic Insights

조재홍

대구경북과학기술원(DGIST) 신물질과학

Oxygen-coordinating metal intermediates, such as metal[?]superoxo, [?]peroxo, [?]hydroperoxo, and [?]oxo species, are frequently invoked as plausible oxidants in the oxidation of organic substrates. In biomimetic studies, iron(III)[?]superoxo species have been proposed as a potent oxidant in the C-H bond activation of hydrocarbons by mononuclear nonheme iron(II) complexes. An iron(III)[?]superoxo intermediate is also proposed as an active oxidant that attacks the sulfur atom of the ligand with the terminal oxygen atom of the superoxo group, followed by the O-O bond cleavage to form an iron(IV)[?]oxo species. In the case of copper(II)[?]superoxo species, a number of synthetic copper(II)[?]superoxo complexes have shown reactivities in ligand oxidation and the oxidation of organic compounds with weak C-H, O-H, and N-H bonds. In this presentation, we have shown the first structurally characterized end-on chromium(III)-superoxo complex, [Cr(O₂)(TMC)(Cl)]⁺ (TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane), which was synthesized by reacting [Cr(TMC)(Cl)]⁺ with O₂. The Cr(III)-superoxo intermediate has shown reactivities in C-H cleavage of alkylaromatics via an H-atom abstraction mechanism. In addition, we report that [Cr(O₂)(TMC)(Cl)]⁺ is able to transfer its oxygen atom to organic substrates (e.g., PPh₃ and sulfides), yielding the corresponding oxygenated products and a chromium(IV)[?]oxo complex, [Cr(O)(TMC)(Cl)]⁺. An electrophilic character of [Cr(O₂)(TMC)(Cl)]⁺ is also demonstrated in the oxidation of *para*-substituted thioanisoles.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR2-4

발표분야: Bioinorganic Chemistry: Recent Trends and Outlooks

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 이석중

Recent novel cysteine and Fenton chemistry probing systems towards addressing molecular aspects in neurodegenerative disease research

D.G.Churchill

한국과학기술원(KAIST) 화학과

Our laboratory is engaged in designing and uncovering new modalities in small molecules for selective molecular recognition and chemosensing (molecular probes). While this area is often explored by analytical, biological, and organic chemists, many molecules we have studied involve metal ions or heavier main group atoms as analytes or part of a sensing ensemble; therefore, the tenets of coordination chemistry and main group chemistry are very much relevant. Small fluorogenic molecules and sites for metal ion chelation / substrate reactivity can allow for optimal selectivity, reversibility, etc. While there is still no perfectly operating molecular probe, we can find ways to optimize certain sensor characteristics while still thinking in “small molecule” terms. There are also opportunities to involve more than one analyte. In this talk, recent pursuits in selective cysteine (Cys) and Fenton chemistry probing ($\text{Fe}^{2+}/\text{Fe}^{3+}$) will be presented. The fluorogenic systems were typically studied in live neuronal cells to help address relevance of these molecular aspects to neurodegenerative disease research. Finally, the optical signal patterns based on the chemical input can be interpreted in “logic gating” patterns in both cuvettes and neuronal cells.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR2-5

발표분야: Bioinorganic Chemistry: Recent Trends and Outlooks

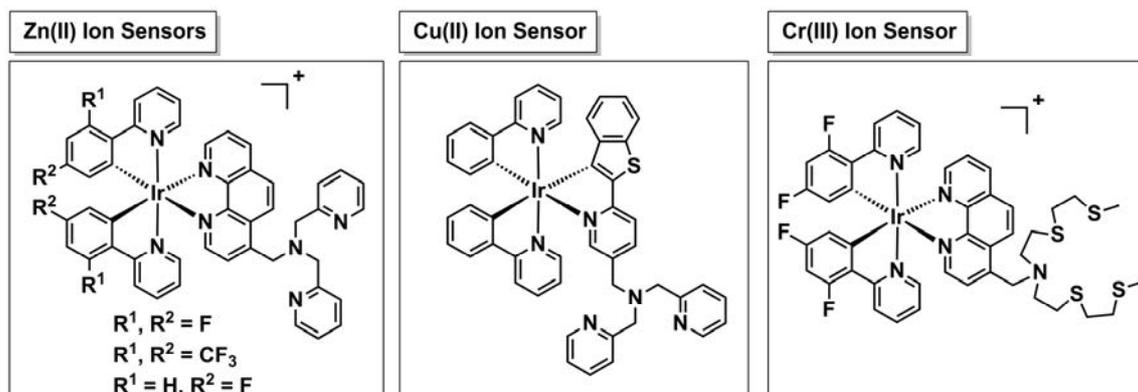
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 이석중

Cyclometalated Ir(III) Complexes for Phosphorescence Sensing of Biological Metals

유영민

경희대학교 정보전자신소재공학과

Phosphorescent sensors are useful alternatives to the conventional probes relying on fluorescence because the phosphorescence signaling can eliminate background noises through time-gated acquisition. We have developed phosphorescent sensors based on cyclometalated Ir(III) complexes. The constructs contained two or three cyclometalating (C[^]N) ligands, and the electron densities and bandgap energies of the ligands were systematically controlled. We incorporated a metal-chelating di(2-picolyl)amino receptor to the Ir(III) complexes to create Zn(II) sensors. We observed phosphorescence turn-on responses to labile Zn(II) ions, which were attributed to the effective suppression of photoinduced electron transfer. The photophysical mechanism strictly adhered to the Rhem-Weller principle. Utility of the phosphorescence signaling was further extended for the creation of phosphorescence ratiometric sensors of redox-active biometals, such as Cu(II) ions and Cr(III) ions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-1**

발표분야: Recent Trends in Theoretical Chemistry

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김우연

Fast and accurate electronic structure methods for intermolecular interactions

John Herbert

Ohio State University, USA

Accurate calculation of non-covalent interactions is a challenging problem for ab initio quantum chemistry. Density-functional methods often fail badly at describing van der Waals interactions, and wave function methods require high level of electron correlation and large basis sets, both of which quickly become intractable for large molecules or for clusters of polar molecules where many-body polarization effects are important. I will describe several new theoretical methods aimed at surmounting these challenges. By means of monomer-based calculations, we achieve sub-kcal/mol accuracy in binding energies (based on comparison to high-level benchmarks), at a cost lower than that required to perform density functional theory on the entire non-covalent assembly of molecules.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-2**

발표분야: Recent Trends in Theoretical Chemistry

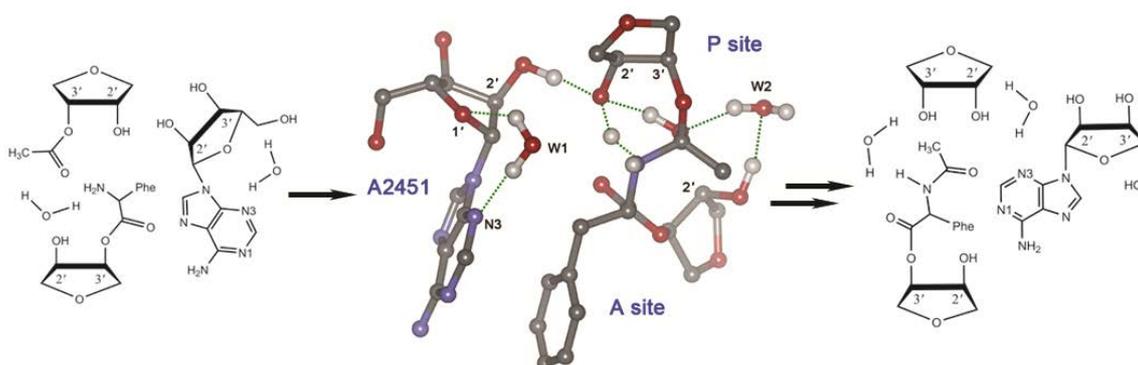
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김우연

A Mechanistic Study for Peptide Bond Formation on the Ribosome

강영기

충북대학교 화학과

Peptide bond formation is one of fundamental reactions in biology, which is catalyzed by the ribosome within the peptidyl transferase (PT) center of its large subunit. Although there has been considerable progress in the mechanistic study of the PT reaction, the detailed pathway is still unclear. We report the feasible pathways of the quaternary model system for the ribosome-catalyzed PT reaction obtained by density functional calculations. Our results indicate that the step from the reactant complex to the first six-membered TS involving a proton shuttle via the 2'-OH of the P-site A76 in the stepwise pathway is the most favored rate-limiting in solution. It is found that the C-O3' bond-breaking of A76 is not significant but the C-N bond formation with a tetrahedral intermediate occurs in the rate-limiting step and that the fast breakdown of the C-O3' bond is followed in the second transition state. These are consistent with recent kinetic experiments.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-3**

발표분야: Recent Trends in Theoretical Chemistry

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 김우연

DFT studies on the intramolecular magnetic couplings of organic diradicals

이진용* 고정철 조대흠

성균관대학교 화학과

DFT calculations often overestimate the magnetic coupling constant (J) of diradicals when compared with experimental values. I would like to introduce a couple of ways to obtain reliable magnetic coupling constants. Recently, we proposed a way of standardization of radicals which induce ferromagnetic or antiferromagnetic coupling through four different couplers. Based on our strategy, a new series of neutral radicals based on diazaphenalenyl were designed via heteroatomic modifications. We divided eight monoradicals into α -group and β -group according to Mulliken spin density values of the connected atoms. The overall trends in the strength of magnetic interactions of diradicals were found to be identical in three different model systems. The diradicals with para-substituted phenyl acetylene coupler resulted in almost twice stronger intramolecular magnetic coupling interactions of the corresponding diradicals as compared to the meta-substituted one with opposite magnetism. NN-Ethylene-PO (nitronyl nitroxide radical coupled to phenoxy radical via ethylene coupler) was calculated to have the strongest magnetic coupling constant with ferromagnetism, and to be even stronger (more than twice) than NN-ethylene-NN (nitronyl nitroxide diradical with ethylene coupler), which was reported to have strong antiferromagnetic interactions in a previous experiment. In addition, for diradicals tested, a remarkable linear relationship between the calculated and experimental J values was found. We suggest that the slope (0.380) of the linear relationship can be utilized as a scaling factor for estimating J values. By applying this scaling factor and calculating J values, we could predict the reliable J values of four dithiadiazolyl (DTDA) diradicals coupled with an aromatic ring.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-4**

발표분야: Recent Trends in Theoretical Chemistry

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 김준수

QM/EFP and QM/MM-MD Methods for Condensed Phase Dynamics(A New Way of Quantum Mechanical Molecular Dynamics)

최철호

경북대학교 화학과

A new way of quantum mechanical molecular dynamics study has been recently developed by integrating QM methods and Effective Fragment Potentials(EFP)[1] as well as classical force fields. The applicability of the hybrid QM/EFP1 to a long-time MD simulation of chemical reaction in aqueous solution has been recently examined[2], where it was demonstrated that the QM/EFP-MD yields accurate free energy change and barrier associated with the zwitterion to neutral tautomerization of glycine in aqueous solution. The same approach has been also successfully utilized for NaCl association/dissociation dynamics[3], hydrophobic association of methanol dimer[4], and anharmonic vibrational properties[5] in aqueous solutions. A REMD (Replica-Exchange MD) version of QM/MM and QM/EFP has also been established using GDDI(Group Distributed Data Interface) technology.[6] In this talk, we introduce our hybrid QM/EFP and QM/MM Molecular Dynamics (MD) techniques as implemented in GAMESS. References:(1)Day, P. N.; Jensen, J. H.; Gordon, M. S.; Webb, S. P.; Stevens, W. J.; Krauss, M.; Garmer, D.; Basch, H.; Cohen, D. J Chem Phys 1996, 105, 1968.(2)Choi, C. H.; Re, S.; Feig, M.; Sugita, Y. Chemical Physics Letters 2012, 539-540, 218-221.(3)Ghosh, M. K.; Re, S.; Feig, M.; Sugita, Y.; Choi, C. H. J Phys Chem B 2013, 117, 289-295.(4)Ghosh, M. K.; Uddin, N.; Choi, C. H. J Phys Chem B 2012, 116, 14254-14260.(5)Ghosh, M. K.; Lee, J.; Choi, C. H.; Cho, M. J Phys Chem A 2012, 116, 8965-8971.(6)Fedorov, D. G.; Sugita, Y.; Choi, C. H. J Phys Chem B 2013, 117, 7996-8002.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-5**

발표분야: Recent Trends in Theoretical Chemistry

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 김준수

Space-time phase transitions in the trajectory space of glassy systems

정연준

서울대학교 화학부

The glass transition is a phenomenon that a liquid freezes to an amorphous phase showing abnormally slow dynamics. Although glassy materials are well characterized by a number of experiments, the existence of actual phase transition is not yet verified. However, recently, a numerical first-order dynamical phase transition in the trajectory space has been reported. The dynamical phase transition is controlled by variables that bias the trajectory of a system to make it out of equilibrium state. In this study, we applied the above method, called an s-ensemble method to kinetically constrained models with additional short-ranged attractive interactions. We report that the first order phase transition in the trajectory space is observed in these models. We also discuss how the additional attractive interactions affect the dynamic heterogeneity of the system by varying the bias variable.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS1-6**

발표분야: Recent Trends in Theoretical Chemistry

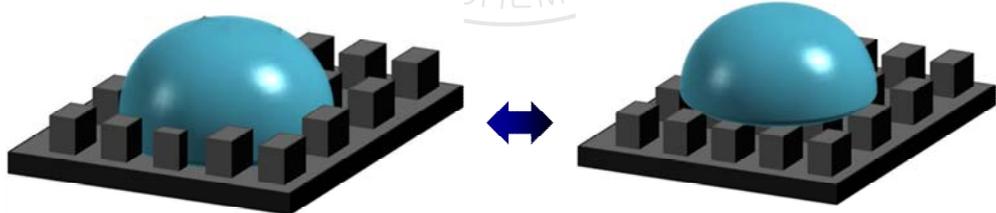
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 김준수

Wetting and Drying Transitions of Water Confined between Hydrophobic Pillars

장준경

부산대학교 나노소재공학과

The phase behavior of the water confined between hydrophobic pillars was studied by using a thermodynamic theory and a molecular Monte Carlo simulation. The drying transition of water with decreasing spacing between pillars is related to the Wenzel (WZ) to Cassie-Baxter (CB) transition of droplet. The intermediate states between the WZ and CB states are revealed in our simulation. We also examine the structure of the confined liquid water. By including the line tension, the present theory agrees with both experiments and the atomistic MD simulations.



Wenzel (WZ) state

Cassie-Baxter (CB) state

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-1**

발표분야: Recent Trends in Physical Chemistry

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 황현석

Got excited? Get Relaxed!

이영민

포항공과대학교 화학과

Following the dynamics of various molecular systems after their electronic excitations has served as a grand challenge in physical chemistry for many decades. Here, we will discuss our recent efforts in advancing methodologies for studying electronically excited molecules, with a focus on their applicability toward large and complex systems. We first show how a semiclassical approach can be applied to studying the excitation energy transfer dynamics of a relatively large photosynthetic complex, even with a simple potential energy model for the complex. Both of its promising and devastating aspects are discussed, with some prospects for its future developments. We then move on to the way of constructing more delicate potential models, which are essential for studying wider range of complex systems. Results of nonadiabatic dynamics simulations based on these models are presented as a demonstration of its applicability and reliability.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-2**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 안태규

Mapping magnetic fields using a radical pair reaction

이호재

광주과학기술원(GIST) 화학

I used a fluorescent chemical indicator of magnetic field to visualize the magnetic field around ferromagnetic structures. The indicator was a chain-linked electron donor-acceptor molecule, phenanthrene-(CH₂)₁₂-O-(CH₂)₂-dimethylaniline, that forms spin-correlated radical pairs upon photoexcitation. The magnetic field altered the coherent spin dynamics, yielding an 80% increase in exciplex fluorescence in a 0.1 T magnetic field. The magnetic field distributions were quantified to precision of 1.8×10^{-4} T by image analysis and agreed with finite-element nanomagnetic simulations.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-3**

발표분야: Recent Trends in Physical Chemistry

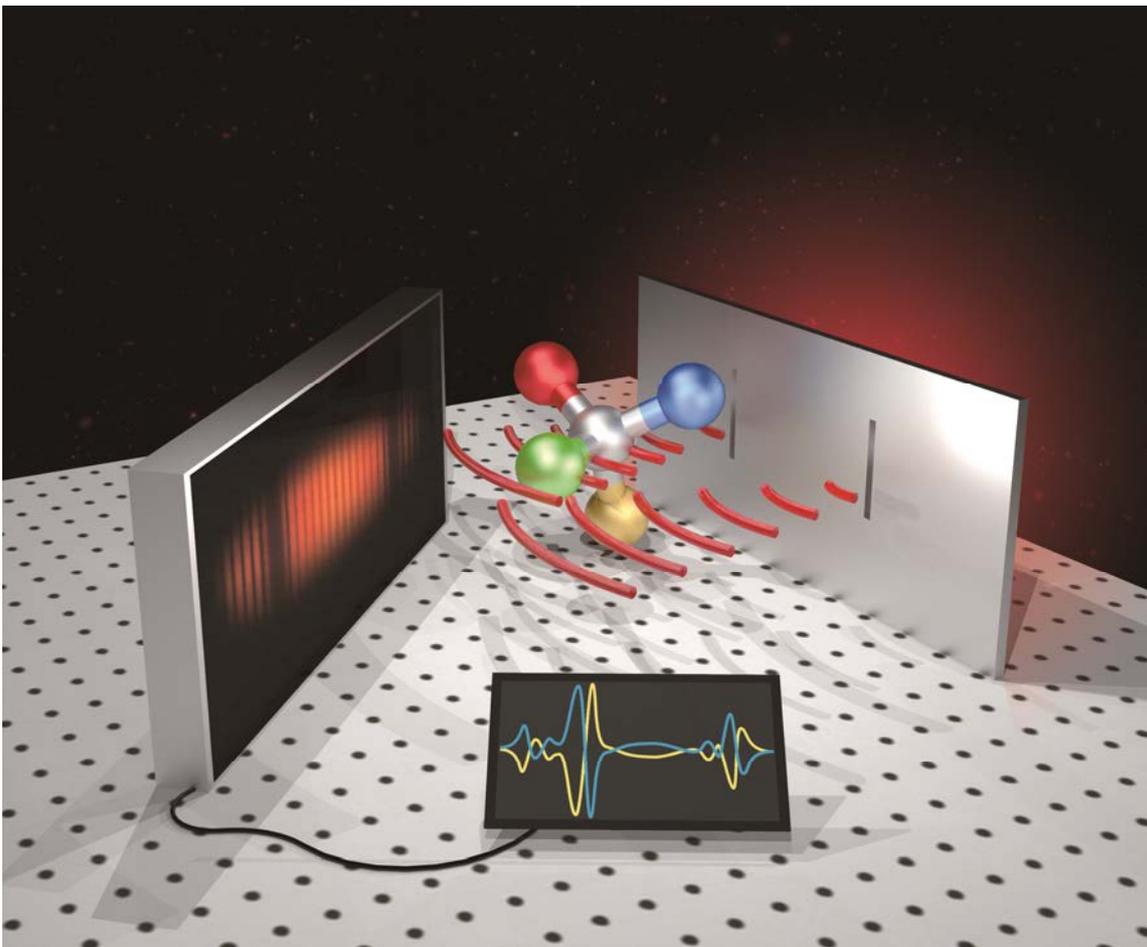
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 안태규

Interference methods in chiroptical spectroscopy

이한주* 조민행^{1,*}

한국기초과학지원연구원 서울센터 ¹고려대학교 화학과

Molecular chirality plays an important role in many chemical and biological processes including asymmetric synthesis, enzyme catalysis, ligand binding to biomolecules. Naturally, its characterization is essential for understanding their functions and mechanisms. However, optical activity resulting from the differential interaction of chiral molecule with left- and right-circularly polarized light is a very weak effect by which further applications are limited. Signal amplification in chiroptical spectroscopy is a necessary step to implement time-resolved chiroptical experiments which requires high sensitivity. Recently, interference methods have been developed to enhance chiroptical signals by properly controlling polarization states and designing detection scheme. Here, basic concepts and experimental details of these techniques are presented and future applications are also introduced and discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-4**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:05, 좌장: 한상우

Fabrication of Nanodevices of Photocatalytic Nanoparticles for Artificial Photosynthesis

강영수

서강대학교 화학과

In this talk, the basic concept and fabrication technology for the nanodevices for artificial photosynthesis was introduced. Based on the synthesis and alignment of the nanoparticles and nano-sized monolayers of photocatalytic materials, vectorial electron transport from the higher conduction band energy to lower conduction band energy could be accelerated by suppressing the defect and optimizing the electron transport distance and diffusion capacity. The fabrication of the photocatalysts was done to get the largest exposed surface area of the most photoactive facets for TiO₂, Cu₂O, Fe₂O₃ and ZnO. Especially, α -Fe₂O₃ monolayer fabrication of visible light sensitive layer on FTO and the measurement of the photocurrent density are the basic approach for the artificial photosynthesis through water splitting and CO₂ reduction. For the efficient electron transport through the TiO₂ nanotubes, SrTiO₃, Fe₂O₃, Cu₂O were doped into the pores of the TiO₂ nanotubes and photocurrent was measured.

1. Chang Woo Kim, Jong Hwa Sohn, a Hyun Gil Cha, a Do Kyoung Kim a and Young Soo Kang, Fabrication of Hollow Metal Oxide Nanocrystals by Etching Cuprous Oxide with Metal (II) Ions : Approach to the Essential Driving Force Nanosclae. 2013, 0000 (in press)
2. Hyun Gil Cha, † Jieun Song, † Kyu Joon Lee, ‡ Hyun Sung Kim †, *, Myung Hwa Jung, ‡ Woon-sup Shin, † Kyung Byung Yoon, † Young Soo Kang †, * Simple Fabrication of (012) Plane Oriented Continuous α -Fe₂O₃ Film : Secondary Growth of Nanocrystal Monolayer J. Am. Chem. Soc. 2013, 0000. (submitted)
3. Long Quoc Pham, Jin you Zheng, Hyungil Cha and Young Soo Kang*, Facile method to improve photoelectrochemical properties of CdS/ZnO nanorod arrays with CdO layer, J. Mater. Chem.C 2013, 0000 (in press)
4. Chang Woo Kim, Minhyuk Kang, Bongjin Moon, Jin Heung Kim and Young Soo Kang, Manganese Doped Highly Ordered Mesoporous Silicate Structure with High Efficiency of Oxidation Suppression Function Chem. Eur. J. 2013, 19,

135.5.Chang Woo Kim, Young Hwan Kim and Young Soo Kang, Facile Synthesis and Magnetic Phase Transformation of Ln-TM-B Nanoclusters by Oxygen Bridging J. Material Chemistry C 2013, 1, 275



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-5**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 한상우

Supra- Quantum Dots

김성지

포항공과대학교 화학과

'Bottom-up' assembly of small building blocks such as atoms, molecules and nanoparticles into hierarchically organized structures can be ubiquitously found in nature. The building blocks can be designed with a precision that cannot be achieved by current lithographic techniques. Colloidal quantum dots (QDs) can be tailored by the size and shape typically in a few nm size regime, and they can be also assembled into three-dimensional superlattices of artificial metamaterials. Herein we intend to introduce unique structure of colloidal nanocluster which is composed by three dimensionally self-assembled QDs. Because of the similarity with supramolecule formation, we name the cluster as 'supra- quantum dot (SQD)'. Slightly truncated zinc-blende QDs of a few nm in size can self-assemble into a relatively uniform size cluster of tens of nm via oriented attachment growth process which is often found in biomineralizations. The clusters evolve into larger clusters via a few discrete stages because of the topological uniqueness of its space filling incapability, and finally become nearly spherical SQDs of typically ~100 nm in size. SQDs can be obtained with near monodispersity and can form superlattices of SQDs. SQDs have excellent colloidal properties allowing precipitation-based size selection, surface ligand exchange, and cation exchange process. As the result, uniquely structured SQDs of desired composition can be dispersed in any medium. For example, SQDs can be applied for photovoltaic devices for enhanced exciton migrations and carrier extractions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS2-6**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:55, 좌장: 한상우

Spatially-resolved chemistry at molecular junctions: the atomic scale study with a scanning tunneling microscope

한재량

전북대학교 화학과

The scanning tunneling microscope (STM) is an ideal tool for probing and control of chemical reactions at the spatial limit of individual atoms and molecules. The ability to visualize single molecules at the sub- \AA scale and control energy of tunneling electrons in the STM junction can be used to understand and manipulate single molecules. Furthermore, investigation of single molecular vibrations by STM inelastic electron tunneling spectroscopy (STM-IETS) provides a way to understand the chemical bond and characteristics of individual atoms and molecules. In this talk I will present several examples of surface chemical reactions studied using STM and STM-IETS. Firstly I will show that tunneling electrons in the STM junction are used to induce the local and nonlocal dissociation of O_2 molecules adsorbed on Ag(110) surface at 13 K. Tunneling of charge carriers from the STM tip into the O_2 causes dissociation of the molecule, giving rise to two adsorbed O atoms separated in different direction. Secondly the reaction characteristics of (R,R)-2,3-butanediol and R (and S)-1,3-propanediol molecules on a Si(001)- 2×1 surface will be presented. Thirdly I will talk about the ability to obtain vibrational characteristics of single CO molecule on the STM tip, which makes it possible to study the effect of electric field on the vibration of single molecules in an STM junction. The electric field modifies the binding characteristics of CO on silver as a result of a change in the charged states of the species, which leads to an increase (or a decrease) of the energies of the hindered rotation and the C-O stretch on silver. The chemical shift of vibration energy of CO varies with the charge states of adsorbate where the CO-terminated STM tip is placed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL1-1**

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 강성호

Advanced Separation of Structural Isomers in the Gas Phase using Ion Mobility Spectrometry (Plasma Chromatography)

김준곤

포항공과대학교 화학과

Ion mobility spectrometry (IMS), or used to be called as plasma chromatography, has been grown from atomic species for fundamental physical studies to nano-scale materials due to its unlimited detection size range. The development of electrospray ionization (ESI) has further expanded the application of IMS to the investigation of structural isomers and isobaric molecules of nonvolatile biomolecules in the gas phase combined with mass spectrometry (MS). ESI, which is a soft ionization method, transfers samples intact from the solution phase to the gas phase. Using this distinctive advantage of ESI, the shapes and sizes of various biomolecular ions from monomeric molecules to macro size complexes have been investigated. In this presentation, fundamental and applied studies of structural dynamics using IMS will be introduced. For example, correlation between van der Waals interaction and collision cross section values of molecules with various sizes will be introduced. Then, its unique applications to isolate and separate structural isomers will be further introduced.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL1-2

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 강성호

Comprehensive 2-dimensional Gas Chromatography for High Resolution Analysis

Mikiko Asakawa

SHIMADZU Corporation

Comprehensive 2-dimensional Gas Chromatography, called “GCxGC” is the latest separation technology with capillary gas chromatography. GCxGC is applicable to various fields, including analysis of complex matrices such as Petrochemical, food, flavor, Fragrance and Environmental samples. GCxGC uses two columns having different separation characteristics (non-polar and polar columns). These columns are connected in series via a modulator having trap and release function. As all of peaks eluting from first column can be separated by second column having different polarity once more, the separation capability of GCxGC becomes very high. It is an extremely effective system for analysis which requires higher separation of target substance in complex matrices. GCxGC covers many kinds of applications and realize a high resolution analysis which is difficult with ordinary capillary column system.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL1-3**

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 강성호

DNA Damage Analysis on Single Molecules

조규봉

서강대학교 화학과

Single molecule approaches are revolutionizing biochemical analysis because they pinpoint measurements to individual molecules in place of bulk assays, thereby engendering new molecular insights. Moreover, the capability of providing individual information makes single DNA molecule approaches useful for stochastic event analysis. For example, ultraviolet (UV) induced DNA damage is a stochastic event as well as a biologically important issue. Thus, here we present a single DNA molecule approach how to visualize UV-induced DNA damages such as double strand breaks (DSB) and single strand breaks (SSB) on DNA molecular backbones. Our molecular observations provide a map of DNA radiation-mediated breakages, revealing the sequence dependency of DNA damages rather than random occurrences. Consequently, our single molecule observations, along with simple genome analysis, imply that essential genes in bacteriophage may have a tolerance to UV irradiation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL1-4

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 차상원

Application of Metabolomics to High Resolution Phenotype Analysis

Eiichiro Fukuzaki

Osaka University

Metabolomics is applicable without genome sequence information. Therefore, Metabolomics would be powerful analytical tool for commercially available plant and microorganisms. According to the above context, Metabolomics means exhaustive relationship analysis between 'data matrix of metabolic profile' and 'data matrix of performance of samples'. Among those operation of Metabolomics, metabolic fingerprinting, in which metabolic profile is used as fingerprint for samples' performance prediction and classification, is one of the most important application of Metabolomics. On this occasion, practical operation of Metabolomics for high resolution phenotype analysis would be presented. To reveal a power of Metabolomics, a possibility of Metabolomics based prediction of "Life span", which is highly integrated and complicated quantitative phenotype, was studied to find strong relationship between metabolome and lifespan by means of PCA. Orthogonal projection on latent structure (OPLS) based model can predict yeast life span using metabolome as fingerprint. Using information of principal component vector in PCA life span related metabolites were nominated and life span related genes were speculated. The result imply Metabolomics would be applicable for high resolution analysis of a complicated quantitative phenotype, and metabolome information might be useful for strategic enhancement of useful quantitative phenotype for biomass production.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL1-5

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

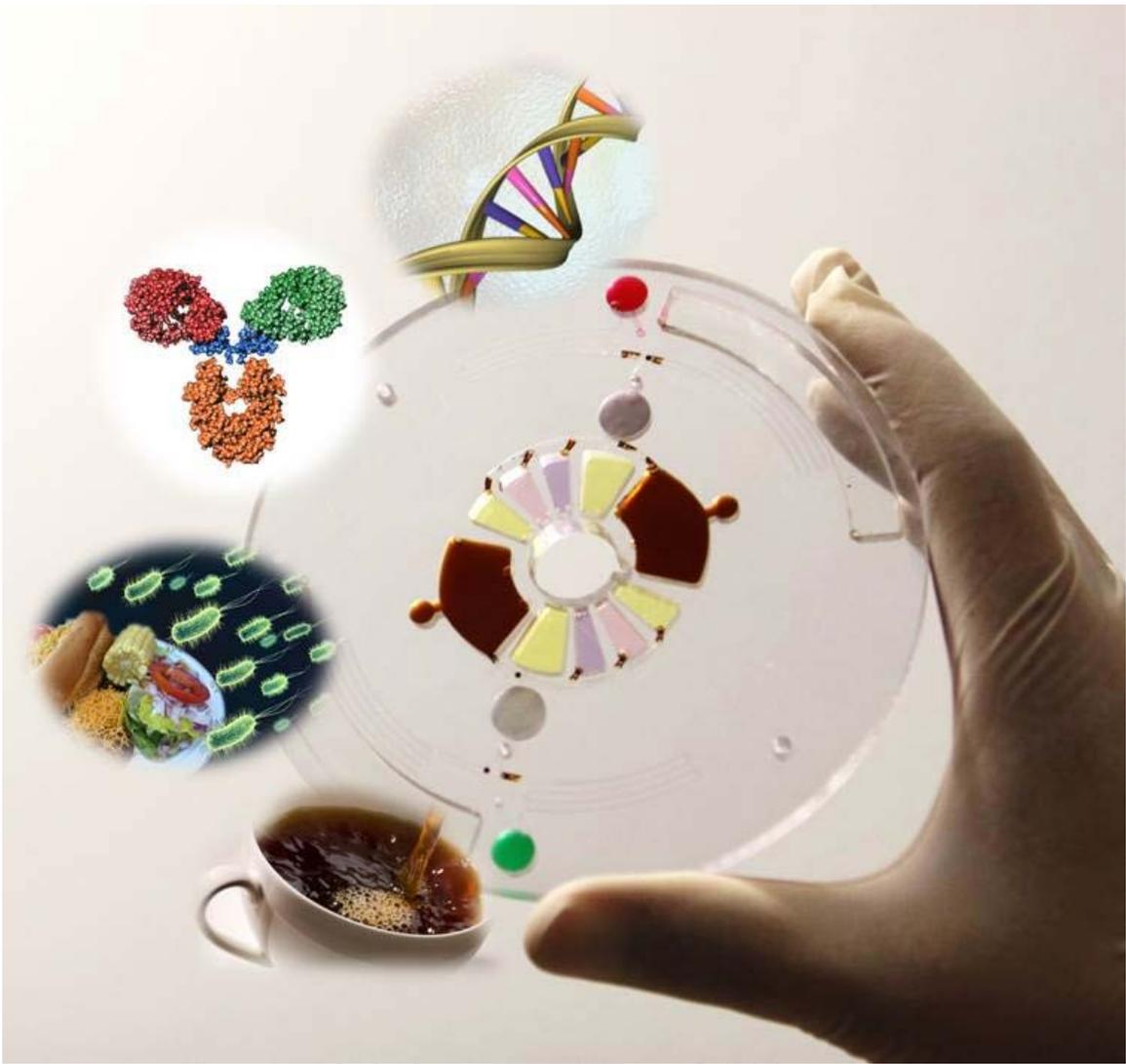
발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 차상원

Lab-on-a-disc for Analytical Chemistry

조윤경* 김태형 박양석 김유빈

울산과학기술대학교(UNIST) 생명공학과

We present a novel fully integrated centrifugal microfluidic device, “Lab-on-a-disc”, for various kinds of applications in analytical chemistry. In biomedical applications, a bead-based enzyme-linked immune-sorbent assay was fully integrated on a disc starting from whole blood for the analysis of multiple protein biomarkers for cardiovascular diseases [1]. The detection sensitivity could be enhanced significantly by using electrochemical detection on a spinning disc and employing nanomaterials such as electrospun nanofibers [2]. In molecular diagnostics, pathogen specific DNA could be extracted from whole blood on a disc within 12 minutes [3] and for the food safety application, a further research fully integrated all the process for Salmonella detection from the milk within 30 minutes by using an isothermal DNA amplification method, Recombinase Polymerase Amplification. Lab-on-a-disc was also employed to automate solid phase extraction of caffeine from real beverages such as a coffee or a soft drink for the quantitative analysis of caffeine concentration [4]. The “Lab-on-a-disc” technology is advantageous because of the capability to integrate and automate all the process into a disc-shaped device with simple, size-reduced, and cost-efficient instrumentation. Integration with microfluidic technology allows more precise control of fluids while also reducing the reagent consumption, the required analysis time and handling errors. We believe these approaches will not only improve the performance of the target analysis but also potentially have great impact on global healthcare. References [1] J. Park et al. Anal. Chem., 84, 2133, 2012 [2] T. Kim et al, Lab Chip, 13, 3747, 2013 [3] Y. Cho et al., Lab Chip, 7, 565, 2007 [4] W. Xu et al., Scientific Reports, 3, 2255



KOREAN CHEMICAL SOC

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL1-6

발표분야: KCS-JASIS Joint Symposium: Advanced Separation Science

발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 차상원

Separation Analysis Technology Using Supercritical Fluid Chromatography

Yoshiteru Horikawa

JASCO Corporation

Supercritical Fluid Chromatography (SFC) offers high speed analysis due to high diffusivity of solutes in the low-viscosity supercritical mobile phase. Generally, the separation mode in SFC is regarded as normal phase with a combination of non-polar CO₂ mobile phase and polar stationary phase. Therefore, separation of water-soluble polar compounds is considered to be difficult to separate by using SFC. However, the elution and peak shapes of polar compounds can be improved by adding a small amount of acid, base, volatile salt and ion pair reagent to the modifier solvent such as alcohol. Supercritical carbon dioxide evaporates when it is released in the air. This takes the advantage of easy solvent removing for fractionation. SFC has become popular for separation and fractionation of chiral substances. The screening method, which comprehensively analyzes the interests by the combinations of various solvents and columns, has been used to achieve a suitable separation of chiral substances. We demonstrate the rapid screening of several chiral medicines. It took only 6 hours to search a suitable separation. In chiral preparative SFC, samples are often over-loaded and it is difficult to determine when to start and end fractionation from Ultra Violet (UV) chromatographic data. A Circular dichroism (CD) detector can differentiate enantiomers and generate positive/negative chromatographic peaks. In addition, CD detector can simultaneously generate CD, UV and g-factor signals. The g-factor is a signal defined as CD/UV whose level is independent of the peak concentration but dependent only on enantiopurity. Therefore, enantiopurity of g-factor triggered fractions is very high.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL2-7**

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 분과기념강연, 발표일시: 목 16:40, 좌장: 김영환

단일분자의 선택적 형광/비형광 검출기술의 개발 및 응용

강성호

경희대학교 응용화학과

일반적으로 개개 분자의 분석이나 통계적인 현상은 평균값에 기본을 둔 보편적인 측정방법에 기본을 두고 있으나, 단일분자 검출기술은 화학 혹은 생화학 반응에서 중간단계는 물론, 각 단계마다 분자 수준에서 직접 시료를 측정하고 분석 할 수 있는 장점을 가지고 있다. 지금까지의 단일분자 검출기술은 주로 형광 검출기술을 사용하여 성공적으로 시행되고 있고, 드물게 전기화학적 방법을 사용하고 있다. 하지만, 최근에는 분자 자체의 화학발광이나 금속 나노결정체의 광전기적 성질을 이용하여 특정 단일분자나 단일입자를 형광표지없이 선택적으로 실시간 검출할 수 있는 새로운 단일분자 검출기술들이 개발되고 있다. 본 발표에서는 최근에 개발된 형광 및 비형광 단일분자 혹은 단일 나노입자의 검출기술과 응용에 대해 소개한다. 이러한 검출기술은 화학은 물론, 생명과학, 신약개발, 미세분리, 질병진단 분야와 분자유전체, 단백질체학, 바이오센서, 면역학을 비롯한 다양한 분야에서 응용이 가능하다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL2-1**

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 조원련

[발표취소] Single Drop Microextraction for Capillary Electrophoresis

정두수

서울대학교 화학부



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL2-2

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 조원련

형광면역크로마토그래피를 이용한 수중 남조류독소, 마이크로시스틴의 새로운 미량분석법 개발

표동진

강원대학교 화학과

본 발표에서는 최근 우리나라 여름철에 호수나 하천에서 녹조현상(남조류의 대량번식)이 발생할 때 수중에 인체에 유해한 독소가 존재하게 되는데 이러한 조류독소를 고감도로 간편하게 검출하는 새로운 분석법을 소개하고자 한다. 이 새로운 분석법은 2013년 8월 29일 산업통상자원부 장관으로부터 신기술 인증(NET)을 획득하였다. 현재까지는 호수나 하천의 극미량 조류 독소인 마이크로시스틴을 검출하기 위해서는 HPLC 나 ELISA 등의 시간이 많이 소요되고 번거로운 방법들이 사용되고 있었다. 새로운 분석법의 분석원리 및 방법은 다음과 같다. 크로마토그래피 매질상의 한 쪽 말단에 조류독소, 마이크로시스틴이 함유된 것으로 예상되는 물 시료를 적하하여 물 시료가 크로마토그래피 매질을 통해 이동되도록 하고, 물 시료중의 분석물은 물 시료가 적하된 구획으로부터 크로마토그래피 매질을 따라 전개하는 방향으로 일정한 간격을 두고 위치한 구획에 흡착되어 있는 표지된 탐지자와 반응하여 분석물-표지된 탐지자의 결합체를 형성하며, 분석물-표지된 탐지자의 결합체는 크로마토그래피 매질을 통해 이동하면서 상기 탐지자와 동일하거나 상이하거나 비표지되어 상기 크로마토그래피 매질상의 중간 정도 위치에 설정된 검사창에 고정된 포획자와 반응함으로써 표지된 마이크로시스틴-BSA 비표지된 포획자 사이에 분석물이 결합되어 형성된 복합체를 형성하고, 이에 따라 형성된 복합체의 양을 측정하여 시료중의 분석물을 정량한다. 세분화된 내용은 아래와 같다. (a) 형광으로 표지된 MCLR-BSA 복합체와 분석 시료 안에 존재하는 MCLR 이 같이 존재한다. (b) 이 두 물질은 크로마토그래피 매질상의 검사창에 선으로 분주되어 있는 항체와 경쟁적으로 결합한다. (c) 경쟁 반응에 참여하는 형광으로 표지된 MCLR-BSA 의 양적인 변동에 따른 시그널의 변화를 줄이기

위해서 사용된 형광과 동일한 형광이 표지된 biotin-BSA 복합체를 MCLR-BSA 형광 복합체와 혼합하여 준비한다. 그리고 MCLR 에 대한 단일 클론 항체가 선으로 분주되어 있는 매질상의 앞쪽에 avidin 을 일정한 농도로 분주한다. (d)최종적으로 나온 결과값은 avidin-biotin-BSA-형광 값을 비교하여 나타낸다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL2-3

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 조원련

분석화학자가 주도하는 임상생화학의 기술혁신

박상열* 이화심¹

한국표준과학연구원(KRISS) 바이오임상표준센터 ¹한국표준과학연구원(KRISS) 바이오/임상센

터

임상화학 또는 임상생화학 분야는 환자로부터 채취한 다양한 검체를 대상으로 생화학분석을 수행하여 결과를 의료진에 제공함으로써 질병의 진단 또는 예후 판단이 정확하게 이루어지도록하는 매우 실용적인 학문분야이다. 주로 화학분석 기법이 사용되었기 때문에 임상화학 (Clinical Chemistry)로 시작되었지만 최근 고도로 발달한 생화학 분석기법이 활발히 적용되면서 임상생화학(Clinical Biochemistry) 으로 확대되었다. 질병의 원인이 불분명할수록 생화학분석이 치열하게 수행되며 많은 경우, 이러한 결과로부터 질병을 치료하는 결정적인 단서가 찾아진다. 최근에는 다중을 대상으로 한 질병예방 성격의 건강검진이 확대되면서 저렴하고 정확한 임상분석의 필요성이 크게 부각되고 있다. 이러한 변화에 따라 분석화학자들이 이분야의 발전에 기여할 수 있는 기회가 더욱 확대되고 있다. 임상진단과 관련하여 신속성, 정확성, 경제성, 그리고 정보의 유용성을 크게 향상시킬 수 있도록 다양한 새로운 분석기법의 개발하고 실용화 하는데 분석화학자들이 크게 기여할 수 있을 것으로 기대된다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL2-4

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 조원련

Generalized preparation protocol of MIP based open tubular CEC columns for chiral separation of profen drugs

정원조

인하대학교 화학과

It will require a huge amount of time to develop a useful molecule imprinted polymer (MIP) for chiral separation of a new pair of enantiomers if optimization is mandatory in both MIP formation and chromatographic elution. Thus, foundation of a generalized preparation protocol regardless of the types of template will reduce such burden dramatically. A generalized preparation procedure of open tubular (OT) MIP columns has been developed for a number of templates including acidic (such as profen drugs), basic (such as atenolol and sulpiride), and neutral drugs. The template (S-enantiomer) was mixed with methacrylic acid, ethylene glycol dimethacrylate and 4-styrenesulfonic acid, dissolved in a porogen mixture of ACN/2-propanol (9/1), and incubated in a pretreated and silanized fused silica capillary by the thermal non-covalent polymerization procedure. The whole preparation procedure was exactly the same for all the MIP capillaries except for the selection of template. Nevertheless, the morphologies of the MIP layers were markedly variant depending upon the choice of template. The separation efficiency of each OT-MIP column for chiral separation of R- and S-enantiomers was examined and tuned to obtain the best separation efficiency by changing the chromatographic parameters such as eluent composition and pH. The chiral and non-chiral separation of this study resulted in very good separation efficiencies. In addition, some empirical rules of eluent optimization based on our studies are summarized as follows for the OT-MIP CEC columns prepared by the generalized protocol. The eluent composed of acetonitrile and an aqueous buffer (either acetate or phosphate) will be useful and the optimized acetonitrile composition is in the range of 70-92% (v/v). The optimized buffer pH is 3-5 for weak acid templates, 2-3 for strong acid templates, 6-8 for neutral templates, and ca. 9 for basic templates. The above description may help reduce efforts and time in eluent optimization.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL2-5**

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 김영환

Flow Field-Flow Fractionation for Blood Proteins and Lipid Analysis

문명희

연세대학교 화학과

This presentation will show recent results of FIFFF for proteomic and lipidomic analysis of human blood using off-line and on-line combination with MS. Asymmetrical FIFFF (AF4) was utilized for the size sorting and simultaneous enrichment of N-linked glycopeptides of human serum by utilizing a dual lectin-based strategy in which two different lectin-glycopeptide complex groups are separated by sizes in AF4 channel while non-glycosylated peptides are depleted by crossflow during separation. Collected lectin-glycopeptide complex fractions from lung cancer sera were analyzed by nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS/MS). Secondly, it demonstrates that high density lipoprotein (HDL) and low density lipoprotein (LDL) from plasma samples from patients having coronary artery disease (CAD) can be separated and collected in their intact forms on a semi-preparative scale using multiplexed hollow fiber FIFFF and that collected fractions can be examined for the lipidomic analysis of various lipids using nLC-ESI-MS/MS. A recently developed on-line chip-type AF4 is utilized for the top-down lipidomic analysis of human lipoproteins at a microflow rate regime which enables the direct coupling with ESI-MS/MS. The developed AF4-ESI-MS/MS provides separation of HDL/LDL with the simultaneous desalting of lipoproteins which enhances ionization of lipid molecules from AF4 separation. It demonstrates the high speed screening of lipid species (phospholipids, regioisomers of triacylglycerols, and cholesteryl esters, etc) in HDL/LDL can be achieved depending on the disease status of CAD.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL2-6

발표분야: Advanced Bioanalysis for Biomedical and Clinical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 김영환

Mass Spectrometric Analysis of Glycoproteins in Human Plasma for Cancer Biomarker Discovery

유종신

한국기초과학지원연구원 질량분석연구부

Human plasma is clinically the most important sample for the study of cancer biomarker. Glycosylation is one of the post-translational modifications of proteins secreted in plasma, which is related to protein folding, quality control, sorting, degradation, and secretion. More than half of plasma proteins are N-linked glycoproteins and their analysis is a major challenge in mass spectrometry. The glycoform distribution and degree of glycosylation of a glycoprotein can be significantly altered by diseases such as cancer, therefore, quantitative analysis of the glycosylation in proteins may be useful in discovering biomarkers. It is challenging to perform the identification and the quantification of N-glycopeptides from mass spectrometry analysis because the instrumental sensitivity and concentration of N-glycopeptides are a lot lower than those of the general peptides due to the intrinsic property and microheterogeneity of glycopeptides. We report the development of a high-throughput method for glycoproteomics analysis, named GlycoProtein Analysis (GPA), which can automatically identify the glycan compositions, glycosylated sites and glycopeptide sequences of N-glycopeptides tryptically digested from glycoproteins. The GPA platform and algorithm were applied to identify the different site-specific glycoforms of a N-glycopeptide tryptically digested from glycoproteins. Here we describe a new label-free quantitative method that can be applied to target glycoproteins in order to discover a cancer biomarker in human plasma. The change and quantification of site-specific N-glycosylation in cancer progression are discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-1**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 이민재

Protein Post-Translational Modification in Biological Research

이상규

경북대학교 약학대학

Post-translational modification (PTM) represents an important mechanism for diversifying and regulating the cellular proteome. Among of known ~ 300 PTMs, acylation at lysine residue and phosphorylation at serine, threonine and tyrosine residues are representative PTMs. Here we will represent the results for identification of crotonyllysine, as novel PTM in histones, and phosphorylation in *Daphnia pulex*, as novel model for PTM research. First of all, we report the identification of 67 previously undescribed histone modifications, increasing the current number of known histone marks by about 70%. We further investigated one of the marks, lysine crotonylation (Kcr), confirming that it represents an evolutionarily-conserved histone PTMs. The unique structure and genomic localization of histone Kcr suggest that it is mechanistically and functionally different from histone lysine acetylation. In male germinal cells immediately following meiosis, Kcr is enriched on sex chromosomes and specifically marks testis-specific genes, including a significant proportion of X-linked genes that escape sex chromosome inactivation in haploid cells. Second, Waterflea, Daphnids, have been used as ecology or ecotoxicology, a small planktonic crustacean. Among several daphnia species, *D. pulex* is a key constituent in the aquatic ecosystems and in the food web. Here, we investigated the 105 phosphorylation sites on 92 daphnia proteins by phosphopeptide enrichment using titanium dioxide and online 2D-LC system with high accuracy mass spectrometer. This is the first in-depth phosphoproteome research of *D. pulex* showing that Ser/Thr/Tyr phosphorylation is also present on many essential *Daphnia* proteins.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-2**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 이민재

Micro-scale Depletion of High Abundance Proteins and Ultra-high Pressure Enzymatic Digestion for High-throughput Analyses of Human Bio-fluids

형석원

한국표준과학연구원(KRIS) 유기분석표준센터

Reduction of protein complexity and follow-up sample digestion are necessary for protein identification by mass spectrometry in bottom-up proteomics studies. Bio-fluids such as plasma and cerebrospinal fluid (CSF) have been considered to be good sources for finding biomarker candidates due to the close relations to human diseases. This presentation describes a methodology in terms of depletion of high abundance proteins and high-throughput protein digestion using human bio-fluids. A vast dynamic range of protein concentration in plasma is required to be depleted for high abundance proteins which inhibit the detection of low-abundance proteins by LC-MS/MS. Immunoaffinity is one of the most frequently used protein depletion methods, however, that requires the sacrifice of high expenses for the purchase of depletion column and sometimes, undesired high sample loading as well. As an alternative to those problems, micro-scale depletion column (volume, 346 μ L) was prepared using Seppro IgY 14 resin and then the feasibility was demonstrated using human plasma. Further study was carried out with CSF as a limited bio-fluid sample which can be more appropriately applicable to the micro-scale immunoaffinity column. In another study, ultra-high pressure enzymatic digester (UPED, XStreamTM) was developed and demonstrated the effectiveness in respect to digestion time and protein identifications. Moreover, this UPED system was integrated with a custom nano-liquid chromatography system for direct LC-MS/MS analysis upon digestion that can span the automation at a time from protein digestion to LC-MS/MS analysis for high-throughput analysis of proteins.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-3**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 이민재

Glycoproteome Profiling of Human Gastric Cancer Tissue Using FACE (Filter Aided Capture and Elution) and UPLC-MS/MS

이후근* 박종문¹

가천대학교 메디컬캠퍼스 약학대학, 이길여 암당뇨연구원 ¹가천대학교 메디컬캠퍼스 이길여
암당뇨연구원

Protein glycosylation is the most important post-translational modifications (PTMs). Glycoproteins are often important integral proteins that play a role in cell-cell interactions,, developmental biology, cell signaling and inflammation in cell membrane. Because of low stoichiometry of modified proteins, for identifying the numerous glycoproteins, the proteomics analysis of these PTM requires powerful and indispensable technology. To detect low abundant glyco-peptides or proteins in complex mixture among the high abundant non glycopeptide equivalents with LC-MS technologies, enrichment methods have to be applied. For example hydrazide bead, ERLIC (Electrostatic Repulsion Hydrophilic Interaction Chromatography), HILIC (Hydrophilic Interaction liquid Chromatography), lectin affinity chromatography method have widely been used for enrich glycol- peptides or proteins. In this study, we introduce a powerful protocol for enrichment of glycopeptides, and analyzed glycosylation of human gastric cancer tissue using membrane based modified FACE (filter aided capture and elution) method. So we were identified 3,000 N-glycosylated peptide. And then, we functional studies of the normal samples compared with cancer sample using IPA (Ingenuity Pathway Analysis) from the list of identified glycopeptides.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-4**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 이민재

Probing Protein Function with Quantitative Mass Spectrometry

이진환

한국표준과학연구원(KRISST) 바이오임상표준센터

Proteins rarely function as individual entities; they form multi-subunit complexes to carry out a diverse range of biological processes. Yet, mechanisms governing assembly/disassembly of most protein complexes remain ambiguous, which poses one of the key challenges in gaining a comprehensive understanding of how cellular activities are controlled. To address this issue, we developed novel quantitative mass spectrometry-based methodologies, which were applied to probe the dynamics of the SCF complex regulation. The modular SCF (Skp1, Cul1, and F box) ubiquitin ligases feature a large family of F box protein substrate receptors that enable recognition of diverse target proteins for proteasome-mediated degradation. Real-time measurements of formation and disassembly indicated that SCF^{Fbxw7} is extraordinarily stable, but the Cul1-binding protein Cand1 accelerated its dissociation by one-million-fold. Binding and ubiquitylation assays showed that Cand1 is a protein exchange factor that accelerates the rate at which Cul1 equilibrates with multiple F box proteins. Depletion of Cand1 from cells impeded recruitment of new F box proteins to pre-existing Cul1 and profoundly altered the cellular landscape of SCF complexes. We suggest that catalyzed protein exchange may be a general feature of dynamic macromolecular machines.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-5**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 이진환

Application of MALDI tissue imaging of Phospholipids and Metabolites

김광표

경희대학교 응용화학과

Recent developments in imaging mass spectrometry (IMS) have allowed complete mapping of the biological molecules including phospholipids (PLs) that are the major building block molecules of cellular membranes. The IMS technique can detect different classes of PLs as well as their location information directly from tissue sections. PL head groups carry either positive and/or negative charges; therefore, IMS experiments must be conducted in both positive- and negative-ion mode to detect all types of phospholipids. Recently, we developed an optimized matrix preparation for IMS experiments in both ion modes that maximize PL identification from a single brain tissue section. The optimized matrix showed improved stability and consistency during both ion mode experiments and successfully identified >100 peaks of PLs determined by parent ion m/z value. Further tandem mass spectrometric analysis (MS/MS) was performed to those PLs that are anatomically important according to their distribution on rat brain tissue section.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-6**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 이진환

Integrated N-terminal Enrichment for Comprehensive Profiling of Proteolytic Cleavage Sites

김종서

서울대학교 생명과학부 RNA 연구단

We report a strategy for enriching protein N-terminal peptides that integrates positive and negative selection methods to obtain a comprehensive coverage of the N-terminome. A novel resin-assisted positive enrichment method with high specificity (>97%) was developed to complement an optimized negative enrichment method. Applications of these methods to cell lysates of *Aspergillus niger* resulted in the identification of 2991 unique protein N-termini and proteolytic cleavage sites from 1051 proteins.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO1-7**

발표분야: Mass Spectrometry for Biological Applications

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 이진환

Measurement of Protein Turnover Rates on a Proteomic Scale by Metabolic Heavy Water ($^2\text{H}_2\text{O}$) Labeling

김태영

광주과학기술원(GIST) 기초교육학부

All proteins are turned over through dynamic processes consisting of synthesis, degradation, import from or export to other cellular compartments. Protein turnover is delicately controlled to adapt to healthy states and contributes to maintain protein function and pool size. Previously available approaches to calculate protein turnover rates have mainly focused on the most abundant protein or proteins correlated with a single biological pathway, and a global analysis of protein kinetics is still challenging. The advent of highly sensitive biological MS techniques enables to perform protein kinetic studies more systematically and globally. Among available technologies, heavy water ($^2\text{H}_2\text{O}$) labeling is a promising method to study biological kinetics, because it is non-toxic to animals and human up to a certain level for a prolonged period of time, results in universal labeling of biomolecules in a body, and is also the most cost-effective tool compared with other isotope labeling approaches. To understand mitochondrial protein dynamics *in vivo*, we designed a novel approach to calculate protein turnover using heavy water. We characterized the turnover rates of 458 proteins in mouse cardiac and hepatic mitochondria, with median turnover rates of 0.0402 and 0.163 d^{-1} , respectively. Our proteomics platform demonstrates the first large-scale analysis of mitochondrial protein turnover rates *in vivo*, with potential applications in translational research.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-1**

발표분야: Imaging of Biological Molecules

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 최수혁

Single-molecule FRET studies on replication fork regression dynamics of WRN helicase

홍성철

서울대학교 물리학

During DNA replication, the replication machinery frequently stalls at various DNA damages. Regression of stalled replication forks by ATP-driven molecular motors is an indispensable process for reactivation of the stalled replication. To elucidate the fork regression mechanism of Werner syndrome protein (WRN), we studied unwinding and fork regression dynamics of single WRN molecules at various DNA forks. Surprisingly, WRN is a bidirectional motor which dynamically switches its branch migration direction at various roadblocks on DNA. Our data suggest that WRN might work as a coordinator of the whole reactivation process of the stalled replication fork.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-2**

발표분야: Imaging of Biological Molecules

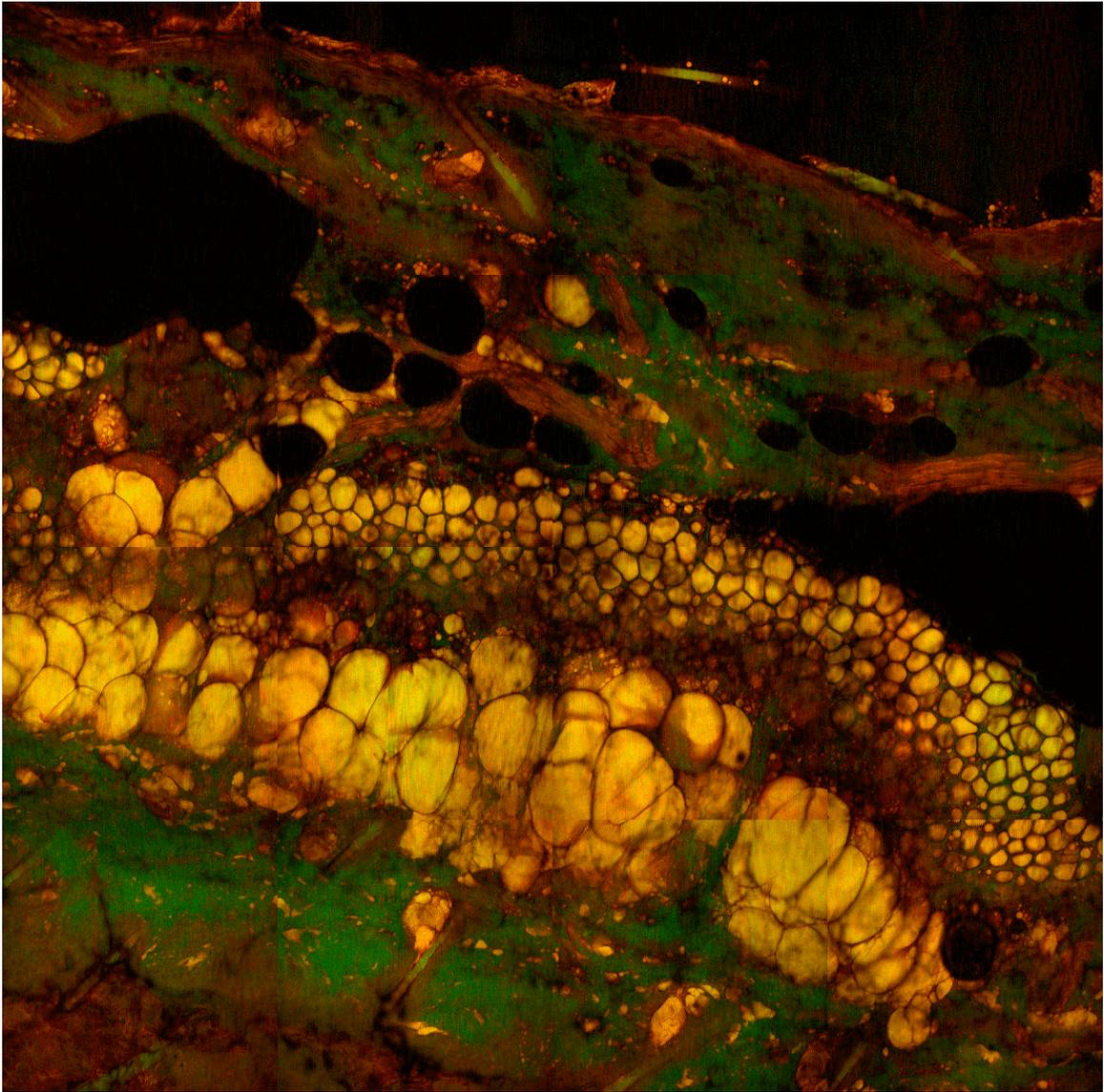
발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 최수혁

Coherent Raman Scattering with Chirped Broadband Laser Pulses

임상현

광주과학기술원(GIST) 환경공학부

Coherent Raman Scattering (CRS) is a powerful spectroscopy technique that can offer the same chemical information as spontaneous Raman scattering, but with orders of magnitude higher sensitivity. Its applications to biomedical imaging and ultrafast spectroscopy, however, have not been wide spread due to the complexity and difficulties of its experimental implementations. In this talk, I will introduce an alternative CRS methods (the so-called "Spectral Focusing" mechanism), which utilized the interference between two identically chirped ultrafast pulses to achieve high spectral resolution with femtosecond laser pulses. I will present its application to the coherent anti-Stokes Raman scattering (CARS) imaging, which can map out the distributions of proteins, saturated and non-saturated fats inside the unlabeled animal tissues. Preliminary imaging of skin, retina and brain tissues will be presented.



TEAN CHEMICAL

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-3**

발표분야: Imaging of Biological Molecules

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 최수혁

Nanoplasmonic Spectroscopic Imaging for Living Cells

최연호

고려대학교 생체의공학과

Label-free, sensitive and selective detection methods with high spatial resolution are critically required for future applications in chemical sensor, biological sensor, and nanospectroscopic imaging. Here I describe the development of Plasmon Resonance Energy Transfer (PRET)-based molecular imaging in living cells as the first demonstration of intracellular imaging with PRET-based nanospectroscopy. In-vivo PRET imaging relied on the overlap between plasmon resonance frequency of gold nanoplasmonic probe (GNP) and absorption peak frequencies of conjugated molecules, which leads to create 'quantized quenching dips' in Rayleigh scattering spectrum of GNP. The position of these dips exactly matched with the absorption peaks of target molecules. As another innovative application of PRET, I present a highly selective and sensitive detection of metal ions by creating conjugated metal-ligand complexes on a single GNP. In addition to conferring high spatial resolution due to the small size of the metal ion probes (50 nm in diameter), this method is 100 to 1,000 folds more sensitive than organic reporter-based methods. Moreover, this technique achieves high selectivity due to the selective formation of Cu²⁺-complexes and selective resonant quenching of GNP by the conjugated complexes. Since many metal ion ligand complexes generate new absorption peak due to the d-d transition in the metal ligand complex when a specific metal ion is inserted into the complex, we can match with the scattering frequency of nanoplasmonic metal ligand systems and the new absorption peak

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-4**

발표분야: Imaging of Biological Molecules

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 최수혁

Ratiometric Two-Photon Fluorescent Probes for Biomedical Research

김환명

아주대학교 에너지시스템학부

Ratiometric imaging with small molecule fluorescent probes is a powerful tool for quantitative analysis of biological events in cells. In recent years, two-photon microscopy (TPM), which employs two near-infrared photons as excitation source, has become indispensable to the study of biology and medicine due to its capability for molecular imaging deep inside intact tissues. TPM offers a number of advantages over conventional microscopy including greater penetration depth ($> 500 \mu\text{m}$), localization of excitation, and longer observation times. As such, there is a strong need to explore various ratiometric two-photon (TP) probes for quantitatively assessing biomolecules and their activities. Recently, we have developed ratiometric TP fluorescent probes based on small molecule that can detect cellular ions and signaling molecules in live cells, live tissue slices and living mouse brain. The molecular design and evaluation of a selection of our recent studies, and their use in biomedical research will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-5**

발표분야: Imaging of Biological Molecules

발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 최수혁

Imaging of membrane protein interactions by single-protein tracking in a single living cell

이남기

포항공과대학교 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.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO2-6**

발표분야: Imaging of Biological Molecules

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 최수혁

Quantitative MR imaging of microvasculature

조형준

울산과학기술대학교(UNIST) 나노생명화학공학부

It is anticipated that the ability to image the spatial distribution of tumor microenvironments (perfusion, necrosis, hypoxia, cellularity, vessel diameter/tortuosity etc.,) in vivo will provide prognostic information including assessment factors that influences response to treatment. Functional imaging modalities such as MRI and PET offer unprecedented opportunities to study in vivo tumor microenvironments and physiology with the development of new imaging techniques and molecular imaging agents. For example, extravasating Dynamic Contrast Enhanced MRI using Gd-DTPA provides vascular/perfusion information of tumor and thus, not only offer complementary information to PET hypoxia markers but also address the relationship between tumor hypoxia and vasculature. Susceptibility contrast MRI utilizes intravascular superparamagnetic imaging agents such as iron oxide nanoparticles to visualize tumor vessel diameter and tortuosity to obtain information regarding tumor angiogenesis. In this talk, a few examples of translational imaging research activities will be introduced, including developments of new imaging methods followed by its application to both neurological and oncological preclinical imaging.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN1-5**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

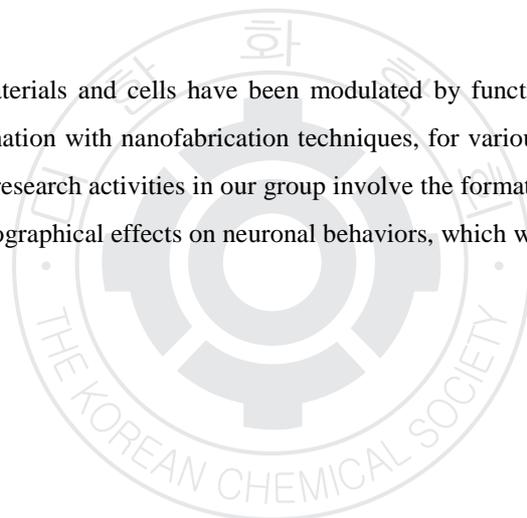
발표종류: 분과기념강연, 발표일시: 목 11:20, 좌장: 이필호

Controlling the Cell-Material Interfaces

최인성

한국과학기술원(KAIST) 화학과

The interfaces between materials and cells have been modulated by functionalizing the materials, cell surfaces, or both in combination with nanofabrication techniques, for various purposes in chemistry and related disciplines. Recent research activities in our group involve the formation of cell-in-shell structures and the study on chemotopographical effects on neuronal behaviors, which will be discussed in this talk.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN1-1

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

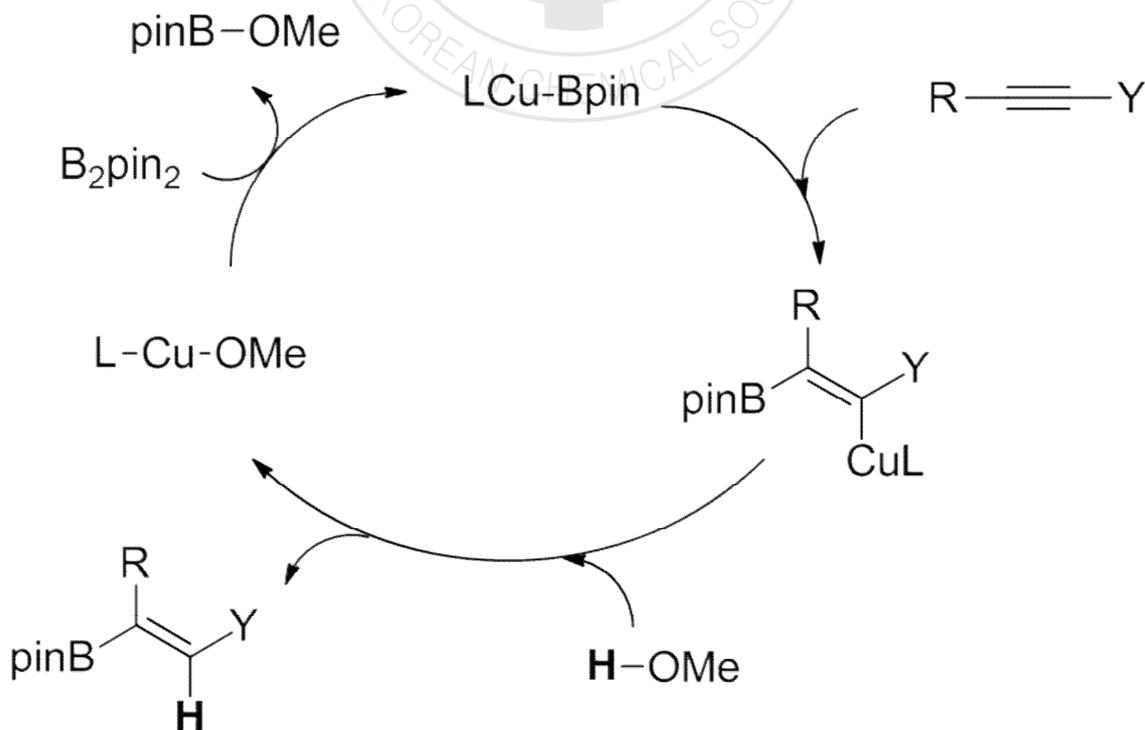
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 박재욱

Ligand-Controlled Regioselective Borylcupration and protonolysis of Alkynes

윤재숙

성균관대학교 화학과

Alkenylboron compounds are versatile intermediates that have been employed for a wide range of organic synthesis applications. Recent progress in the copper-catalyzed addition of boron (borylcupration of copper⁺boryl complexes) has made this protocol an important tool for the direct generation of alkenylboronates. In this presentation, reactions of copper⁺boryl complexes with various types of alkynes will be presented, which proceed with high chemo-, regio- and stereoselectivity.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGNI-2**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 박재욱

Asymmetric Organocatalyses using *N*-Centered Heteroaromatic Nucleophiles

조창우

경북대학교 화학과

Nitrogen-containing heterocycles and their derivatives have broad applications in organic, biological, and materials chemistry and, accordingly, synthesis of *N*-heteroaromatic compounds, especially optically pure ones, via catalytic routes has been a subject of active research. In organocatalytic asymmetric cascade reactions, the use of *N*-centered heteroaromatic nucleophiles remains almost unexplored in contrast to the widely studied *C*-centered nucleophiles. Specifically, pyrroles have never been used as the *N*-centered nucleophiles in the cascade reactions, in spite of the importance of pyrroles as optically pure *N*-heteroaromatic pharmacophores in biologically active natural products. In addition, pyrazole itself has never been used as the *N*-centered nucleophile in organocatalytic asymmetric reactions, although pyrazole derivatives have been recognized as important pharmaceuticals. Here, the first uses of pyrroles and pyrazole itself, respectively, as the *N*-centered heteroaromatic nucleophiles to α,β -unsaturated carbonyl compounds in the organocatalytic asymmetric reactions and their application to the asymmetric formal synthesis of biologically active natural products will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN1-3**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박재욱

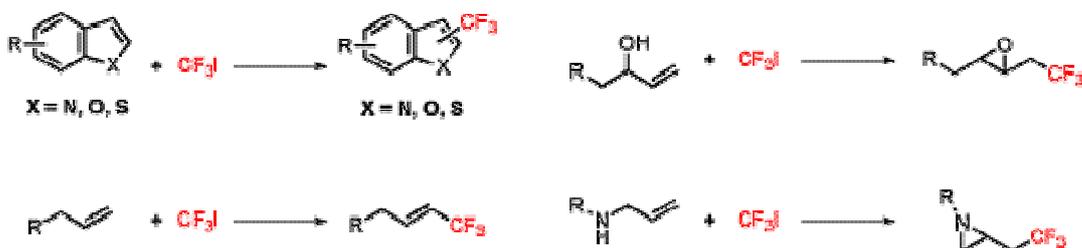
Visible Light-Induced Photocatalysis

조은진

한양대학교 응용화학과

Visible light-driven photocatalysis has been of great interest in the last few years as these methods do not require specialized equipment, but rather use irradiation sources such as sunlight, fluorescent bulbs, or blue LEDs. We have developed several types of visible light-induced reactions. Trifluoromethylation of organic molecules is of vital importance especially in the fields of pharmaceuticals and agrochemicals due to the unique physical and biological activities of compounds containing trifluoromethyl groups. We investigated visible light-induced trifluoromethylations of heterocycles, alkenes, and alkynes. In addition, efficient methods for the generation of CF₃-containing epoxides and aziridines, which are potential trifluoromethylated building blocks, have been developed. Benzofused heterocycles are another interesting class of molecules in many applications. Efficient methods for synthesis of 2-substituted benzothiazoles and benzimidazoles have been developed.

Trifluoromethylations



Synthesis of benzofused heterocycles



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGNI-4**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 이필호

Direct One-Pot Synthesis of Polycyclic Heterocycles

허정녕

한국화학연구원 의약화학연구센터

Dibenzo[b,f]oxepin is an important motif in natural and medicinal compounds. For example, aristoyagonine occupies a special interest since it is the only example to date of a natural cularine alkaloid incorporating a five-membered lactam. Due to low natural occurrence in conjunction with its biological activity against various cancer cell lines, several synthetic tactics have been disclosed for the synthesis of these structurally unusual alkaloids. Notably, molecules containing the dibenzo[b,f]oxepin moiety have received considerable interest from the medicinal community due to these compounds' potent biological properties, such as antipsychotic, antidepressant, antihypertensive, antiestrogenic, anti-inflammatory, and insecticidal activities. We have developed a direct one-pot strategy of phenanthrenes that employs a Suzuki-Miyaura coupling/aldol condensation cascade sequence. Then, we reported the application of this procedure to the total synthesis of aristolactams, including aristolactam BII, aristolactam BIII, aristolactam FI, N-methyl piperolactam A, and sauristolactam. In addition, we have successfully achieved the total synthesis of laetevirenol A. As part of a research program to develop a one-pot metal-catalyzed reaction/aldol condensation reaction, we sought to develop an efficient synthesis of dibenzo[b,f]oxepin via a one-pot Cu-catalyzed aryl ether formation/aldol condensation reaction. Herein, we will discuss the synthetic methodologies for the construction of diverse polycyclic heterocyclic scaffolds via an efficient one-pot procedure.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이건형

Design of Porphyrin-based Functional Materials

장우동

연세대학교 화학과

Porphyryns and chlorophylls are essential pigments in natural system. In biological systems, porphyryns and chlorophylls perform many essential functions, such as oxygen transport, active site in enzyme, and light harvesting. The functional porphyryn derivatives in biological systems provide various motivations for the design of biomimetic functional materials. Using the porphyryn moieties, we recently have designed several types of receptor molecules for the bindings of anionic and cationic species. As mimicry of biological suparmolecular assembly system, porphyryns were utilized as a building block to creat artificial receptors for specific molecules and light harvesting antenna systems. In this symposium, we are going to introduce several porphyryn-based functional materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN2-2**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이건형

Peptoids as Chemical Tools for Biological Applications

권용익

이화여자대학교 화학·나노과학과

It is essential to explore the biological functions of each protein including the protein-protein interaction events in the post-genomic era. In addition, glycosylation plays vital roles in cell-cell recognition, protein folding, stabilization, cell growth regulation, cell differentiation, immunological response, metastasis, bacterial and viral infections, etc. Therefore, it's also important to understand the biological functions of glycomes. In chemical biology and drug discovery, various chemical tools with a high affinity and a high specificity against proteins must be developed. Although peptides are an attractive class of molecules that contain protein-binding properties, they possess several undesirable flaws such as sensitivity to proteases, limited cell permeability and poor bioavailability. Thus, the development of new peptidomimetics with improved pharmacokinetic characteristics is increasingly needed. Peptoids, N-substituted oligoglycines, have emerged as attractive molecules which possess many characteristic advantages over peptides, including easy synthesis of libraries, a myriad of chemical diversity, proteolytic resistance and improved cell permeability. Especially, cyclic peptoids which usually exhibit enhanced cell permeability, higher protein-binding affinities and resistance to proteolytic degradation, are of considerable potential interest as protein ligands. Additionally, glycopeptoids as glycopeptide mimetics could also be potential chemical tools for glycomics and chemical biology. In this presentation, the several solid-phase synthetic approaches for the development of peptoid-based chemical tools including cyclic peptoids and glycopeptoids will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN2-3**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 이건형

Design and Synthesis of π -Conjugated Polymers for Molecular Actuators and Sensors

송창식

성균관대학교 화학과

Electronic properties of π -electronic materials, such as π -conjugated polymers (e.g., polythiophenes) and carbon nanotubes, depend on π -electrons; we can tune their bandgaps and electron/hole transfer rates through modifying π -electrons' energy levels. Molecular design and synthesis play a important role in controlling such π -electrons. If those π -electronic systems are coupled to well-designed molecular structures, we may create novel functions or properties. I will discuss how new properties emerge in π -conjugated polymers and small molecular systems, especially by designs at the molecular level. I will propose novel molecular structures for π -conjugated polymer actuators and sensors, and discuss their synthesis and interesting properties.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN3-1**

발표분야: The Future of Organic Chemistry

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 서홍석

Development of the Metal-Catalyzed Direct C-H Amination Reactions

장석복

한국과학기술원(KAIST) 화학과

Aryl amines are a key synthetic unit widely utilized in organic synthesis, coordination chemistry, materials science and pharmaceutical industry. Current routes to those compounds require either prefunctionalized starting materials or external oxidants, thus inevitably generating stoichiometric amounts of side wastes. We have developed direct amidation and amination reactions of arene carbon-hydrogen (C-H) bonds using sulfonyl and aryl azides as the source of the nitrogen group to release molecular nitrogen as the single by-product. The reaction is catalyzed by a cationic rhodium complex under external oxidant-free conditions, and a broad range of chelate group-containing arenes are selectively amidated and aminated with excellent functional group tolerance, thereby opening a new avenue to environmentally benign carbon-nitrogen (C-N) bond formation which can be immediately applied in synthetic chemistry, medicinal, and materials science.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN3-2**

발표분야: The Future of Organic Chemistry

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 서홍석

Organic Functional Materials

윤주영

이화여자대학교 화학·나노과학과

Supramolecular chemistry, molecular recognition and host-guest chemistry emerged as active research fields in last few decades. In this regards, the Nobel Prize in 1987 was awarded to Charles J. Pedersen, Jean-Marie Lehn and Donald J. Cram "for their development and use of molecules with structure-specific interactions of high selectivity". Especially, organic chemistry has played a key role in these research fields. Basic studies in the fields of supramolecular chemistry, molecular recognition and host-guest chemistry have been nicely applied to the development of chemosensors, molecular devices and other functional materials in recent years. Certainly, organic chemistry has been a key factor in the recent development of multidisciplinary research. Organic chemistry is also closely related to medicinal chemistry, polymer chemistry, material chemistry, etc. In the current presentation, the history of supramolecular chemistry and its successful applications in recent years will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN3-3**

발표분야: The Future of Organic Chemistry

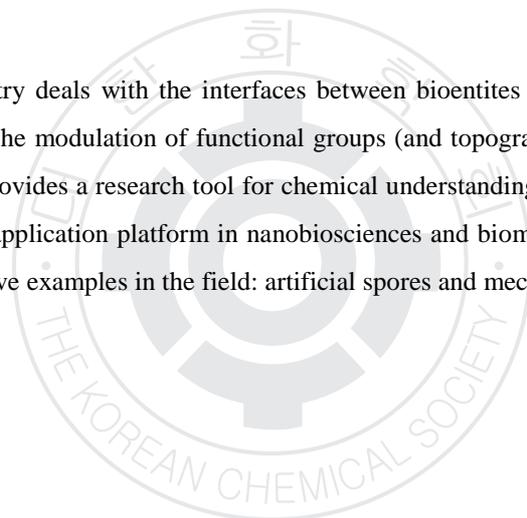
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 서홍석

Biosurface Organic Chemistry

최인성

한국과학기술원(KAIST) 화학과

Biosurface organic chemistry deals with the interfaces between bioentities (DNAs, proteins, cells, etc.) and man-made materials. The modulation of functional groups (and topography) of materials, as well as cell-surface engineering, provides a research tool for chemical understanding of biological processes, not to mention generating the application platform in nanobiosciences and biomedical engineering. This talk focuses on two representative examples in the field: artificial spores and mechanoneurochemistry.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN3-4**

발표분야: The Future of Organic Chemistry

발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 서홍석

Discovery of Novel Therapeutic Agents using Chemical Biology and Molecular Diversity

박승범

서울대학교 화학부

The importance of molecular diversity has been clearly recognized to identify specific bioactive small molecules for the elucidation of mysterious biological processes. The diversity-oriented synthesis (DOS) was introduced for efficient population of molecular diversity in untapped chemical space using complexity-generating synthetic route. To maximize the molecular diversity with high relevance in biological space, we pursued privileged-substructure-based DOS (pDOS) strategy to emphasize the importance of maximized skeletal diversity through the creative reconstruction of core skeletons containing privileged substructures. Our divergent pDOS strategy can provide an efficient approach for the discovery of novel small-molecule modulators with excellent specificity in chemical biology and drug discovery. Secondly, a systematic study of Seoul-Fluor will be presented. During our continuous efforts on the construction of drug-like small-molecule libraries using pDOS strategy, we aimed to develop a novel fluorescent core skeleton for the development of bioprobes, applicable for image-based screening. Seoul-Fluor analogs were successfully applied in HCS. Lastly, we developed a new target identification platform, FITGE, which aims to preserve protein-small molecule interactions under the intact cellular environment. After a series of failures using conventional target ID methods, we successfully identified the protein target of anti-proliferative compound with FITGE only under the live cell condition and observed the environment-dependent binding events of a functional small molecule by direct comparison between live cells and cell lysates.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-1**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 민선준

희귀질환 연구 및 치료제 개발 전략

Jangik I. Lee

연세대학교 약학대학

희귀질환이란 일반적으로 그 유병율이 인구 일만 명당 5명 이하인 질환을 말한다. 세계에는 약 7000여종의 희귀질환이 알려져 있고 학술지에 매 주 대략 5종의 새로운 희귀질환이 보고되고 있다. Orphan 의약품이란 희귀질환치료제 또는 수익성이 없어 제약회사가 생산을 기피하는 일반질환 치료제로서 정부가 지정한 의약품을 말한다. Orphan 의약품의 개발에는 여러가지 장점이 있다. Orphan 의약품으로 정부의 지정을 받으면 세금감면을 통한 연구비 지원, 임상시험 비용 지원, 신약허가 심사비 면제, 시장독점권 부여 등의 특혜가 주어진다. 희귀질환의 대부분은 단순한 유전적 결함에 의하는 경우가 많아 치료제의 표적발견이 비교적 쉬우므로 개발 성공률이 높고, 임상시험기간이 짧으며, 시판허가를 받을 확률이 높아 연구개발비용이 적게 든다. 그 결과 전세계 orphan 의약품 시장은 2009년 약 850억 달러에 이르렀고 매년 6%씩 성장하여 2014년에는 약 1120억 달러의 시장을 형성할 것으로 추정된다. Orphan 의약품 시장은 현재 매년 8.9%씩 성장하고 글로벌 시장의 51%를 점유하는 미국을 중심으로 성장해 가고 있으며, 총매출액의 64.3%가 유전자재조합의약품에 의한 것으로 알려져 있다. 이러한 의약품시장의 변화와 사회적 요구에 부응하여 한국 또한 희귀질환 치료제 개발의 활성화를 위해 재정적 지원체계를 구축하고, 허가관리를 개선하며, 법률적 제도를 완비하는 과정에 있다. 희귀질환의 치료적 타겟을 찾아 신물질이나 기존의 약물을 발굴하는 과정이 주로 대학이나 연구 중심 병원에서 이루어지고 있고 최근에는 신약의 상업화에도 대학과 병원이 크게 기여하는 추세이다. 신약개발 인프라가 취약한 제약산업의 입장에서 볼 때, 제도가 잘 정립되어 있어 성장하는 미국 의약품 시장을 겨냥하여 희귀질환 연구 및 orphan 의약품 개발을 전략적으로 수행한다면 큰 성공을 거둘 수 있을 것으로 기대된다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-2**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 민선준

Contributions of the tumor microenvironment to anti-HGF resistance

박종배

국립암센터 특수암연구과

Drug resistance has been noticed as a great challenge for most anticancer therapies, especially on targeted therapies. Many of the experimental approaches and clinical studies have implicated that the tumor-associated microenvironment contribute huge role on both a protective shield that block drug effect and a inducible microenvironment that encourages a tumor growth niche where tumor cells overcome treatment- and cancer-induced stresses. Better understanding of the effects of the tumor microenvironment on cancer cells in drug resistance condition will be essential to design new therapies aimed at targeting this tumor-protective niche. To address this question, we generated animal model for the drug resistance of anti-HGF with glioma model system. In this model we analysed genesexpression profile which was changed during the acquisition of drug resistance. Based on the species of these genes, we can separate genes which were changed in cancer cells vs stromal cells. From the results, we have found interesting molecular signature of stromal gene expression. Especially, we have identified many interesting genes which is linked to microglia signature. Here, I will discuss about the molecular cross-talk between glioma cells and glial cells during drug resistance.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-3**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 민선준

Discovery of Q203, a potent clinical candidate for the treatment of tuberculosis

김재승

한국파스퇴르연구소 의약화학그룹1

There is an urgent necessity for the development of new therapeutic options for TB. Despite existing cheap and effective treatments, TB remains a global emergency with 8.7 million new cases and 1.4 million deaths in 2011. The situation is aggravated by the HIV/AIDS pandemic and the emergence and alarming spread of multidrug-resistant (MDR) and extensively drug-resistant (XDR) TB. Therefore the development of more potent drugs that inhibit new targets and exhibit no unfavorable drug-drug interaction with anti-HIV medications or existing TB drugs is highly warranted to shorten the duration of therapy and allow the treatment of MDR and XDR TB. Institut Pasteur Korea (IP-K) in collaboration with its affiliated biotech company, Qurient, Co. Ltd., published in Nature Medicine, on the identification of a promising new drug candidate for the treatment of TB termed Q203. The novel drug candidate exhibits remarkable potency in preclinical animal models of Mycobacterium tuberculosis infection at comparably low doses and the high potency of Q203 is importantly conserved against a panel of clinically relevant M-XDR isolates. The drug constitutes a new chemical class with a novel mechanism of action targeting a protein called QcrB, which is an essential component of a vital cellular process termed 'cellular respiration' that generates the majority of a cell's chemical energy in the form of adenosine triphosphate (ATP). Q203 also demonstrates very favorable safety and pharmacokinetic profiles in rodents including a long half-life and target tissue levels suggesting a potential for shortened treatment regimens. (Nature Medicine, published online on August 4th, 2013, doi:10.1038/nm.3262)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-4**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 박기덕

Human ABC Transporters and Pharmacogenomics

이민구

연세대학교 의과대학 약리학교실

ATP-binding cassette (ABC) transporters constitute a superfamily of membrane proteins. The ABC proteins protect cells from a wide range of toxic compounds, and regulate basic biologic processes of essential organs. Consequently, mutations affecting ABC-transporters have been found to be the underlying causes for a large number of human inherited diseases including cystic fibrosis. Currently, 49 ABC transporter genes were identified in human genome and classified into 7 subfamilies according to their sequence homologies. The multi-drug resistance 1 (MDR1) and multidrug resistance proteins (MRPs) genes were originally identified as a gene that confers multi-drug resistance to cancer cells. They have a physiological role of protecting cells and organisms from various toxic substances including commonly prescribed medications. Thus, identifying the individual genetic variations of these transporters carries significant meaning in pharmacotherapy of post-genomic era, since such genetic variants are likely to be an important source for the inter-individual variability in toxicity and response of many drugs. Our results of genetic association studies revealed that genetic variations in the ABC transporters are associated with drug response and toxicity of antidepressants, antiepileptics and cardiovascular agents. Further identification of the functional genetic variations in ABC transporters and other major drug-response genes using the state-of-the-art technologies will improve the predictive value of genetic tests for tailored drug therapy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-5**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 박기덕

The discovery of XL019 as a potent and selective Janus kinase 2 (JAK2) inhibitor

김병규

LG 생명과학 기술원

Janus kinase 2 nonreceptor tyrosine kinase, a member of the JAK2 family of kinase has garnered a tremendous amount of attention in recent years since the discovery of a somatic mutation of the gene encoding JAK2. The V617F mutation occurs in the auto-inhibitory JH2 domain and is thought to disrupt its negative regulatory function. This leads to constitutive activation of JAK2, downstream signal transducer and activator of transcription (STAT), and activation of gene transcription. A frequent point mutation of JAK2 was identified in myeloproliferative disorder (MPDs) including polycythemia vera (PV), essential thrombocythemia (ET), and primary myelofibrosis (PMF). Recent approval of ruxolitinib (JAK1/2 inhibitor), developed by Incyte and Novartis, has clinically validated JAK2 for the treatment of MPDs. Not surprisingly, several JAK2 selective inhibitors have been developed and are currently being tested in clinical trials. Herein, the discovery of XL019 as a potent and selective inhibitor will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI-6**

발표분야: Current Trends in Medicinal Chemistry: Orphan Drugs

발표종류: 심포지엄, 발표일시: 목 17:15, 좌장: 박기덕

Introduction of services for high throughput screening of small molecule libraries in biological assays

최용문

(재)경기과학기술진흥원 연구개발팀

A drug discovery program involves target identification and validation, assay development and high throughput screening, hit identification, lead optimization and finally the selection of a candidate for clinical development. Gyeonggi Bio-Center has established infrastructure for high throughput screening including small molecule libraries, liquid handler, and plate reader, and provided a range of screening services to support pharmaceutical researchers to identify hit compounds in the drug discovery process. Among the well recognized services are identification of modulators of GPCR signaling, Ca²⁺ mobilization, and nuclear translocation of NFκB, and the results from the high throughput screening efforts to identify either inhibitors or stimulators of such signaling pathways will be presented during the talk.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT1-1

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 주상훈

Proving and Exploiting Catalytic Functions of Hydrogen Spillover with Well-Defined Model Catalysts

최민기

한국과학기술원(KAIST) 생명화학공학과

Hydrogen spillover has been extensively studied in catalysis field for several decades, but the nature and its catalytic functions still remain a topic of vigorous debate. Here we used well-defined Pt/LTA zeolite nanocrystals as a model catalyst for rigorously studying the catalytic functions of spillover hydrogen. LTA zeolite was chosen as a support for Pt clusters because the small pore aperture of the zeolite (0.4 nm) allows the selective diffusion of H₂ over organic molecules, which makes the catalytic interpretation very straightforward. We also deliberately control the zeolite crystallite size and the density of hydroxyl defect sites within the zeolite frameworks in order to study the effect of diffusion path length and the effect of defect sites on the migration of activated hydrogen. The results show that the presence of surface hydroxyls (e.g., Bronsted acid) and external surface area of catalysts are the governing parameters for the catalytic use of spillover hydrogen. We propose a long-range H migration mechanism mediated by Bronsted acid sites based on quantum mechanical energetics. The spillover catalysts showed very high activities in hydrogenation/dehydrogenation, but virtually zero activities in hydrogenolysis. The distinct behavior indicates that the spillover and reverse spillover can be used for the addition and subtraction of H to or from organic molecules, but cannot break C-C bonds. It is reasonable to expect that the understanding on the catalytic functions of spillover hydrogen can be used to design advanced catalysts with enhanced catalytic activities, tolerance against thermal sintering and chemical poisoning, and distinct catalytic selectivity by choosing proper supports and metal encapsulation strategies.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT1-2

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 주상훈

Structure of Nanoporous Materials and Their Physical or Chemical Properties

정낙천

대구경북과학기술원(DGIST) 신물질과학과

In this talk, two nanoporous materials - a zeotype material, ETS-10 and a metal-organic framework material, CDMOF-2 - in particular, the relationship between their structures and physicochemical properties will be presented. As a representative zeotype material which contains quantum wires, ETS-10 has been received great interests in zeolite society. In ETS-10 crystal, the TiO₃²⁻ quantum wires (QWs) are running along the [110] and [1-10] directions, respectively. Due to a large number of inherent defects, the TiO₃²⁻ QWs with varying lengths and local densities are expected to be positioned along the [110] and [1-10] directions. However, there have been no methods to analyze the distribution pattern of their relative lengths, length homogeneities, and local densities within a crystal. In this talk, how to analyze the distribution pattern of the wires in a big ETS-10 crystal will be discussed. A metal-organic framework (MOF), CDMOF-2 contains γ -cyclodextrins (γ -CDs) and Rb⁺ linker. It features reversible chemical binding of CO₂ to primary hydroxyl groups on γ -CD. As a broad, fundamental investigation, we observed high ionic conductivity, relatively, with the "as synthesized" version of CDMOF-2 following sorption of methanol as a pore filling solvent. Unexpectedly, however, a substantial decrement (~550-fold) of the ionic conductivity was rendered by the CO₂ binding. As an extension, the concentrations of chemisorbed CO₂ were varied and the electrochemical output showed a ratiometric relationship between conductance and CO₂ concentration, showing promise for a new MOF-based CO₂ sensor.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT1-3

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 주상훈

Developing Mesoporous Carbon-Based Supports for Fuel Cell Application: Surface and Framework Structures

김지만* JINXING¹

성균관대학교 화학과 ¹성균관대학교 자연과학대학 화학과

Since the first report on the successful synthesis of ordered mesoporous carbon (OMC) using a mesoporous silica template, OMCs have been of great interest due to their regular mesopore sizes, high surface areas, and high pore volumes. Vast progress has been made in the preparation of OMC materials with modified surfaces, graphitic frameworks, and pore structures, which enable their utilization for various applications such as adsorbents, catalyst supports, nano-templates, materials for advanced electronics, etc. Here, the synthesis of mesoporous carbon-based materials with controlled surface and framework structures, which play key roles for the application to catalyst supports of DMFC, will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT1-4

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 최민기

결정성 하이브리드 나노세공체 합성 및 가스흡착 응용

황영규 장종산^{1,*}

한국화학연구원 그린화학공정연구본부 ¹한국화학연구원 그린화학촉매연구센터

배위고분자로 구성된 결정성 하이브리드 나노세공체, 즉 다공성 유기-금속 골격체 화합물 MOF 는 현재 개발된 물질 가운데 표면적과 다공성이 가장 높은 초다공성 소재로서 재료화학 분야에서 가장 연구가 활발히 진행되고 있는 물질 가운데 하나이다. 하이브리드 나노세공체는 금속이온과 유기 리간드 화합물이 골격을 구성하고 있어 금속 이온과 리간드의 기능성, 소수성/친수성, 불포화 배위자리 생성, 골격 유연성 등 다양한 특성을 갖고 있어 흡착, 분리, 저장, 촉매, 센서, 멤브레인, 약물전달 등에 응용성을 갖고 있다. 본 연구팀에서는 수열안정성이 우수하고 세공구조가 독특한 새로운 하이브리드 나노세공체 물질을 개발하였고, 다양한 합성, 표면기능화 및 불포화배위자리 응용기술을 개발해 왔다. 또한 고표면적의 Fe-MOF 물질의 골격구조 내에서 철이온의 불포화 배위자리와 환원성을 동시에 조절함으로써 2 가지 산화상태를 유도하여 올레핀, 일산화탄소와 같은 불포화결합 기체의 흡착 분리능을 향상시킬 수 있었고, 기존 상업용 수분 흡착제 대비 2 - 4 배 이상의 흡착량을 나타내는 수분흡착제용 MOF 를 개발하는 등 다양한 개발 경험을 갖고 있다. 본 발표에서는 최근 화학(연)에서 수행한 하이브리드 나노세공체 합성, 기체 또는 액체의 흡착 및 분리, 저장 등에 관한 결과를 중심으로 국제적인 연구 및 기술개발 동향을 소개하고 토의하고자 한다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT1-5

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 최민기

Microporous organic networks for energy and environmental applications

손성욱

성균관대학교 화학과

In this talk, several approaches for the synthesis of microporous organic networks (MONs) will be presented. Especially, the tailored synthesis of MONs using pre-designed building blocks, tandem synthetic process based on the C-C coupling reaction and cyclization and the shape-controlled synthesis of MONs will be presented. In addition to synthetic issues, several applications of MONs for energy and environmental technologies will be introduced. First, photocatalytic chemical conversions using MONs and visible light will be presented. Second, carbon dioxide capture or chemical fixation using MONs bearing active sites will be presented. Third, the application of MONs for the template synthesis of inorganic anode materials for in lithium ion batteries will be addressed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT1-6**

발표분야: Functional Nanoporous Materials

발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 최민기

Nanoporous Materials for Gas Sorption and Separation: MOFs, Metal Oxides, and Carbons

문희리

울산과학기술대학교(*UNIST*) 친환경에너지공학부

Nanoporous materials are ubiquitous in the material sciences because of their numerous potential applications in various areas, including adsorption, catalysis, energy conversion and storage, optoelectronics, and drug delivery. For appropriate purposes, we have developed new synthetic methods of novel nanoporous materials such as metal-organic frameworks (MOFs), metal oxides, and carbon materials. In this talk, we will present a novel synthetic strategy that exploits a metal-organic framework (MOF)-driven, self-templated route towards nanoporous metal oxides and graphitic carbon materials via thermolysis under inert atmosphere. Upon temperature, guest molecules, and pressure, structural flexibility of porous MOFs studied by in situ X-ray diffraction analysis will be also discussed. These novel nanoporous materials exhibit exceptional carbon dioxide adsorption capacity as well as high gas selectivity under conditions mimicking flue gas.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT2-1

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 유효종

Shape-tuning of 2-dimensional metal nanoplates: nanodisk, nanoprism, nanofrisbee, and nanomesh

박성호

성균관대학교 화학과

We present a simple synthetic method for hexagonal Au nanoplates in pure form. Selective etching of specific facets of triangular nanoplates has led to the shape transformation. This contribution exemplifies how the site-dependent reactivity of nanoparticles can be used to fine-tune the shape of nanoparticles. The site-dependent reactivity of nanoparticles was used for selective etching and growth of specific facets by controlling experimental conditions. Also, the high quality of hexagonal Au nanoplates allows one to identify the higher-order plasmon resonance bands in addition to the dipole mode, which is important in terms of physical property characterization as well as their optical applications. Armed with the obtained synthetic strategy, we found the methodology to fine-tune the metal nanoplates by using a thin-layer of Ag as an electron shuttling mediator, leading to nanofrisbees. Additionally, we will briefly introduce two-dimensional ordered arrays of honeycomb morphology of platinum that are fabricated by using anodized aluminum oxide template and metal sputtering methods.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT2-2

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 유효종

Fabrication of size-controlled polymer vesicles through cooperative self-assembly of nanoparticles and amphiphilic polymers

박소정* Robert J. Hickey¹ Jason Koski¹ Xin Meng² Robert A. Riggleman¹ Peijun Zhang²

이화여자대학교 화학나노과학 ¹University of Pennsylvania, USA ²University of Pittsburgh, USA

The ability to fabricate size-controlled polymer vesicles is important for their biological and medical applications. Here, we present a new approach to prepare polymer vesicles with controllable diameter through the cooperative self-assembly of nanoparticles and amphiphilic polymers. Polymersomes densely packed with magnetic nanoparticles (magneto-polymersome) were fabricated with a series of different sized iron oxide nanoparticles. The binary self-assembly behavior was strongly dependent on the size of incorporated nanoparticles. The yield of magneto-polymersomes increased with increasing the diameter of incorporated nanoparticles, and the size of polymersomes was effectively controlled by varying the size of nanoparticles. In this presentation, we will discuss the origin of the unique size-dependent self-assembly behavior.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT2-3

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 유효종

Functionalization of a Hollow Nanoreactor with Catalytic Metal Nanocrystals inside the Cavity

이인수

포항공과대학교 화학과

Hollow nanoparticles that encapsulate catalytic species inside the permeable porous shell of chemically inert materials are promising candidates for nanoreactors that efficiently catalyze the chemical reactions of selected molecules while preserving the exposed surface area of the entrapped catalysts even under harsh reaction conditions or during the recycling process. To increase the potential applications of such nanoparticles in nanoreactors, it is essential to develop a new method for functionalizing the internal cavity, which allows chemical reactions to occur within the protective void space. In this presentation, I will discuss the functionalization protocol based on galvanic replacement at the Mn_3O_4 surface, which leads to the high-density deposition of ultrafine metal nanocrystals on a interior surface of the hollow silica nanosphere. The fabricated hollow nanoreactor exhibited highly enhanced activity, selectivity, and recyclability in catalyzing organic reactions, which are attributable to the synergistic combination of the porous nanoshell and the immobilized catalytic nanocrystals inside the cavity.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT2-4

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 심포지엄, 발표일시: 목 16:05, 좌장: 이민형

Light Engineering by Metal-Semiconductor Hybrid Nanostructures

송현준

한국과학기술원(KAIST) 화학과

Surface plasmon resonance (SPR) that is significantly observed in noble metals is a phenomenon involving the coupling of irradiated light and conducting electrons. It leads to intense light scattering, which is highly dependent upon the dielectric constants of conducting elements and surrounding media, as well as the morphology of conducting nanostructures. On the other hand, semiconducting nanostructures can absorb light in the ranges of UV and visible to near infrared and generate electron-hole pairs by precise tuning the band gap of the materials. Therefore, it is very interesting to investigate the plasmon and charge generation behaviors in the combined system of metal and semiconductor nanostructures. Direct contact of metal and semiconductor exhibits the complete quenching of electrons generated from the photon absorption in the semiconductor to the metal domains. The chemical conversion from metal to semiconductor leads to huge difference of the corresponding dielectric constant, which changes scattering property of the nanostructures. The introduction of plasmonic domains on metal and semiconducting nanostructures can either monitor the change occurred on the surface, or enhance the electron excitation under the visible light irradiation. Herein, we present three representative structures containing metal and semiconductor hybrids. In Au@Ag nanocubes, Ag on the shell was converted to semiconducting Ag₂S, which exhibited controllable scattering colors over a full visible range. In platinumized CdS hollow nanocubes, the introduction of Au probes could monitor the reaction progress of hydrogen generation on the Pt surface at a single-particle level. In Pt-tipped CdSe nanorods, a unidirectional single-tipped structure yielded higher catalytic activity than that of the double-tipped one on the hydrogen generation reaction. Such a well-designed combination of metal and semiconductor components would pave a new way to maximize the photoconversion efficiencies on visible photocatalysts and solar cells.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT2-5

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 이민형

Spherical nanoparticles with a silica shell and gold nanodots assembly as the core

유효종

한림대학교 자연과학대학 화학과

Highly spherical nanoparticles with a core comprising multiple gold (Au) nanodots assembly and a silica shell (multi-Au@SiO₂ NPs) 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 solution. Multiple Au nanodots with a maximum diameter of ~5 nm could be assembled and encapsulated within a silica matrix during the growth process. The size of the multi-Au@SiO₂ NPs and the number of Au nanodots doped could be controlled by varying the water-to-Brij35 ratio and the amount of the precursor of cationic gold ions. In an endeavor to develop the availability of multi-Au@SiO₂ NPs, we fabricated multiple gold (Au) nanodots core-mesoporous silica shell nanoparticles (multi-Au@mesoporous-SiO₂ NPs) through a green technology without using any surface-protective or etching agents. Thermal treatment of multi-Au@SiO₂ NPs in an aqueous media lead to generation of mesopores over the silica shell without any change in the size and number of the Au nanodots. 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 (single-Au@SiO₂ NPs and single-Au@mesoporous-SiO₂ NPs). The enhanced catalytic activity is mainly due to the efficient diffusion of reactants onto the multiple Au nanodots through mesopores within the silica shell as well as the higher surface area of multiple Au nanodots. We also present the incorporation of Au nanoclusters (Au NCs) into a porous silica matrix to generate fluorescent Au NC-doped silica nanoparticles. Stable and highly emissive Au NCs were successfully synthesized by means of stabilization with PIPES (PIPES-Au NCs, where PIPES = 1,4-piperazinediethanesulfonic acid) using a thermal synthetic strategy. By varying the amount of PIPES, two Au NCs with different emission maxima were obtained. Sequential doping of the

PIPES-Au NCs with tetraethylorthosilicate (TEOS) and 3-(aminopropyl)triethoxysilane (APTS) furnished a double-layer silica matrix, which effectively protected the PIPES-Au NCs during repeated washing with aqueous solvent and the composite of which exhibited enhanced emission.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT2-6**

발표분야: Synthesis and Application of Particulate Nanomaterials

발표종류: 심포지엄, 발표일시: 목 16:55, 좌장: 이민형

Nanocrystal Quantum dots for Photovoltaics: Understanding the Size-dependent Stability

정소희

한국기계연구원 나노기계연구본부

Lead chalcogenides have been extensively investigated lately with a hope for realizing next-generation photovoltaics. Their large exciton Bohr radius provides strong confinement effects, and the band gap tunability from infrared to ultraviolet could enable a multi-junction solar cell absorbing entire solar spectrum. Furthermore, a successful utilization of high energy photons above band gaps could promise a single-junction solar energy conversion efficiency over the Shockley-Queisser limit. In spite of these advantages as light absorbing materials for next-generation solar cells, a working device has long been a challenge because of uncontrolled surface defects and thus degradation during post-processing for device fabrication. Here, the microscopic understanding of QD surface chemistry exclusively derived from ultrasmall PbS QDs will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC-1**

발표분야: Recent Advances in Electrochemiluminescence (ECL) Technique

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 김종원

미정

정택동

서울대학교 화학부

미정



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC-2**

발표분야: Recent Advances in Electrochemiluminescence (ECL) Technique

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김종원

Molecularly electrochemiluminescent sensor for in-vitro analysis

신익수* 김효기 서혜진

승실대학교 화학과

Recently, electrochemiluminescence (ECL) have made significant advances in chemical analysis such as DNA determination, immunoassay, food testing, and biowarfare determination. As it possesses the simplicity of electrochemistry and the inherent sensitivity and wide linear range of chemiluminescence method, tremendous effort has been devoted to develop new analytical techniques based on ECL. Our group has studied the ECL analysis, and in the talk I will review some of our recent results on it. In our approach, no separation or washing step which was typically needed in ECL analysis was required. Instead, we designed a molecular probe which selectively recognized a specific target generating (or attenuating) the ECL emission upon the presence of the target. These results propose a proof-of-concept for the molecularly ECL sensor for in-vitro analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC-3**

발표분야: Recent Advances in Electrochemiluminescence (ECL) Technique

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 김종원

How can we enhance electrochemiluminescence (ECL)?

김주훈

경희대학교 화학과

Here, we report on the electrochemical grafting of amine-terminated dendrimers encapsulating nanoparticles onto indium tin oxide (ITO) surface, which can be applied for sensitive electrochemiluminescence-based assays. Specifically, we prepared two different dendrimer-encapsulated nanoparticles (DENs), Pt and Au DENs, using amine-terminated sixth generation polyamidoamine dendrimers, and subsequently immobilized the DENs onto ITO surfaces via electrooxidative grafting of the terminal amines of dendrimers to the surfaces. Electrochemical experiments and X-ray photoelectron spectroscopy (XPS) confirmed that the DENs were electrochemically grafted onto the ITO surface and not just physisorbed. The resulting DEN-modified ITOs exhibited highly improved catalytic activity for electrochemical oxidation of Ru(bpy)₃²⁺ (bpy, 2,2'-bipyridine)/ tri-n-propylamine (TPrA), leading to significantly increased electrochemiluminescence (ECL) emission while preserving the good optical transparency of ITOs.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC-4**

발표분야: Recent Advances in Electrochemiluminescence (ECL) Technique

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 방진호

Electrochemistry and Electrogenerated Chemiluminescence of Organic Nanoparticles

석정돈 Allen J. Bard^{1,*}

한국화학연구원 차세대전지소재연구그룹 ¹University of Texas at Austin

Electrogenerated chemiluminescence (ECL) is a type of luminescence which involves the generation of oxidized and reduced species, radical ions, which undergo a fast electron transfer at electrode surfaces to produce an excited state. The electrochemical and emission properties of organic nanoparticles (NPs) have been the subject of relatively few studies compared to inorganic NPs. For inorganic materials the physical and chemical properties observed in the corresponding bulk forms are very different when the particle size is reduced to the nanometer regime. The size effect of the properties of organic NPs is not expected to produce large changes in characteristics compared to the bulk crystal, because electrons are largely confined within single molecules and do not delocalize or transfer over nanometer and micrometer domains. In principle, organic NPs might have practical applications because their fluorescence spans a wide wavelength region. ECL studies were performed on several interesting compounds. Several new anthracene derivatives such as a variety of 2- and 4-fold anthracene-functionalized tetraarylbimesityls and a series of 9-naphthylanthracene based dimer and trimer were studied. They showed one wave on the oxidation and reduction because of a sequence, two or more electron transfers during the annihilation of the radical ions. Depending on the structure, some of them exhibited excimer formation on ECL spectra. Azide-BTA compound which consists of two triphenylamine and 2,1,3-benzothiadiazole groups at the ends bridged by a fluorene moiety was synthesized and examined. The compound is a newly synthesized D-A-?-A-D molecule which had reversibility upon electrochemical oxidation and reduction, and also showed intense red fluorescence and stable red ECL emission. Using a simple reprecipitation method, well-dispersed and spherical organic nanoparticles of Azide-BTA and 9-naphthylanthracene based dimer were prepared in an aqueous solution. Controlling the preparation condition, the size of nanoparticles can be minimized to 15 nm. Especially we prepared the organic nanoparticles of 9-naphthylanthracene based

dimer dispersed in organic solvent, MeCN, one of the preferred solvents for electrochemical studies and ECL.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC-5**

발표분야: Recent Advances in Electrochemiluminescence (ECL) Technique

발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 방진호

Biosensing of Determination of Glycated Hemoglobin (HbA_{1c}) Based on Boronic Acid Modified Gold Electrode and Luminol Chemiluminescence

이원용

연세대학교 화학과

Diabetes, a disorder in the metabolism of glucose due to the lack or inability to use insulin to regulate the glucose level, is one of the major health concerns worldwide. Therefore, the monitoring of glucose level is necessary to diabetic patients. Hemoglobin A1c level has been used as one of the reliable markers of glycemic control. The detection of hemoglobin A1c is very important because it indicates the average blood glucose level over 3 months. A chemiluminescence flow injection system was used to detect the hemoglobin A1c containing iron inside. In this study, we have used luminol chemiluminescence in the presence of H₂O₂, to measure Fe content inside of hemoglobin A1c. First, hemoglobin A1c was selectively bound into the SAM of boronic acid on a gold electrode surface, and then luminol and H₂O₂ were flown into the observation cell where the CL reaction take place and the light is measured. The present sensor responded linearly to HbA1c in the wide % range from 2.5% to 17% with a good sensitivity. Furthermore, the HbA1c % in human plasma samples was successfully determined and compared to the result obtained with other methods. Therefore, the chemiluminescence flow injection system detection of HbA1c sensor might be applied for the determination of HbA1c in the human blood samples.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR1-1**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 박현웅

Photocatalytic CO₂ Reduction in Ionic Liquids

최지나 김범식*

한국화학연구원 환경자원연구센터

Photocatalytic reduction of CO₂ to value-added chemicals or fuels by using solar energy is an attractive but still a challenging process to address both energy and environmental issues. Photocatalytic CO₂ reduction has been mostly conducted by TiO₂-based photocatalysts in aqueous solution. However, the solubility of CO₂ in water is very low and it causes low conversion efficiency and a problem for practical application. Here, we have investigated the ionic liquid-mediated system for the photocatalytic and (photo-)electrochemical CO₂ reduction since CO₂ solubility in ionic liquids is relatively high. We have developed the synthetic system of high purity (>99.9%) ionic liquid and several physicochemical/photochemical properties of ionic liquids, which should be considered for the photocatalytic CO₂ reduction, have been also investigated. The synthesized ionic liquids have been used as a reaction medium and it was observed that the photocatalytic CO₂ reduction could effectively occur in ionic liquid system.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVRI-2**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 박현웅

New Manganese Phosphate Crystal as Water Oxidation Catalyst

남기태

서울대학교 재료공학부

Splitting water to generate hydrogen and oxygen is one of the promising pathways for solar to energy conversion. The oxygen evolution reaction (OER) has been regarded as a major bottleneck in the overall water splitting process due to the high activation energy barrier for O-O bond formation and the slow transfer rate of four electrons. Therefore, the development of water oxidation catalyst has been a demanding challenge to realize overall water splitting systems. Interestingly, nature has a water oxidation complex (WOC) in photosystem II (PSII) comprised of the earth-abundant elements Mn and Ca which generates oxygen efficiently under neutral condition. The asymmetric geometry and flexible ligation of the biological Mn_4CaO_5 cluster are important properties for the function of photosystem II, and these properties can be applied to the design of a new inorganic water oxidation catalyst. Inspired from the WOC in nature, we identified a new crystal structure, $Mn_3(PO_4)_2 \cdot 3H_2O$, that precipitates spontaneously in aqueous solution at room temperature and demonstrated its superior catalytic performance at neutral pH. Computational analysis indicated that phosphate ligations in our crystal make Mn-O bonding longer and more distorted than in other Mn-based oxides. Such structural flexibility can stabilize Jahn-Teller distorted Mn(III) and thus facilitate Mn(II) oxidation, as monitored by electron paramagnetic resonance spectroscopy. This study provides valuable insights into the interplay between atomic structure and catalytic activity.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR1-3**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박현웅

Electrochemical Synthesis of Photoelectrodes for Efficient Photoelectrochemical Water Splitting

박이슬

대구경북과학기술원(DGIST) 에너지연구부

Development of efficient and practical photoelectrodes for use in a water splitting photoelectrochemical cell involves simultaneously satisfying multiple requirements, which remains a challenge. The photoelectrode must absorb visible light, preferably with a direct bandgap transition, and then efficiently separate and utilize the photogenerated carriers to drive desired reactions. In addition, it is important to develop simple and low-cost methods for electrode preparation. One promising photoanode material is bismuth vanadate (BiVO_4), an n-type semiconductor with a direct bandgap of 2.4 eV and the appropriate valence band position for O_2 evolution. Its conduction band edge position and flat band potential are fairly negative compared with most other narrow bandgap (i.e., $E_g < 2.6$ eV) oxide-based photoanode materials, located just short of the thermodynamic level for H. As a result, complete water splitting with BiVO_4 requires only a small amount of external bias. On the other hand, p-type CuFeO_2 is promising photocathode which has a suitable conduction band position to photoreduce water to H_2 while having a bandgap that utilizes the entire range of visible light ($E_g = 1.5\text{-}1.6$ eV). In this study, a new electrodeposition route is proposed to produce n-type BiVO_4 photoanode and p-type CuFeO_2 photocathode for the water splitting. Electrodeposition has the distinctive advantages of being simple, low cost, and easily scalable while enabling deposition of the material of interest only on the conductive substrate and not on the chamber wall. BiVO_4 is doped with Mo^{6+} to improve the electron transport by increasing the carrier density. The electrochemical route provided an effective way of doping BiVO_4 , and the optimally doped sample increased the electron-hole separation yield from 0.18 to 0.58 at 0.6 V vs. RHE, which is a record high separation yield achieved for BiVO_4 -based photoanodes. Various photoelectrochemical properties of the p-type CuFeO_2 photocathode were investigated and its photoelectrochemical hydrogen production was confirmed by gas chromatography.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR1-4**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 박이슬

Efficient Solar Light Harvesting: Electricity Generation and Hydrogen Production

박종혁

성균관대학교 화학공학부

The development of new types of energy generation devices is promoted by increasing public awareness that the Earth's oil reserves could run out during this century. As the energy needs of the planet are likely to double within the next 50 years, the stage is set for a major energy shortage, unless renewable energy can cover the substantial deficit left by fossil fuels. Our group has developed new methods to increase light harvesting efficiency to generate electricity and hydrogen production from solar light by applying nano-concepts to materials and/or devices. Some of these approaches could be used as to form nanostructured active materials for organic solar cells, dye-sensitized solar cells and photoelectrochemical cells. In this seminar, the unique materials and processes for efficient solar water splitting will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVRI-5**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 박이슬

Nanoporous Si for H₂ Production by Photoelectrochemical Water Splitting

오지훈

한국과학기술원(KAIST) EEWS

Hydrogen production at a semiconductor/water interface by photoelectrochemical (PEC) reaction is a promising route to direct conversion of solar energy to a storable and clean fuel. For PEC H₂ production on a semiconductor using only sunlight and water, materials must have energy bandgap > 1.23 eV, its conduction and valence band edge must straddle the water reduction and oxidation redox potentials, it must operate over long time without corrosion, and it must be earth-abundant. While various materials and systems have been tested for PEC H₂ reaction, unfortunately, very few materials and systems meet those stringent requirements. Silicon is an earth-abundant and environmentally benign element and has a promising band edge position for H₂ evolution reaction. Therefore, it can be used to build un-assisted water splitting system combining a metal oxide photoanode or external photovoltaic cells. However, Si suffers from high reflection (about 25 %) of incident solar photon that can not be used to produce H₂. In addition, charge transfer rate at Si/water interface to produce H₂ is sluggish. Here, we report that a nanoporous Si photocathode can significantly improve the H₂ production rate by minimizing reflection and also enhance the sluggish charge transfer rate at the nanoporous layer. We also present various approaches to further improve the PEC H₂ reaction by modifying a Si photocathode. We will also present recent results on stability of silicon photoelectrode in water during PEC reaction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR1-6**

발표분야: Solar Fuel Production: Challenge, Evolution, and Advancement Towards the Future

발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 박이슬

Semiconductor Nanowire for Solar Water Splitting

황윤정

한국과학기술연구원(KIST) 청정에너지 연구센터

One-dimensional nanostructure such as nanowire is a promising geometry for photoelectrochemical (PEC) application in light absorption and charge separation. Nanowire allows light absorption and transport of charge carriers along the wire while hole-electron pairs can be separated across the wire with short travel distances. Si/TiO₂ heterojunction shows the nanowire arrays give enhanced photoanodic current compared to thin film because of the higher surface area and the reduced reflection. The suggested charge separation within dual band gap system was observed with specially designed Si/TiO₂ asymmetric nanowire in a single nanowire level. The observed charge separation is desirable for the hydrogen reduction on Si surface and water oxidation on TiO₂ surface. We also demonstrate the charge collection efficiency can be improved when the surface of the hydrothermally grown TiO₂ nanowire was coated with atomic layer deposition (ALD) TiO₂ shell. The epitaxial grains of ALD shell contribute to increase the quantum efficiency in short wavelength region where poor charge collection limits the quantum efficiency. Based on the previous studies, this talk suggests a design of the nanostructured photoanode for solar to fuel conversion.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-1

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 한승희

Potential applications of zero-valent magnesium in environmental remediation

이기현

연세대학교 지구시스템과학과

Zero-valent magnesium (ZVMg) was tested as a reductant for the removal of Cr(VI) from water. The kinetics of ZVMg dissolution and of Cr(VI) reduction by ZVMg were examined in a simple electrolyte solution (10 mM NaCl) with 50 mM MOPS buffer at pH 7 with varying doses of reactants. The dissolution of ZVMg obeyed a first order kinetics with respect to $[Mg^0]_0$ with a rate constant, $k_{Mg} = 1.05 \pm 0.06 \times 10^{-2} \text{ min}^{-1}$. Cr(VI) was effectively removed from solution via reduction not directly by ZVMg but by an intermediate product of ZVMg-water interaction. The reduction of Cr(VI) mediated by ZVMg was rapid and followed a fractional order ($n = 0.19$) with respect to $[Cr(VI)]_0$ and the observed rate constant was determined as $k_{obs} = 1.07 \times 10^{-6} \text{ M}^{0.81} \text{ min}^{-1}$. The results showed a potential that ZVMg may be employed as an effective reductant for the treatment of various redox-sensitive contaminants.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-2

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 한승희

X선흡수분광법을 이용한 몬모릴로나이트 층간 구리(II)의 배위 연구

현성필

한국지질자원연구원 지구환경연구본부/지하수연구실

평운성 점토 광물인 몬모릴로나이트 층간의 구리(II) 배위를 연구하였다. 산성의 pH 조건에서 몬모릴로나이트 층간에 삽입한 층간 구리를 X 선흡수분광법, 전자상자성공명, 그리고 X 선회절법을 이용하여 분석하였다. 실험적으로 측정된 XANES 와 EXAFS 스펙트럼을 Feff 코드를 이용하여 순이론적(*ab initio*) 계산으로 재현하였다. 층간 구리의 배위 상태는 층간의 수화 상태와 구리 부하량(*loading*)에 의해 변화하였다. 구리로 포화된 완전히 수화된 몬모릴로나이트는 특징적인 단일선의 1 차 도함수 XANES 스펙트럼을 가진다. 계산 결과는 이 단일선이 층간 구리 원자에 결합된 물 분자의 정팔면체 배위에 기인함을 제안한다. 다른 모든 시료와 표준 물질들—구리 포화 탈수 몬모릴로나이트, 구리 불포화 수화/탈수 몬모릴로나이트, 구리 수용액 이온, 질산염구리, 수산화구리 침전물—은 모두 이중선의 1 차 도함수 XANES 스펙트럼을 가진다. 이는 양-텔러 효과에 의해 축 방향으로 신장된 팔면체 배위와 사각 평면 배위 구조에 기인한다. 축 방향 산소 결합 길이의 함수로 계산한 EXAFS 스펙트럼은 축 방향 결합 산소에 의한 후방 산란과 수평 방향 결합 산소에 의한 후방 산란의 상쇄 간섭이 정방 배위에서 예상되는 6 보다 낮은 산소 배위수를 야기함을 보여준다. 전자상자성공명과 X 선흡수분광법은 완전히 수화된 불포화 층간의 구리가 수용액 중의 구리와 유사한 배위 상태를 가지며, 탈수된 층간에서는 사각 평면 배위체를 형성함을 보여준다. X 선회절로 결정한 구리로 포화된 몬모릴로나이트의 d_{001} 층간 거리는 수화된 몬모릴로나이트와 탈수된 몬모릴로나이트가 층간에 각각 평균적으로 네 층과 한 층의 물 분자를 가짐을 보여준다. 이 연구는 층간 구리(II)가 정팔면체 배위, 축 방향으로 신장된 정방 배위, 그리고 사각 평면 배위를 가지며 구리 부하량과 수화 정도에 따라 이들

배위 구조가 서로 호환됨을 보여준다. 층간 구리(II)의 정팔면체 배위는 이 연구에서 새롭게 제안되었다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-3

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 한승희

Sorption Mechanism of Iodine Species by Black Carbon

정성욱

포항공과대학교 첨단원자력공학부

Natural organic matter (NOM) plays an important role in determining the fate and transport of iodine species such as iodide (I^-) and iodate (IO_3^-) in groundwater system. Although NOM exists as diverse forms in environments, prior iodine studies have mainly focused on uptake processes of iodide and iodate to humic materials. This study was conducted to determine the iodide and iodate uptake potential for a particulate NOM (i.e., black carbon [BC]). A laboratory-produced BC and commercial humic acid were used for batch experiments to compare their iodine uptake properties. The BC exhibited >100 times greater uptake capability for iodide than iodate at low pH~3, while iodide uptake was negligible for the humic acid. The uptake properties of both solids strongly depend on the initial iodine aqueous concentrations. After uptake reaction of iodide to the BC, X-ray Absorption Fine Structure spectroscopy results indicated that the iodide was converted to electrophilic species, and iodine was covalently bound to carbon atom in polycyclic aromatic hydrocarbons present in the BC. The computed distribution coefficients (i.e., K_d values) suggest that the BC materials retard significantly the transport of iodide at low pH in environmental systems containing even a small amount of BC.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-4

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 한승희

Cation exchange of Co^{2+} -substitued zeolite X: thermal treatment effect

정훈영

부산대학교 지질환경과학과

Heavy metals and nuclides are effectively sequestered by zeolite due to the high cation exchange capacity. However, the sequestered cations by zeolite are likely to be re-exchanged by other cations (Ca^{2+} , Mg^{2+} , Na^+) in groundwater. Consequently, it is of environmental significance to understand the mechanism involved in re-exchange reactions to predict the fate and behavior of the metal cations sequestered by zeolite. In the present study, a series of cation exchange experiments were performed by equilibrating Co^{2+} -substitued zeolite X (Co-X) in concentrated CaCl_2 solutions. The radioactive isotope of cobalt ($^{60}\text{Co}^{2+}$), present in low-to-intermediate level nuclear wastes, is subjected to radioactive decay, altering the physicochemical properties of zeolite by producing heat and irradiation. To simulate such effects, Co-X was thermally treated at 400 and 600°C prior to re-exchange experiments. At the higher treatment temperature, the re-exchanged amount of Co^{2+} in Co-X by Ca^{2+} was found to decrease. From X-ray diffraction, the re-exchange reaction led to little change in the zeolite crystallinity for thermally untreated samples, but the significantly decreased crystallinity was resulted in among re-exchanged, thermally treated samples. Nonetheless, ^{27}Al MAS NMR spectra of all re-exchanged samples indicated that the peaks corresponding to 4-fold coordinated Al became broader along with their positions shifting as a result of the re-exchange, suggesting that the re-exchange reaction caused a short-order structural distortion for both thermally untreated and treated samples. Also, Co-K edge X-ray absorption spectroscopy (XAS) was employed to examine the mechanism associated with the re-exchange. By comparison of XAS spectra between re-exchanged samples and model compounds, Co^{2+} was thought to be either present as an extraframework cation within zeolite or incorporated into a cobalt hydrotalcite ($\text{Co}_6\text{Al}_2(\text{OH})_{16}(\text{A}^n)_{2/n}$ where A^n is an interlayer anion) phase. The relative contribution of an extraframework Co^{2+} versus cobalt hydrotalcite in re-exchanged samples was determined by the least squares fitting of EXAFS spectra. The formation of cobalt hydrotalcite became more intensive with the

increasing treatment temperature. In conclusion, thermal distortion of zeolite promoted the dealumination of zeolite and the subsequent formation of cobalt hydroxide.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-5

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 현성필

Extracellular electron shuttle-mediated biotransformation of contaminants

권만재

한국과학기술연구원(KIST) 환경연구그룹

This presentation will discuss the potential for extracellular electron shuttles (EES) to stimulate the reduction of Fe(III), cyclic nitramines (e.g., hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)), or U(VI) in the presence of Fe(III)- and/or EES-reducing microorganisms. EES have been proposed as an electron transfer mediator between microorganisms and solid-phase minerals to stimulate Fe(III) reduction by eliminating the need for physical contact between the cell and the Fe(III) (hydr)oxide. EES can be present as synthetic compounds (e.g., anthraquinone-2,6-disulfonate (AQDS)), naturally occurring compounds (e.g., humic substances) and/or as microbially produced and excreted compounds (e.g., flavin mononucleotide (FMN) and riboflavin by *Shewanella* species). Our studies demonstrated that Fe(III)- and EES-reducing microorganisms utilized EES to stimulate contaminant reduction at rates significantly faster than those previously reported. In addition, contaminant reduction was directly stimulated by the EES in Fe(III)-poor environments and indirectly stimulated by reactive minerals such as magnetite in Fe(III)-rich environments. The approach for contaminant reduction with EES will provide an opportunity to study the complexity of subsurface systems, thereby providing a more thorough understanding of the coupled biological and geochemical processes controlling the fate and transport of various contaminants.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-6

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 현성필

Biotransformation of Fe(III)-containing minerals and its effect on contaminant degradation

배성준

한국과학기술원(KAIST) 건설 및 환경공학과

The bioreduction of Fe(III)-containing minerals by iron-reducing bacteria has been an active area of research due to the formation of reactive Fe(II)-containing minerals such as magnetite and green rust. This biotransformation of Fe(III)-containing minerals has been shown to be significantly affected by electron transfer mediators (ETMs) which can enhance the bioreduction of Fe(III)-containing minerals. ETMs can be divided by exogenous (mostly quinones) and endogenous (mostly flavins) ETM which is introduced/formed by natural organic matters and bacteria, respectively. In this study, bioreduction of lepidocrocite (γ -Fe₃O₄) by *Shewanella putrefaciens* CN32 (CN32) was examined in the presence of different types of ETMs. A variety of Fe(II)-containing minerals (i.e., green rust, vivianite, and goethite) formed depending on the types of ETMs and Fe(II) production rate was found as a key factor controlling the formation of specific secondary mineral phases. The degradation of carbon tetrachloride (CT) was also conducted using Fe(III)-containing minerals (i.e., magnetite and lepidocrocite) with CN32. The dechlorination of CT was significantly enhanced by magnetite and lepidocrocite with CN32 compared to the microbial transformation of CT by CN32. Chloroform, carbon monoxide, and formate were measured as main products for the degradation of CT. The results of X-ray diffraction and electron microscope analysis and transformation products of CT suggest that biogenic vivianite can play a pivotal role for the enhanced dechlorination of CT in this study.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-7

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 현성필

Accelerated Geochemical Processes in Ice and their Environmental Impacts

김기태 최원용^{1,*}

한국해양과학기술원 부설 극지연구소 극지기후연구부 ¹포항공과대학교 환경공학부

The understanding of redox processes in the environment is an important part in environmental chemistry and provides basic information for preserving and remediating the affected environment. The redox speciation of inorganic compounds controls their mobility, bioavailability, toxicity, and environmental fate. Geochemical reactions and mechanisms in aquatic environments have been extensively investigated but those in ice phase have rarely been studied despite their importance in the environment, especially in the cold regions (e.g., upper troposphere, permafrost, polar/high latitude environment, and midlatitudes during winter season) where freeze-thaw cycles take place. In this talk, the unique and interesting geochemical processes accelerated in ice media (dissolution of iron oxides and manganese oxides in ice under dark and irradiation conditions, simultaneous conversion of Cr(VI)/As(III), oxidation of iodide, and iron oxide dissolution by iodide) will be visited

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR2-8

발표분야: Current Topics in Environmental Geochemistry

발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 현성필

Hg(II) reduction by reduced natural organic matter in anoxic environments

한승희

광주과학기술원(GIST) 환경공학과

Divalent Hg reduction in anoxic water and sediment may limit the production of monomethylmercury, a highly toxic and bioaccumulative form of Hg. Based on literature reviews, natural organic matter (NOM) seems to play an important role in microbial metal reduction, e.g., Fe(III), As(V), U(VI), and Tc(VII), as extracellular electron shuttles; however, the possibility of Hg(II) reduction by NOM electron shuttles is largely unknown. Current study describes the results of laboratory experiments designed to identify the role of NOM (Suwannee River humic and fulvic acids, and Elliott soil humic acid) in microbial and chemical Hg(II) reduction. In the microbial Hg(II) reduction test using *Shewanella oneidensis* MR-1, Hg(II) reduction efficiency was significantly increased in the presence of NOM, possibly due to quinone electron shuttles. In the chemical Hg(II) reduction, NOM composition, particularly free radical content, was critical in determining Hg(II) reduction efficiency. The ubiquitous presence of natural NOM and their active involvement in bacterial electron flow suggest that quinone-containing NOM may play a significant role in anaerobic Hg(II) reduction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS1-1**

발표분야: ICT 미래소재 심포지엄(Flexible, Touch) - 감성은 부드럽게 Touch하고, 생각은 Flexible하게!

발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 권장혁

금속 소재를 이용한 고 투과 터치센서 제조기술

양대근 곽민기^{1,*} 서대식

연세대학교 ¹전자부품연구원

요즘 스마트폰 및 Tablet PC 의 입력장치로 사용되는 터치센서는 정전용량방식의 터치(Projected capacitive touch)가 사용된다. 정전용량 방식의 터치센서는 투명전극이 형성된 필름 기판을 사용하는 타입(GFF, GF2, GF1), 필름기판과 유리 기판을 사용하는 타입(G1F), 유리 기판만을 사용하는 타입(GG, GG2, G2)등으로 분류된다. 이와 같은 터치센서들은 주로 투명 전도막으로 ITO(Indium Tin Oxide) 박막을 사용한다. 투명 전도막, 즉 ITO 박막은 저항이 낮고, 고 투과 특성을 가지기가 어렵다. 따라서 본 연구에서는 저항이 낮은 금속 소재를 이용하는 고 투과 특성을 가지는 터치센서(Projected capacitive touch sensor)를 제작하여 전기 광학적 특성을 조사하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS1-2**

발표분야: ICT 미래소재 심포지엄(Flexible, Touch) - 감성은 부드럽게 Touch하고, 생각은 Flexible하게!

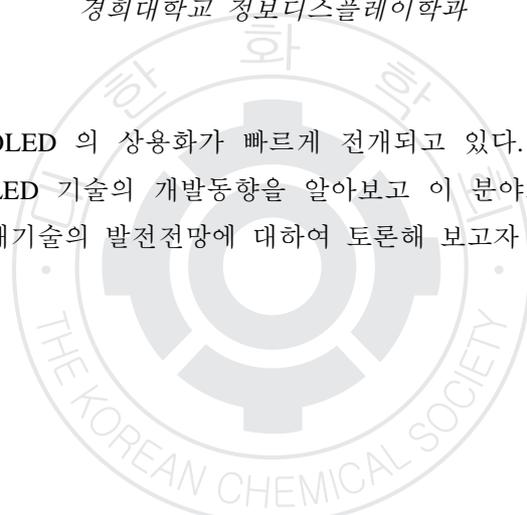
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 박상희

Flexible OLED 기술개발 동향

권장혁

경희대학교 정보디스플레이학과

최근 들어 flexible AMOLED 의 상용화가 빠르게 전개되고 있다. 현재 개발되어 상용화가 추진중인 flexible AMOLED 기술의 개발동향을 알아보고 이 분야가 가지고 있는 문제점과 향후 개발해야 되는 미래기술의 발전전망에 대하여 토론해 보고자 한다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS1-3**

발표분야: ICT 미래소재 심포지엄(Flexible, Touch) - 감성은 부드럽게 Touch하고, 생각은 Flexible하게!

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 권장혁

고해상도 대면적 산화물 TFT

박상희

한국전자통신연구원

지난 8 여년간 눈부신 발전에 힘입어 모바일용 고해상도 TFT-LCD 와 대면적 AMOLED 의 양산제품에 산화물 TFT 가 구동소자로 진입하였다. 산화물 TFT 가 기존 Si 기반의 TFT 의 시장을 대체하여 최근 디스플레이의 큰 이슈인 고해상도, 대면적, 플렉시블 디스플레이에 사용되기 위해 반드시 개발되어야 할 BCE TFT 와 Self-align TFT 소자 구조 및 이를 확보하기 위한 반도체, 저저항 배선 및 이들의 에천트 및 플라스틱 기판 등의 이슈들에 대해 고민해본다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS1-4**

발표분야: ICT 미래소재 심포지엄(Flexible, Touch) - 감성은 부드럽게 Touch하고, 생각은 Flexible하게!

발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 권장혁

Flexible Display용 기판 및 Encapsulation 기술

윤종근

LG Display

차세대 미래 Display 인 Flexible OLED Display 에 사용되는기판 종류 및 제작기술을 알아보고,
Flexible OLED 에 사용할 수 있는 Encapsulation 최신 기술을 소개함.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS2-1**

발표분야: 국가와 기업이 원하는 과학기술 인재상

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 석차옥

화학산업발전전략과 한국화학연구원의 비전

김재현

한국화학연구원

- 화학산업의 해외 동향
- 산업의 화학화(chemicalisation)
- 한국의 화학산업 성과와 문제점, 주요 이슈
- 우리나라 화학산업의 미래발전전략과 주요 과제
- 한국화학연구원의 역할
- 우수인재 육성의 필요성과 여성 과학기술인의 역할

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **KCS2-2**

발표분야: 국가와 기업이 원하는 과학기술 인재상

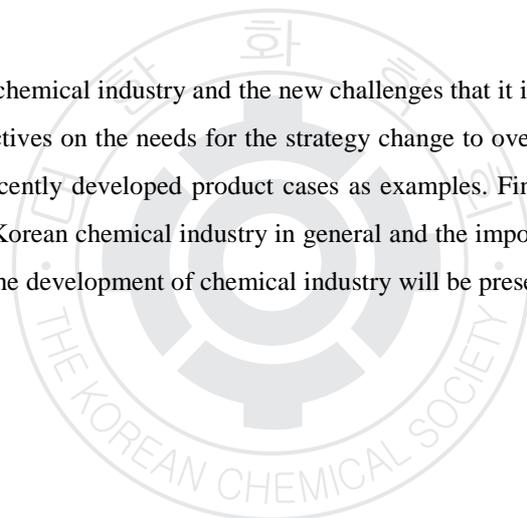
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 석차욱

Korean chemical industry and technology innovation

유진녕

LG화학기술연구원 기술연구원장

The importance of Korean chemical industry and the new challenges that it is facing for the future will be discussed. Personal perspectives on the needs for the strategy change to overcome the challenges will be shared with LG Chem's recently developed product cases as examples. Finally, the directions of future technology innovation for Korean chemical industry in general and the importance of human resources in science & engineering for the development of chemical industry will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-1**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 민사훈

Mussel-inspired adhesive polymer as a binder of Li-ion batteries

김선진 이해신*

한국과학기술원(KAIST) 화학과

In recent decades, rising of oil price caused global energy problem and induced technical progress of alternative of fossil fuels. The development of electric vehicles (EVs) is expected to replace existing automobile which uses petroleum as a fuel. To commercialize EVs, high-performance rechargeable batteries are required. Lithium-ion batteries (LIBs) are considered as power supply of EVs, however, it still needs to be improved for higher energy density and longer cycle life. There have been many researches using Silicon(Si) particles as an anode material because of its higher capacity than that of graphite, which is commercially used in Li-ion batteries. However, Si anodes has poor cycling performance due to its dramatic volume expansion and contraction during the Li alloying-dealloying processes. To improve the stability of electrode, polymeric binders are added for binding Si particles. In this study, we synthesized a new polymer, alginate-catechol (Alg-C) for effective binding performance. Alginate is a polymer that contains more hydrogen bonding sites than conventional binder, and catechol is a well-known adhesive moiety inspired by adhesive mussel foot proteins. The synthesized catechol-conjugated polymer presents excellent wet-resistant adhesion, and single-molecule adhesion force of the polymer was measured in atomic force microscopy (AFM). Alg-C binder LIBs showed higher capacity and better cyclic performance than that of conventional binder batteries.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.O-2

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 민사훈

Complex Arrays of Titania Nanostructures and Metal Nanoparticles Fabricated by Diblock Copolymers and Their Micelles

김성수 손병혁*

서울대학교 화학부

Integration of nanostructures of semiconductors and metallic materials is of interest due to their potential applications in opto-electronic, photonic, magnetic, and chemical devices. To take full advantage of both nanostructured materials, controlled placement of two nanomaterials having different shapes and sizes in large area is highly desirable. One of effective ways to locate nanomaterials can be the utilization of self-assembled nanostructures of diblock copolymers. Diblock copolymers spontaneously assemble into periodic nanostructures, of which the size and morphology can be controlled by the molecular weight and composition of copolymers. In addition, diblock copolymers form nanometer-sized micelles consisting of a soluble corona and an insoluble core in a selective solvent for one block of copolymers. Diblock copolymers and their micelles can be coated on solid substrates to form nanostructured thin films, which can be used as nanotemplates to generate a variety of arrayed nanostructures including particles, cylinders, and lamellae. In this work, we first created cylindrical or lamellar nanostructures of semiconductor titania using perpendicular nanodomains of diblock copolymers in thin films. Then, these titania nanostructures were employed as templates to direct the arrangement of nanoparticles synthesized by diblock copolymer micelles, leading to complex arrays of titania nanostructures and metal nanoparticles.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-3**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 민사훈

Bio-inspired hybrid material for selective oil-spill capture

NAGAPPANSARAVANAN 하창식*

부산대학교 고분자공학과

The bio-inspired materials have been considerable interest in the recent days for their wide variety of usage in various applications. We carried out a pioneer work at the preparation of more fascinating bio-inspired material with superhydrophobic, superoleophilic properties using siloxane polymer and leaf powder hybrid. Our hybrid suspension can produce superhydrophobic properties instantaneously by simple casting the suspension followed by the evaporation of solvents (within few mins). The surface shows almost complete superhydrophobicity (water contact angle (CA) $> 175^\circ$) on a variety of substrates and superoleophilicity (oil CA $< 5^\circ$) for various oils and excellent non-stick and self-cleaning properties. The bio-inspired hybrid material showed excellent thermal stability and mesoporous structure, and became superhydrophilic on curing at 600°C . A dip coated hybrid poly(dimethylsiloxane) (PDMS) sponge exhibited very high selectivity and absorption capacity for a range of oils and organic solvents (2000 to 3600 w/w% to absorbent) in deionized water.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-4**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 민사훈

The Feasibility of Single Molecule Scattering with Worldwide X-Ray Free Electron Laser Facilities

김경태 이문호*

포항공과대학교 화학과

The feasibility of single molecule elastic scattering analysis with the X-ray free electron laser (XFEL) sources in operation and under construction around the world was investigated for various biological and synthetic materials (pepsin, polyethylene, poly(4,4'-oxydiphenylene pyromellitimide), and ferric oxide). This study found that existing XFEL facilities provide coherent pulse X-ray beams with the required energies (8.3-12.4 keV) but their fluxes are too low for single molecule elastic scattering experiments to determine the three-dimensional structures of such molecules; for single molecule scattering, the XFEL facilities need to improve their beam flux density to 2×10^{15} to 7×10^{18} photons pulse⁻¹ μm^{-2} depending on the beam energy. However, the existing XFEL facilities' sources were found to enable the elastic scattering analysis of pepsin and the synthetic polymers in sample sizes of 1-160 μm as well as of ferric oxide in sample sizes ≥ 80 nm. These criteria for the sample size can be extended to other soft (biological, organic, and polymer molecules) and hard (molecules containing heavy metals) materials. In addition, the inelastic scattering, absorption, and radiation damage characteristics of the chosen materials when exposed to the XFEL sources were examined.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-5**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 민사훈

The Fabrication of Organic Semiconducting Nanostructures by Eutectic Reaction

정재연 김주은¹ 권태훈¹ 강영종*

한양대학교 자연과학대학 화학과 ¹한양대학교 화학과

The organic semiconductors with crystalline 1D nanostructures have been used extensively in numerous electronic devices because of their anisotropic optoelectronic properties and their promising applications. By comparison to their inorganic counterparts, organic nanomaterials offer many advantages such as easy and technically infinite ways of modulating band gap simply by changing side functional groups, and which could be effectively lead to new optical properties. The fabrication of well-defined organic semiconducting nanostructures with controlled geometry and alignment, however, has not been well established yet comparing with their inorganic counter parts. Herein, we present fabrication and characterizations of well-defined organic semiconducting nanowires, which can be applied for patterning and alignment. In this presentation, we will demonstrate that highly crystalline rubrene nanowires as well as various organic semiconductors could be formed and crystal growth direction also controlled. The structures and physical properties were confirmed by electron and optical microscopies, MALDI-TOF, GI-WAXD and XRD.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-6**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 정재연

Coarse-grained molecular dynamics simulation for reversible assembly-disassembly behavior of photo-responsive polymeric micelle

민사훈 김병수*

울산과학기술대학교(UNIST) 친환경에너지공학부

Light-induced isomerization between spiropyran and merocyanine has received considerable attention due to their difference in polarity as well as color. This photo-isomerization can provide the strategy for fabricating photo-responsive polymeric materials by introducing the spiropyran moiety into polymers. In particular, there are several reports on photo-responsive polymeric micelle decorated with spiropyran. Although many spiropyran-based polymeric materials have been synthesized, it is still challenging to simulate and visualize the self-assembly of photo-responsive micelle in an aqueous phase, which is hard to observe details on a molecular level experimentally. Thus we propose a coarse-grained model for spiropyran-based polymeric micelle by standard mapping of MARTINI force-field to understand the reversible assembly-disassembly behavior of the micelle with coarse-grained molecular dynamics simulation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-7**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 정재연

pH sensitive Halloysite based hydrogel nanocomposites for colon cancer drug delivery

KUMMARAMADHUSUDANARAO 하창식*

부산대학교 고분자공학과

In this study we synthesized safe and efficient Halloysite-hydrogel nanocomposite for colon cancer drug delivery using biocompatible and biodegradable materials composed from sodium haluronate with poly(hydroxyethyl methacrylate). Further, hydrogel nanocomposites were characterized by various techniques to confirm the formation, crystallinity, thermal and morphological properties. The hydrogels exhibited good swelling property with pH sensitive fashion. 5-fluorouracil is an anticancer drug was successfully encapsulated into these hydrogels as well as inside halloysite nano tubes via equilibrium swelling followed by pulling and breaking the vacuum. TEM results showed 5-FU also encapsulated in the halloysite nanotubes. Furthermore the release studies carried out pH 1.2 followed by 7.4 phosphate buffer media to display the effect of drug release in acidic and alkaline conditions. The kinetics of in vitro release was analyzed using the empirical equations to understand the nature of release mechanism. The release studies indicates these new type of hydrogels are promising controlled release carriers for colon cancer delivery.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-8**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 정재연

Concentration dependent dimer formation of human natural and pyrene-modified i-motif DNA

김미희 김병현* 이문호*

포항공과대학교 화학과

We have investigated the concentration-dependent changes of natural and pyrene-modified i-motif DNA in solution by using synchrotron small-angle X-ray scattering. Detailed data analysis was performed with singular value decomposition and a series of data fitting process. The 3-dimensional structure of natural and pyrene-modified i-motif DNA was similar to each other so that it is possible to use the pyrene-modified i-motif DNA as efficient probe system. As the concentration of DNA increases, the fraction of dimeric i-motif DNA increases. To identify the structure of dimeric i-motif DNA, we created atomic coordinates of dimeric i-motif DNA model and facilitated direct structural comparison with the experimental results. Also, the effect of heating to 90oC and subsequent quick quenching was studied. The natural i-motif DNA become monomeric i-motif DNA after treatment regardless of concentration, while pyrene-modified i-motif DNA still has mixture of monomeric and dimeric i-motif DNA. This study can enable us to conceive 3D structure of i-motif DNA in molecular crowding condition.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-9**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 정재연

Mussel-Inspired Modification of Superhydrophobic Surface for the Formation of Therapeutic Cell Spheroids

이미현 이해신*

한국과학기술원(KAIST) 화학과

We report a mussel-inspired modification of superhydrophobic surface for the formation of therapeutic cellular spheroids. The modified superhydrophobic surface (mSF surface) was prepared by photolithographic patterning of catecholamine on superhydrophobic anodized aluminum oxide (AAO) surfaces. On the mSF surface, homogeneous sizes of cell aggregates (i.e. spheroids) were generated with high efficiency, and size of the spheroids was readily controllable by the hanging drop method. It is reported that the size of cell spheroids affects cell viability, proliferation, cellular functions and stem cell fate, which mainly results from different cell to cell interactions. So, the spheroids size and size homogeneity should be precisely controlled for their therapeutic applications. In this study, spheroids originated both from insulin-secreting, primary islet β -cells and mesenchymal stem cells (MSCs) were formed, demonstrating biological versatility of the mSF surfaces. Both types of cell spheroids showed greater viability than the spheroids produced by the traditional hanging drop method. The diameter of spheroids was efficiently controlled from 50 μm to 250 μm with high size homogeneity. For islet β -cells spheroids, stimulation index (SI), the indicator of glucose sensitivity of β -cells, increased when the spheroids were produced on the mSF surface. Also, the spheroids size dependence of vascular endothelial growth factor (VEGF) secretion of MSCs was demonstrated. The 210 μm size of MSCs spheroids showed highest VEGF secretion, and the VEGF secretion decreased with increasing spheroids diameter. In addition, the catecholamine micropatterns on the superhydrophobic surfaces are stable enough enabling for one to use the mSF surface for many times.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.O-10**

발표분야: New Horizons of Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 정재연

Synthesis of Hydroxyl-Functionalized Polyisocyanate Block Copolymer via Living Anionic Polymerization and Mild Thiol-Ene Click Reaction

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광주과학기술원(GIST) 나노바이오재료전자공학과 ¹광주과학기술원(GIST) 신소재공학과,

PIMS

A well-defined polyisocyanate block copolymer bearing hydroxyl side group was synthesized via living anionic polymerization and sequential thiol-ene click reaction, in order to extend the range of functional polyisocyanates. A modifiable precursor, poly(allyl isocyanate)-b-poly(n-hexyl isocyanate) (PAIC-b-PHIC), which has alkenyl side groups, was synthesized by anionic block copolymerization of allyl isocyanate (AIC) and n-hexyl isocyanate (HIC). The polymerization system offered the living nature including the quantitative yield, predictable molecular weight, and narrow molecular weight distribution, as well as maintained intact allyl side groups. The obtained PAIC-b-PHIC underwent free radical-mediated thiol-ene click reaction with 2-mercaptoethanol using a low temperature-decomposable radical initiator. The simple and mild functionalization method was proved to be highly effective for complete hydroxylation and to be tolerant to the backbone and excess mercaptans. The functionalized block copolymer was characterized by NMR, SEC-MALLS, FT-IR, and TEM analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.O-1**

발표분야: General Oral Presentation

발표종류: 분과기념강연, 발표일시: 금 10:00, 좌장: 이진석

Fabrication of Nanoreactor and Biomedical Imaging Agents Based on the Hollow Nanoparticle Platform

이인수

포항공과대학교 화학과

Hollow inorganic nanoparticles, which have an interior cavity enclosed by an inorganic shell of nanosized thickness, have been receiving a lot of recent attention due to their distinct characteristics that are advantageous in a variety of biomedical and catalysis applications. Their hollow interior structure can be used to selectively encapsulate and release the guest molecules and carry the high payload of the functional molecules at the large surface area, which therefore enriches their potential in the emerging fields such as nanoreactor, drug delivery vehicle, contrast agent for molecular imaging, and energy and gas storage material. Firstly, I will discuss the fabrication of the nanoreactor systems based on the hollow nanospheres which encapsulate catalytic species inside the permeable porous shell of chemically inert materials. I will explain our strategy to transform pre-synthesized nanocrystals into targeted hollow nanostructures and to functionalize the void space of the resulted hollow nanosphere with precious metal nanocrystals. I will also present the successful employment of the catalytically functionalized hollow nanospheres for the high-concentration syntheses of metal nanocrystals and the substrate-selective catalytic reactions. The second part of this seminar will present our recent researches with hollow manganese oxide nanoparticles which show the greatly enhanced MRI relaxivities and drug loading capacity, comparing with those having solid interior. I will discuss the development of a platform protocol based on the HMON for fabricating target-specific multimodality imaging probes for T1 weighted MR imaging.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.O-2**

발표분야: General Oral Presentation

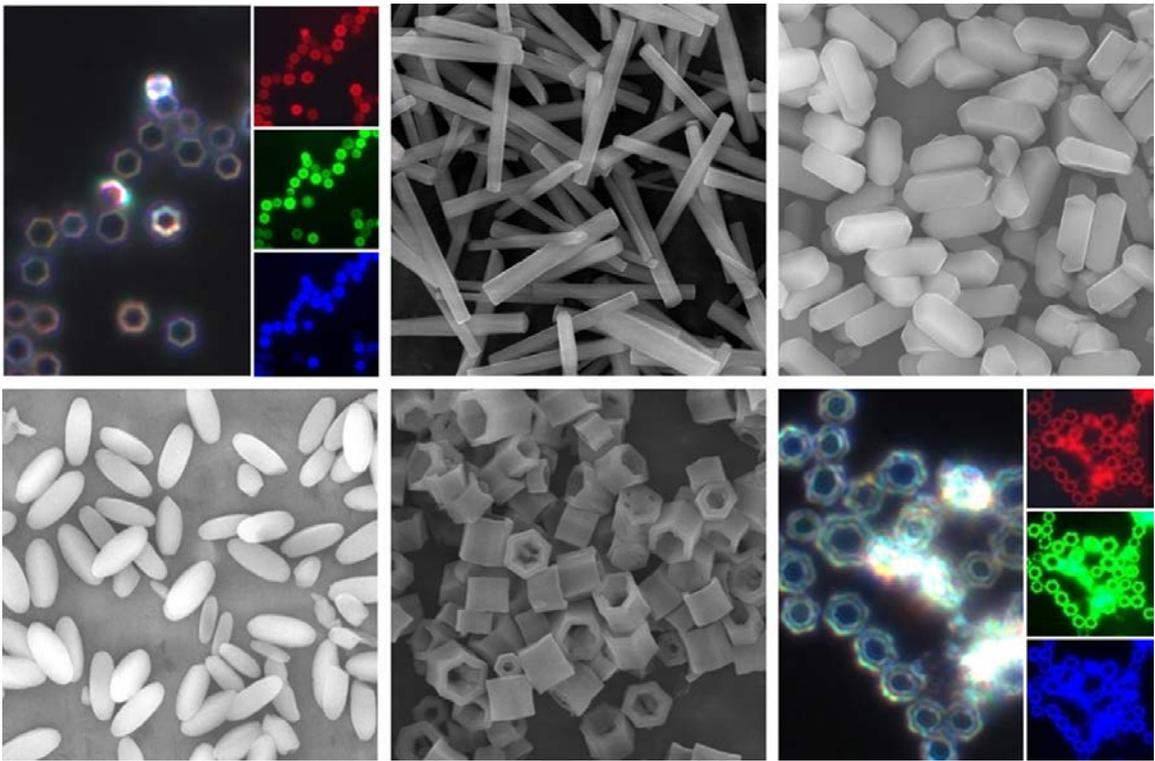
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Coordination Polymer Particles (CPPs)

오문현

연세대학교 화학과

Infinite porous coordination polymers built from metal ions or metal clusters connected by molecular building blocks consisting of organic molecules or organometallic complexes have received a great deal of attention due to their useful applications in gas storage, catalysis, optics, recognition, and separation. Although the majority of coordination polymer materials, including metal-organic frameworks (MOFs), are concentrated on macro-scaled crystalline products, for structural studies based on single crystal X-ray analysis, we and others have recently reported the synthetic strategies for the preparation of nano- and micro-sized coordination polymer particles (CPPs). Here we present the development in CPPs and the utilization of CPPs for the preparation of diverse metal oxides. Metal oxide materials have also received a great deal of attention as a result of their unique properties that have made them of use in a wide range of fields including magnetics, electronics, optics, catalysis, and medical diagnostics. The work described here will provide a way to access a variety of multi-compositional CPPs and metal oxides, something that should facilitate their eventual use in practical applications.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.O-3**

발표분야: General Oral Presentation

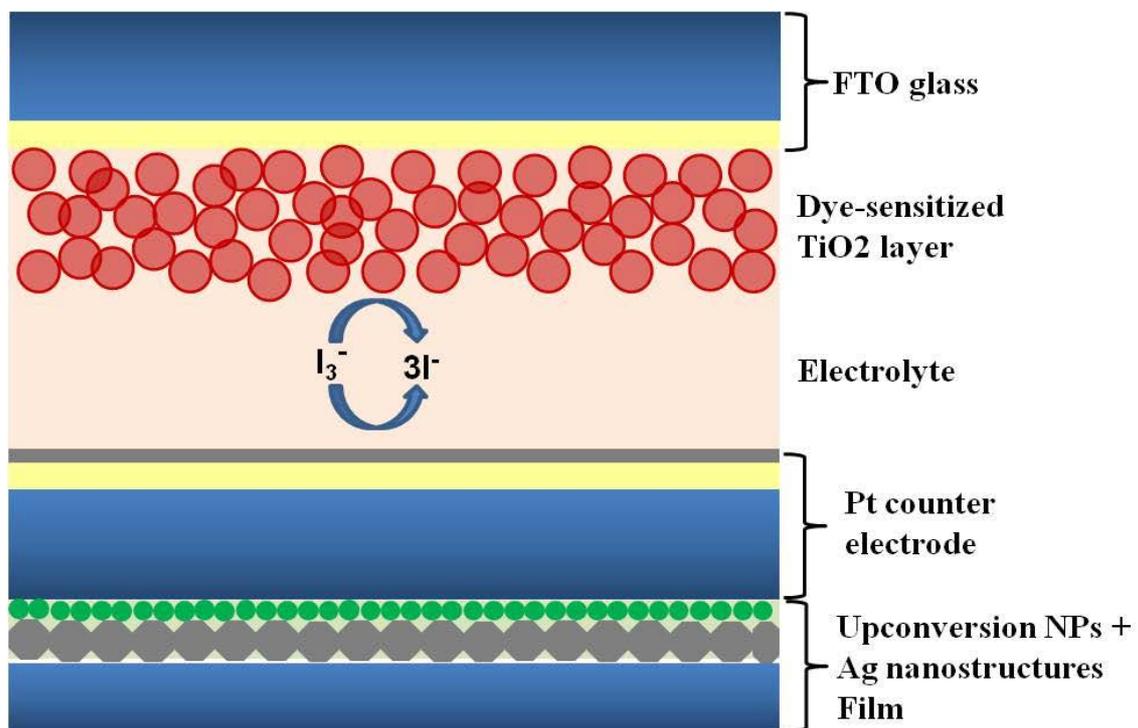
발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 유효종

Combined plasmonic and upconversion rear reflectors for efficient Dye-sensitized solar cells

PARTHIBAN 김진권^{1,*}

공주대학교 화학과, GETRC ¹공주대학교 화학과

Dye sensitized solar cell (DSSC) is a promising technology to replace conventional silicon-based solar cells due to its low cost, simple process and power conversion efficiencies. By the great efforts of researchers working in the DSSC field, the power conversion efficiency of greater than 11% has been achieved [1,2]. However the conversion efficiency is still behind that of the inorganic solar cells. One of the main reasons for this low performance of DSSC is the incapacity of the dyes to utilize the near-infrared (NIR). To overcome this limitation, upconversion nanoparticles (UCNPs), which can transform near infrared photons into visible photons, have been considered as one of the promising solutions and have been applied in DSSCs [3]. However the low upconversion luminescence efficiency limits the practical application of the UCNPs in solar cells. Herein we present a method to increase the efficiency of upconversion luminescence in UCNPs by Fe³⁺ tridoping and used as a rear reflectors in DSSCs to increase the power conversion efficiency of DSSCs.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 유효종

Syntheses, Structures, and Characterizations of New Mixed Metal Selenites and Tellurites

이동우 이은표 옥강민*

중앙대학교 화학과

Mixed Metal selenites and tellurites materials have received a great deal of attention due to their asymmetric coordination environments. Combining local asymmetric coordination units tends to increase an incidence of macroscopic noncentrosymmetric (NCS) crystal structures. NCS materials possess a number of technologically useful characteristics such as ferroelectricity, pyroelectricity, piezoelectricity, and second-order nonlinear optical (NLO) behaviors. Many synthetic chemists continuously have put forth huge efforts to develop superior performing NCS materials. In this presentation, a series of newly discovered mixed metal selenites and tellurites materials will be introduced.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.O-5

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 유효종

Metal-organic frameworks with polar environments exhibiting selective CO₂ adsorption and proton conductivity

방원주 홍창섭*

고려대학교 화학과

Metal organic frameworks (MOFs) are crystalline porous solids being studied for a wide range of applications stemming from their structural tunability. Their designable feature enables us to readily ornament the pore surface of a MOF with special characters such as polarity and acidity. The modifications of the interior of a MOF affect on gas adsorption capability and selectivity. In addition, MOFs have gained researchers' attention as candidate materials for solid state proton conductors. A new two-dimensional (2D) Zn(II) metal-organic framework with flexible aryl ether linkers and water molecules exposed to the pores and its dual properties, such as selective CO₂ adsorption and proton conductivity, originated from polar circumstance will be introduced. Detailed discussions of this material together with other interesting proton-conducting MOFs will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.O-6

발표분야: General Oral Presentation

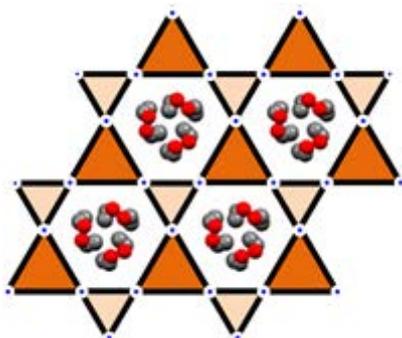
발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 유효종

Constructions of 2D and 3D Kagome-type Copper(II) Coordination Polymers: Thermolysis, Alcohol Reservoirs, and Catalysis

이혜리 정옥상*

부산대학교 화학과

Self-assembly of CuX_2 ($\text{X}^- = \text{Cl}^-$ and Br^-) with a new tridentate ligand, N,N',N'' -tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L), yields a uniquely very thin Kagome-type network consisting of both nano-sized hexagonal (Cu_6L_6) and triangular (Cu_3L_3) motifs as an effective reservoir for small alcohol molecules. When the crystals were calcined for 1 h at 250°C , the resulting contraction via eruption of both solvated and combusted organic molecules produced the shellshape morphology. At 350°C , the crystals changed to the chrysanthemum flower shape, and they took on the convex?concave surface, which forms seemingly as a result of the inner eruption of combusted organic molecules. Finally, above 600°C , copper(II) oxide nanocrystals were formed. Self-assembly of CuX_2 ($\text{X}^- = \text{ClO}_4^-$ and BF_4^-) with 2,3-bis(nicotinoyloxy)naphthalene (L) yields 1D loop-chain skeleton. The 1D loop-chains form an ensemble constituting a unique 3D kagome-type structure with both infinite hexagonal channels and trigonal channels. The unprecedented reversible supra-channel effects on the catalytic oxidation of 3,5-di-*tert*-butylcatechol to 3,5-di-*tert*-butylbenzoquinone were investigated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.O-7

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:40, 좌장: 유효종

Highly tunable and biologically functional nanostructured surfaces for biological application

이효진 남좌민^{1,*}

서울대학교 자연과학대학 화학부 ¹서울대학교 화학부

Cells within a tissue interact with neighboring cells and with the extracellular matrix (ECM) through biochemical and mechanical cues. The cellular environmental factors composited of micro- or nanoscale cues affect cell behaviors. Therefore, over the last decade, micro- or nanofabrication techniques have sufficiently resulting progressed to recapitulate many cellular environmental factors, making them progressively more useful for application in biology and tissue engineering. Recent advances in micro- or nanofabrication techniques pave the way for engineering biomaterial surfaces that control cellular interaction from the micro-to the nanoscale. In particular, studies on the effect of nanomaterials on cell behavior are great important because the length scale of such nanoparticle is physiologically relevant due to consistency with the sizes of many functional biomolecules and their complexes, ranging from a few to hundreds nanometers, including the fibers of ECM proteins, the components of basement membrane, and focal adhesions. Here, we have mainly focused on the development of the nanostructure and bio mimetic system as enabling tools for studying the effects of cell adhesion and signaling on cell function. For fabrication of nano-biomimetic platform, we used metal nanoparticle, nanothickness polymer film, and nanoporous membrane. Using these nano materials, we mimic several bio-events including cell-ECM interaction, metastatic cancer cell focal adhesion, invasion process of cancer cells, and cell-cell communication. This study of nanoscale engineering in controlling cell-material interfaces can have profound implications for future development of tissue engineering and regenerative medicine.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-1**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 곽경원

Dynamical changes in microscopic fluorescence spectra of grana and stroma-exposed regions in chloroplasts of a higher plant protoplast during state transitions

김은철 Shigeichi Kumazaki^{1,*} 안태규*

성균관대학교 에너지과학과 ¹Department of Chemistry, Kyoto University

In chloroplasts of plant and algae, state transition is an important regulatory mechanism to maintain the excitation balance between photosystem I (PSI) and photosystem II (PSII) under fluctuating light conditions in terms of intensity and spectrum. Light harvesting complex II (LHCII) seems to play a key role as the regulated energy distributor to each photosystem. It is widely believed that LHCII migrates in thylakoid membrane to bind with PSI and PSII at state 2 and state 1, respectively. We employed a fluorescence spectral imaging system in order to give a new insight on the state transition based on microscopic fluorescence spectra with a submicrometer spatial resolution. Protoplasts from *Arabidopsis thaliana* has been used to give a better access to the intrachloroplast structures, while maintaining the high physiological activity of the chloroplasts. Near-infrared mode-locked laser-based fluorescence spectral microscopy was applied to obtain fluorescence spectra from grana and stroma-exposed thylakoid regions selectively, as previously demonstrated in the case of leaves of *Zea mays*. It was revealed that two-photon and one-photon excitation of chloroplasts in the wavelength region of 785 ? 820 nm lead to dominance of PSII and PSI in the fluorescence spectrum, respectively, even at around 295 K. It is thus expected that highly pure spectra of PSI and PSII obtained in the identical setup can be utilized for a reliable spectral decomposition between PSII and PSI in measured fluorescence spectra on a submicrometer spatial scale. We succeeded to obtain state-transition induced changes in microscopic fluorescence spectra, which were different between grana and stroma-exposed thylakoid regions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-2**

발표분야: General Oral Presentation

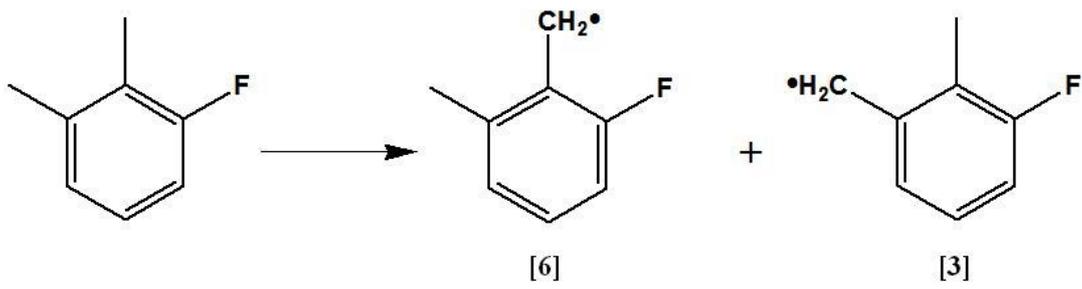
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 곽경원

Spectroscopic identification of isomeric jet-cooled benzyl-type radicals formed from 3-fluoro-o-xylene by corona discharge

윤영욱 채상열¹ 이상국*

부산대학교 화학과 ¹(주)엔지텍 연구개발팀

Spectroscopic identification of isomeric transient species generated from same precursor is an important subject for understanding dynamics of molecules. Over a few years, we have identified several isomeric jet-cooled benzyl-type radicals produced by corona discharge of substituted dimethylbenzene precursors, in which the dissociation of methyl C-H bond of different methyl groups generates isomeric benzyl-type radicals. Vibronically excited but jet-cooled isomeric benzyl-type radicals were generated from the precursor 3-fluoro-o-xylene using a pinhole-type glass nozzle designed for supersonic jet expansion along with corona discharge, from which the visible vibronic emission spectrum was recorded from the discharge system with a long-path monochromator. The spectrum shows a complicate vibronic pattern of two isomers; 2-methyl-3-fluorobenzyl and 2-methyl-6-fluorobenzyl radicals. The vibronic structure was analyzed based on the substituent effect on electronic transition energy which shows very strong dependence of transition energy on the substitution position of methyl group and fluorine atom. From an analysis of the spectrum observed, we identified the formation of two isomers, 2-methyl-3-fluorobenzyl and 2-methyl-6-fluorobenzyl radicals in the corona discharge of precursor, and determined for the first time the electronic energy in the $D_1 \rightarrow D_0$ transition and vibrational mode frequencies in the D_0 state for both isomers.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-3**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 곽경원

Vibrational assignment and structure of acetone cation investigated by vacuum ultraviolet mass-analyzed threshold ionization spectroscopy and quantum chemical calculations

강도원 이유란 김홍래* 권찬호*

강원대학교 화학과

Acetone has attracted much attention as simple model because of two methyl groups causing internal rotations. In this regards, extensive studies on torsional modes for neutral have been carried out but study for cation is lack. We recorded the vibrational spectrum of acetone cation in the electronic ground state using the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. From the VUV-MATI spectrum measured, the accurate ionization energy of acetone was determined to be 9.707 ± 0.002 eV. Nearly complete assignments for the vibrational peaks in the VUV-MATI spectrum were possible by utilizing vibrational frequencies and Franck-Condon factors calculated at the density functional theory (DFT). We observed several low frequency peaks that can be identified as the torsional modes and analyzed successfully them with aid of density functional theory calculations.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 곽경원

IR Dip Spectroscopy of Jet-cooled 3-cyanoindole-(H₂O)_n (-n=0-5) in the Gas Phase

민아름 문철주 안아름 이지훈 최명룡* 김성근¹

경상대학교 화학과 ¹서울대학교 화학부

3-cyanoindole (3-CI), a derivative of indole, has important intrinsic properties which give rise to enormous biological activities. In our previous studies, one conformer of 3-CI-water clusters was identified via the REMPI and UV-UV double resonance spectroscopic methods in the gas phase studies. In this study, we have further investigated the 3-CI-water clusters having up to 5 water molecules, 3-CI-(H₂O)_n (n=0-5). For the 3-CI-(H₂O)₁ clusters, their REMPI spectrum has a strong origin band, red-shifted compared to that of the monomer and a relatively weak origin band attributed to the 3-CI-(H₂O)₂ clusters. The assignment of specific conformers was aided by the combination of UV-UV hole-burning and IR-dip spectroscopy. All mass-selected origin bands of 3-CI-(H₂O)_n (n=0-5) clusters in the REMPI spectra were the targets for the burning frequency in IR-dip spectroscopy. The corresponding IR-dip spectrum in the region of 2800-4000 cm⁻¹ showed clear identification of certain 3-CI-(H₂O)_n (n=0-5) conformers. We have also calculated the optimized structures of 3-CI-(H₂O)_n (n=0-5) clusters using density functional theory (DFT). Further details on the 3-CI-(H₂O)_n (n=0-5) clusters will be discussed by IR dip spectroscopic studies in this poster.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-5**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 곽경원

A Simulation Study on the Rotational Dynamics of Dimers in Random Obstacle Matrices

전희진 성봉준*

서강대학교 화학과

A plasma membrane contains a numerous kinds of proteins and lipids. These elements in plasma membrane generate a heterogeneous environment that influences the dynamic behavior of the membrane proteins. The translational diffusion of dynamics of membrane proteins has been investigated extensively. However, few studies have been performed on the rotational diffusion of proteins. In this work, we elucidate the rotational dynamics by using the dimer tracers in two dimensional (2D) random obstacle matrices to mimic the protein rotation in a plasma membrane. The random matrices are generated by randomly distributing non-overlapping quenched obstacles in 2D. As the area fraction of obstacles, Φ_m , increases, the system becomes more crowded and heterogeneous. Below the pore percolation threshold of obstacles, $\Phi_c=0.22$, both translational and rotational diffusion of proteins follows the normal Brownian diffusion. Above Φ_c , the particles are confined such that they can't move freely. Therefore, the translational diffusion of dynamics becomes anomalous. On the other hands, the rotational dynamics still shows a Brownian motion. This shows clearly that the translational and the rotational diffusion decouple in such crowded environments. More interestingly, when the $\Phi_m > 0.30$, the rotational dynamics shows an oscillatory behavior in the probability distribution of rotational displacement.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-6**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 곽경원

Random Walk Model for the Self-Assembled Monolayer in Dip Pen Nanolithography

김효정 장지혜 장준경^{1,*}

부산대학교 나노융합기술학과 ¹부산대학교 나노소재공학과

The growth of a self-assembled monolayer (SAM) pattern in dip-pen nanolithography (DPN) was simulated by using a simple random walk model. In this model, the SAM pattern grows mainly via the serial pushing of molecules initiated by molecules dropping from an atomic force microscope (AFM) tip. In our model, the serial pushing is taken to be in the same direction for a finite number of consecutive pushing events. We examine various SAM patterns, such as lines, crosses, and letters by changing the tip scan speed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-7**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 곽경원

Control of Osmosis and Desalination by Lower Critical Solution Temperature (LCST) Type Phase Behavior

목영봉 이연*

서울대학교 화학부

Osmotic flows can be reversibly controlled by temperature-sensitive materials. Because temperature-sensitive materials show temperature-driven hydrophilic to hydrophobic transition in aqueous condition, corresponding abrupt changes of effective concentration in the solution containing those materials can induce conversion of osmotic flows. Some temperature-sensitive materials show 'lower critical solution temperature' (LCST) phase transition (miscible at low temp. and not miscible at high temp.). So they can osmotically draw water in feed solution at low temp. and release the water after phase separation at high temp. But most LCST materials are polymers. Because polymers cannot induce high osmotic pressure, new ones having significantly lowered MW is needed. Derived from the structure of temperature-sensitive polymer, we synthesized N-acylated tris(2-aminoethyl)amine (nBu-TAEA). It has MW of 356g/mol and shows phase separation above ~27 Celsius. nBu-TAEA aqueous solution showed clear conversion of osmotic flow at low and high temp. when it was facing saline solution. Also, its possibility for continuous osmotic desalination was checked by circulating LCST mixture at low and high temp. environment, making simultaneous water withdrawal and release.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.O-8**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:15, 좌장: 곽경원

Computational Studies of the Interactions between Poly (Amidoamine) (PAMAM) Dendrimers and Biological Membranes

김용빈 장락우*

광운대학교 화학과

Understanding the interaction of nanoparticles with biological membrane is important for both designing effective nanodevices for medical applications and avoiding unintended consequence from disruption of biological structure. Dendrimers, hyper-branched polymers, represent a novel class of structurally controlled macromolecules. With the advantages such as controlled mass, surface functionality, and easy surface modification, they can be the good candidates for nano materials with biomedical applications such as drug/gene delivery. Especially, poly(amidoamine) (PAMAM) dendrimers are the first complete dendrimer family to be synthesized, characterized and commercialized. For that reason, PAMAM dendrimers are widely studied for both medical and basic science applications. However, the behavior of PAMAM dendrimers near cell membranes is not fully understood. In this study, we have performed full atomistic molecular dynamics simulations to investigate the interactions between amine-terminated PAMAM dendrimers and two model biological membranes such as zwitterionic DPPC and negatively charged POPG lipid bilayer membranes. Using the P2₁ boundary condition, which allows the flip-over of lipid molecules, the asymmetric stress on leaflets in the presence of dendrimer is effectively handled. The free energy calculation of the dendrimer adsorption shows that there exists significant attractive interaction between the positively charged dendrimer and both model membranes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-1

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김준곤

New insight into the inflammation mechanism evaluated by LC-MS based quantitative eicosanoid signatures

이수현 이원용 정봉철¹ 최만호^{2,*}

연세대학교 화학과 ¹한국과학기술연구원(KIST) ²한국과학기술연구원(KIST) 미래융합기술연구
본부

Eicosanoids as metabolites of arachidonic acid (AA) are rapidly biosynthesized and degraded in vascular function, inflammation, hypertension and other pathologies. Simultaneous changes of eicosanoids in the liver S9 fraction with systemic inflammation were therefore investigated. The S9 fraction was obtained from model rabbits consisted of control and 1% carrageenan subcutaneous injection groups. After incubation of the S9 fraction with inflammation mediators, 33 eicosanoids were quantitatively measured by LC-MS combined with the high-resolution selected-ion monitoring (LC-HR/SIM-MS). Among different metabolic pathways of AA, cyclooxygenases (COXs) and lipoxygenases (LOXs) are the major target for the most popular medications used to treat pain, fever and inflammation. Here, the inflammation signatures was confirmed with two inflammation mediators, ibuprofen and celecoxib for inhibition of COX-1/2 and selective COX-2, respectively. Then, the devised technique was successfully applied to identify the new biochemical role of an endogenous steroid, epitestosterone, as inflammation mediator may responsible for the COX-1 inhibition.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-2

발표분야: Oral Presentation of Young Analytical Chemists

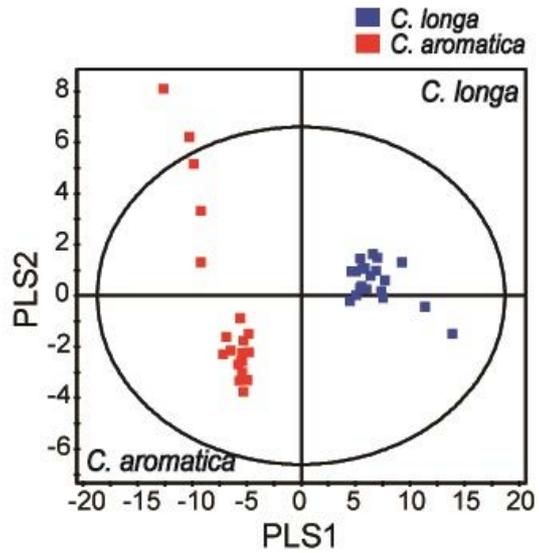
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 김준곤

Secondary metabolite profiling of *Curcuma* species grown at different locations using GC/TOF and UPLC/Q-TOF MS

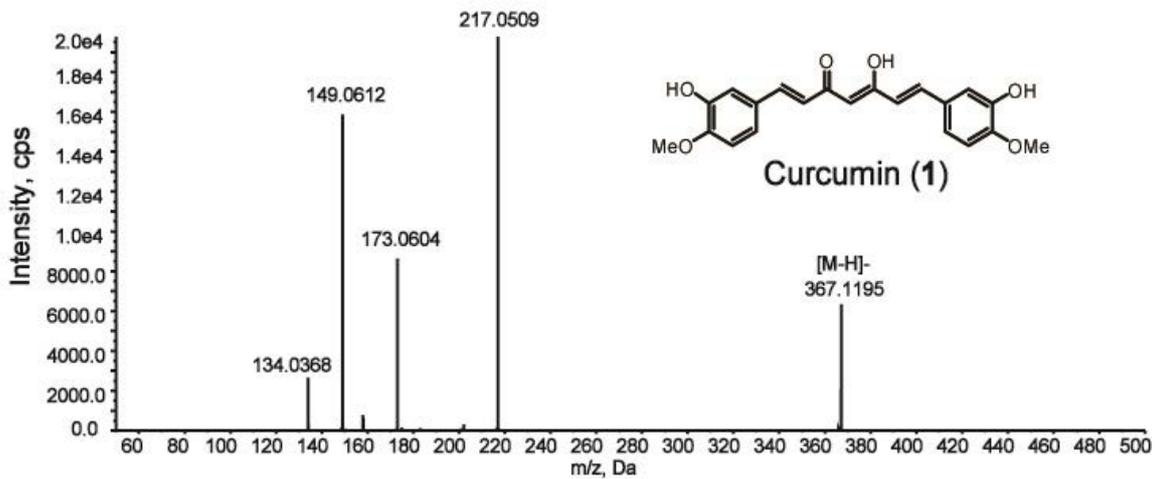
이주은 정영애¹ 류도현* 황금숙^{1,*} 남미소

성균관대학교 화학과 ¹한국기초과학지원연구원 통합대사체연구그룹

Curcuma, a genus of rhizomatous herbaceous species, has long been used as a spice, traditional medicine, and natural dye. Recently, attention has turned to the medicinal properties of Curcuma species for treatment of illnesses such as cancer, and Alzheimer's disease. In this study, the metabolite profile of Curcuma extracts was obtained using gas chromatography-time of flight mass spectrometry (GC/TOF MS) and ultrahigh-performance liquid chromatography-quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF MS) to characterize the differences between Curcuma aromatica and Curcuma longa grown either in the Jeju-do or Jin-do islands of South Korea. Previously, abundant primary metabolite profiling of Curcuma species grown in different regions using NMR based metabolomics had been reported. On the other hand, this study focused on profiling of secondary metabolites from the hexane extract of Curcuma species. This metabolite profiling, coupled with multivariate analysis, was performed by GC/TOF MS to identify different secondary metabolites between C. aromatica and C. longa. Principal components analysis (PCA) and Partial Least Squares Discriminant analysis (PLS-DA) plots showed significant differences between the C. aromatica and C. longa metabolite profiles, whereas geographical location had little effect. A t-test was performed to identify statistically significant metabolites, such as terpenoids. Additionally, targeted profiling using UPLC/Q-TOF MS showed that the concentration of curcuminoids differed depending on the origin of the plant. Through these results, it was demonstrated that global and targeted metabolite profiling using a combination of GC- and LC-MS is useful toward discriminating between Curcuma on the basis of species or geographical origins.



Global profiling by GC/TOF MS



Targeted profiling by UPLC/Q-TOF MS

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-3

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 김준곤

Comprehensive Analysis of Petroleum by Laser Desorption Ionization coupled to Fourier Transform Ion Cyclotron Resonance Mass Spectrometer

조윤주 김성환*

경북대학교 화학과

Many studies have analyzed the chemical composition of petroleum in order to better understand and predict the properties and behaviors of heavy petroleum. However, even using Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS), a complete understanding of the chemical composition of petroleum is not currently available. One of the problems limiting our knowledge is discrimination occurring during the ionization process. To circumvent this problem, it is beneficial to use as many ionization techniques as possible. Therefore, there have been many studies devoted to utilizing various ionization techniques, e.g., electrospray ionization (ESI), field desorption ionization, atmospheric pressure photo ionization (APPI), atmospheric pressure chemical ionization (APCI), easy ambient sonic-spray ionization mass spectrometry (EASI), laser-induced acoustic desorption (LIAD), and atmospheric pressure laser-induced acoustic desorption chemical ionization (AP/LIAD-CI) for oil research. Matrix-assisted laser desorption ionization (MALDI) is a widely used ionization method to analyze biomolecules and polymers. MALDI is limited for the analysis of oils because peaks originating from the matrix are abundant at $m/z < 500$, where many compounds in oil are observed. Therefore, laser desorption ionization (LDI) has been used instead of MALDI to study petroleum. In this study, (+) and (-) mode LDI FT-ICR MS spectra obtained from crude oils have been compared and shown that LDI can be a useful technique to study crude oil. Heavy components of oils contain aromatic ring structures were successfully analyzed because they can absorb laser photons efficiently. For shale oils derived from different source rocks, the comparison results of characterization using (+) mode APPI and LDI FT-ICR MS have shown that LDI is sensitive toward nitrogen class compounds and can be a good method for the analysis of oil shale extracts.

Moreover, vanadyl- and nickel porphyrin complexes in crude oils were detected more effectively by LDI than APPI FT-ICR MS directly from an unfractionated crude oil.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL.O-4**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 김성환

2D correlation analysis for protein nanoparticles

박연주 서용일 표동진 황현석 정영미*

강원대학교 화학과

Two-dimensional (2D) correlation spectroscopy has been attracted a high level of interest in analytical science community, as it provides considerable utility and benefit in many fields of spectroscopic studied. In this work, to investigate secondary molecular structure and thermal behavior for two types of insulin nanoparticles, which were prepared from EtOH and DMSO solution, respectively, by solution enhanced dispersion supercritical fluid (SEDS) process, 2D correlation analysis was applied to the temperature-dependent diffuse reflectance infrared Fourier transform infrared (DRIFT-IR) spectra. To better understand molecular structure of insulin nanoparticles, molecular dynamic (MD) simulation was also performed. In this presentation, results of 2D correlation analysis and MD simulation for two different types of insulin nanoparticles will be discussed more details.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-5

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 김성환

A New Strategy for the Determination of Self-Exchange Rate of Alkanethiolates on Self-Assembled Monolayers on Gold using MALDI-TOF MS

강현욱 여운석*

건국대학교 생명공학과

In this paper, we describe a new method for the determination of exchange rates of alkanethiolates on Self-assembled monolayers (SAMs) on gold using matrix assisted laser desorption/ionization time of flight mass spectrometry (MALDI-TOF MS), by which the composition of alkanethiolates on SAMs can be analyzed rapidly and directly. Particularly, for the investigation of the self-exchange of an alkanethiol, we prepared the deuterated alkanethiol that has the same molecular properties to the non-deuterated alkanethiol but a different molecular weight. Monolayers consisting of deuterated alkanethiolates were immersed into a solution of the non-deuterated alkanethiol, and influences of immersion time, concentration, temperature, and solvent upon the self-exchange rates were investigated. Furthermore, we investigated the exchange rates between alkanethiols which have different carbon chain lengths or ethylene glycol units.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-6

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 김성환

Glycosylated proteins preserved over millennia: N-glycan analysis of Tyrolean Iceman, Scythian Princess and Warrior

김범진 Sureyya Ozcan¹ Rudolf Grimm² 안현주*

충남대학교 분석과학기술대학원 ¹Department of Chemistry, University of California, Davis, California 95616, USA ²Agilent Technologies Inc., Santa Clara, California 95051, USA

An improved understanding of glycosylation will provide new insights into many biological processes. In the analysis of oligosaccharides from biological samples, strict regimen is typically followed to ensure sample integrity. However, the fate of glycans that have been exposed to environmental conditions over millennia has not yet been investigated. This is also true for understanding the evolution of the glycosylation machinery in humans as well as in any other biological systems. In this study, we examined the glycosylation of tissue samples derived from four dominantly natural mummies: the 5,300 years old “Iceman, Oetzi”, found in the Tyrolean Alps; the 2,400 years old “Scythian warrior”, found in the Altai Mountains; the 2,400 years old “Scythian Princess”, also found in the Altai Mountains; and a 4 years old contemporary mummy, found in an apartment in Vienna/Austria. By using a combination of chromatographic retention time and accurate molecular mass from mass spectrometric analyses, we were able to determine the N-glycan composition of all available mummy tissue samples. The number of identified N-glycans depended on both the age and the preservation status of the mummies. The contemporary mummy tissue sample showed significantly more glycan structures than the ancient mummy tissue samples. Interestingly, we found that the ancient mummy tissue samples contained primarily N-glycans with bi- and tri-antennary glycan structures composed of mostly mannose residues, which also happen to be abundant in human cancer tissues. Our findings clearly show the oldest glycans ever discovered suggesting that protein glycosylation persists for thousands of years and that mummies are enabling us to investigate ancient glycosylation opening a window to the far past.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.O-7

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 김성환

Advanced Analytical Methods for the Lipid Analysis from Biological Sample

방대영 문명희*

연세대학교 화학과

Lipids have multiple functions, serving as the building blocks of membranes and playing roles in energy storage and signal transduction between cells, and they are involved in human diseases. Since each group of lipids contains different combination of acyl chains, the simultaneous analysis of the entire lipidome is a complicated task. This presentation shows advanced techniques developed in our laboratory in qualitative profiling of lipids from human urine and plasma samples by using nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS-MS). While MS analysis of most glycerophospholipids (GP) classes is carried out in negative ion mode, analysis of neutral polar lipids is highly efficient in positive ion mode. In order to establish run conditions to carry out a single nLC-ESI-MS-MS for all GPs, the ionization efficiency of 13 different types of GP molecules in nLC-ESI-MS has been evaluated in negative ion mode by varying the modifiers and their concentrations. The optimized conditions were applied to the analysis of GP mixture extracted from a human urine sample. Based on the lipid classification, major lipids have been divided into four categories such as glycerolipids (GL), sphingolipids (SP), sterol lipids (ST) including GP. However, complexity in lipid mixtures still remains a barrier toward a complete identification even with sophisticated HPLC methods. The study demonstrates a separation of different plasma lipid classes on a strong anion exchange (SAX) column in the first dimension and that of plasma lipid molecular species on a reversed-phase (RP) column in the second dimension, so that the ion suppression effects can be reduced and the number of identified lipids can be increased.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.O-1**

발표분야: New Frontiers in Chemical Biology

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이준석

Discovery of potent modulators for circadian rhythms

이재욱

한국과학기술연구원 천연의약센터

The circadian clock underlies daily rhythms of diverse physiological processes and alternation in circadian clock is related with numerous pathologies. To discover new chemical probes for modulating and dissecting the clock mechanism, we performed circadian screen of ~500,000 compounds on human cells which are harboring *Bmal1-dLuc*. [1] The data analysis identified small molecules, which potentially lengthen the circadian period in dose-dependent manner. We selected a carbazole derivatives which named as cryptostar. [2] To improve the potency of these compounds and identification of linker position, we synthesized the derivatives of the carbazole compound. For target identification of a carbazole compound, we performed affinity chromatography coupled with proteomic mass analysis. We identified cryptochrome as targets of cryptostar(KL001) for period regulation. After further analysis of cryptostar, we identified that cryptostar interacted with the FAD-binding pocket of CRY to prevent ubiquitin-dependent degradation. We further demonstrated that KL001 inhibited glucagon induced gluconeogenesis in hepatocytes.

1. Lee JW, Hirota T, Peters EC, Garcia M, Gonzalez R, Cho CY, Wu X, Schultz PG, Kay SA. *Angew Chem Int Ed Engl.* 2011, 50, 45, :10608-11
2. Hirota T, Lee JW, St John PC, Sawa M, Iwaisako K, Noguchi T, Pongsawakul PY, Sonntag T, Welsh DK, Brenner DA, Doyle FJ 3rd, Schultz PG, Kay SA. *Science* 2012, 337, 6098, 1094-7.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.O-2**

발표분야: New Frontiers in Chemical Biology

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 이준석

Albumin-coated ZAIS Fluorescent Nanoparticles for Facile Antibody Conjugation and Target-specific Bioimaging

정종진 이승재¹ 박자영 장혜미 박정규^{2,*}

한국화학연구원 나노기술융합연구단 ¹연세대학교 화학과 ²한국화학연구원 형광물질연구팀

ZAIS - (ZnxAg_yInz)S₂ - fluorescent nanoparticle (NP) has been developed to replace II-VI QDs due to its cadmium free non-toxic nature, and facile synthesis of the fluorescent nanocrystal library by ultrasonic and combinatorial chemistry. In addition, ZAIS shows much stronger fluorescence intensity than QD without photoblinking in single nanoparticle level, which is suitable for a cell imaging probe. However, the lack of methods to coat the surface of ZAIS NP has limited to have stability in a physiological solution as well as to attach targeting molecules. Here, we developed a biocompatible and stable coating method by passivating ZAIS NPs with BSA. BSA-coated ZAIS NP (ZAIS-BSA) shows excellent stability in a high concentration under the physiological condition. Moreover, the best BSA passivation condition and its non-aggregation characteristics were evaluated by running agarose gel electrophoresis. Its increased hydrodynamic size and the change of surface charge were characterized by dynamic light scattering and zeta potential measurements. For the facile antibody conjugation and target-specific bioimaging, we demonstrated the attachment of IgG to ZAIS-BSA by developing both the passivation method and hydrazone based conjugation of IgG. Both approaches are complementary in a sense that the passivation method is simple but the antibody orientation is random, however, the hydrazone conjugation method shows relatively specific orientation of IgG in spite of complicate attachment procedures. The target-specificity of these two approaches were tested by performing the binding experiment of Herceptin conjugated ZAIS-BSA to the Her2 positive breast cancer cell lines such as SK-BR-3 and HCC1954, following the attachment of Herceptin, anti-Her2 antibody onto ZAIS-BSA.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.O-3**

발표분야: New Frontiers in Chemical Biology

발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 이준석

Application of Transition-Metal-Mediated ^{18}F -Fluorination to PET Radiotracer Development

이은성 Jacob. M. Hooker¹ Tobias Ritter^{2,*}

포항공대 화학과 ¹Athinoula A.Martinos Center for Biomedical Imaging, Massachusetts General Hospital and Harvard Medical School ²Department of Chemistry and Chemical Biology, Harvard University

New fluorination methods for the synthesis of ^{18}F -radiolabeled small molecules have the potential impact for clinical positron emission tomography (PET) imaging, if the methods can be successfully translated. However, progression of modern reactions from the stage of synthetic chemistry development to the preparation of radiotracer doses ready for use in human PET imaging is challenging and rare. Here we present the process of and the successful translation of a modern transition-metal-mediated fluorination reaction to non-human primate (NHP) baboon PET imaging?an important milestone on the path to human PET imaging. The method, which transforms $[^{18}\text{F}]$ fluoride into an electrophilic fluorination reagent, provides access to aryl ^{18}F bonds that would be challenging to synthesize via conventional radiochemistry methods.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.O-4**

발표분야: New Frontiers in Chemical Biology

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 이준석

A novel small molecule inducer of cellular antioxidant response

허우영

한국과학기술연구원(KIST) 화학 키노믹스 연구센터

Eukaryotic cells counteract oxidative and other environmental stress through the activation of Nrf2, the transcription factor that controls the expression of a host of protective enzymes by binding to the antioxidant response element (ARE). The electrophilic molecules that are able to activate Nrf2 and its downstream target genes have demonstrated therapeutic potential in carcinogen-induced tumor models. Using a high-throughput cellular screen, we discovered a class of ARE activator, which we named AI-1, that activates Nrf2 by covalently modifying Keap1, the negative regulator of Nrf2. Biochemical studies indicated that modification of Cys151 of Keap1 by AI-1 disrupted the ability of Keap1 to serve as an adaptor for Cul3-Keap1 ubiquitin ligase complex, thereby causing stabilization and transcriptional activation of Nrf2. AI-1 and its biotinylated derivative are useful pharmacological probes for investigating the molecular details of the cellular antioxidant response

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-1**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이선우

Rhodium-Catalyzed Oxidative C-H Activation/Cyclization for the Synthesis of Phosphaisocoumarins and Phosphorous 2-Pyrones

박영철 이필호*

강원대학교 화학과

The rhodium-catalyzed cyclization of phosphinic acids and phosphonic mono-esters with alkynes has been developed. The oxidative annulation proceeded with complete conversion of phosphinic acid derivatives and allowed for the atom economic preparation of useful phosphaisocoumarins with high yield and selectivity. The reaction is tolerant of extensive substitution on the phosphinic acid, phosphonic mono-esters and alkynes, including halides, ketone, and hydroxyl group as substituents. Also, we found that alkenylphosphonic mono-esters proceed to give a wide range of phosphorus 2-pyrones through oxidative annulations with alkynes. Mechanistic studies revealed the C-H bond metalation to be rate-limiting step.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-2**

발표분야: Oral Presentation for Young Organic Chemists

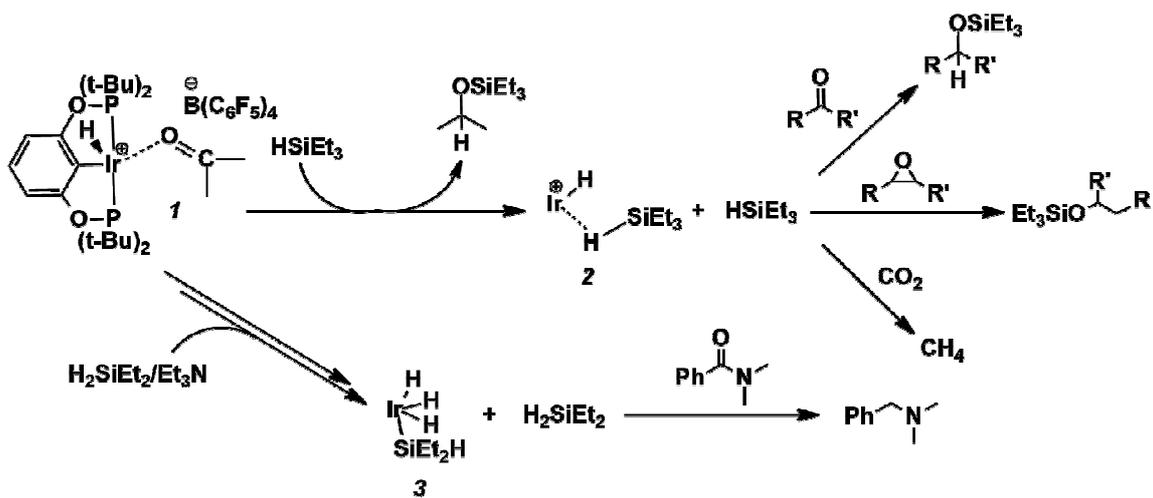
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Development and Mechanistic Investigation of a Highly Efficient Iridium(III) Silane Complex for Hydrosilylation of Various Carbonyl Functionalities

박세훈 David Bezier¹ Maurice Brookhart^{1,*}

IBS 화학과 ¹University of North Carolina at Chapel Hill, U.S.A.

Cationic iridium silane complexes with POCOP ligand {POCOP = 2,6-[OP-(tBu)₂]₂C₆H₃}, 2 generated in situ from the complex 1 in combination with Et₃SiH catalyze hydrosilylations of epoxides and carbon dioxide as well as ketones, aldehydes, and esters. Kinetic study at low temperatures for the hydrosilylation of acetone reveals that the complex 1 is the catalyst resting state and is in equilibrium with low concentration of the silane complex 2. D-labeling study of the hydrosilylation of styrene oxide shows that the epoxide isomerizes to the ketone, followed by hydrosilylation. Surprisingly, it turns out that CO₂ smoothly undergoes reductive hydrosilylation by the complex 2 to convert to CH₄ under mild conditions (23 °C and 1 atm of CO₂). In the course of the study on the reduction of tertiary amides to amines, unexpectedly a neutral iridium(V) silyl trihydride complex, (POCOP)IrH₃(SiEt₂H), 3 has been identified as an active catalyst for the amide reduction. The complex 3 with H₂SiEt₂ in the presence of trialkylammonium salt under 1 atm of H₂ has been shown to reduce tertiary amides to the amines with turnover numbers as high as 10,000 under mild conditions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-3**

발표분야: Oral Presentation for Young Organic Chemists

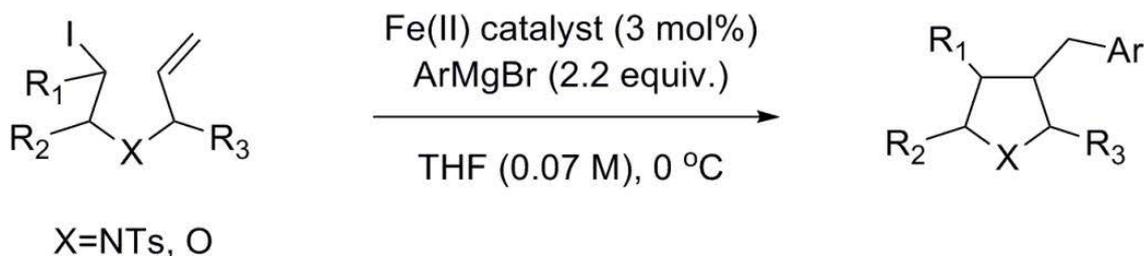
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 이선우

Iron(II)-Catalyzed Tandem Cyclization and Cross-coupling Reaction of Iodoalkanes and Aryl Grignard Reagents

김재곤 강은주^{1,*}

경희대학교 화학과 ¹경희대학교 응용화학과

Iron-catalyzed cross-coupling reactions have been intensely investigated in recent years, while palladium- and nickel-catalyzed cross-coupling reactions of aryl and vinyl halides have evolved over decades into mature tools for advanced organic synthesis. The most valuable characteristic of iron catalysis in cross-coupling reactions may be the unprecedented reactivity toward alkyl halides. Alkyl halides are considered challenging substrates because they resist oxidative addition, and the resulting metal reagents have proclivity for β -hydride elimination. Despite a number of reports on iron-catalyzed cross-coupling reactions of alkyl halides, the tandem reaction protocol was not investigated in detail. We have demonstrated that tandem cyclization and alkyl-aryl cross-coupling of primary and secondary alkyl iodides with aryl Grignard reagents can be realized by using an FeCl₂ catalyst to afford arylmethyl-substituted heterocycles; a range of arylmethyl substituted pyrrolidines and tetrahydrofurans. Several experimental results, such as stereochemical outcome of secondary iodide substrate and intermediate identification with TEMPO, support the radical process of this catalytic system. In future studies, we aim to discover efficient tandem reactions expanded by this versatile iron catalysis to fully explore its preparative scope.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-4**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 이선우

Dual-Color Imaging of Cytosolic and Mitochondrial Zinc Ions in Live Tissue With Two-Photon Fluorescent Probes

RATHORE KAILASH 조봉래*

고려대학교 화학과

Zinc ion is an essential trace metal ion that plays important roles in the mammalian cells as catalytic or structural cofactors.¹ A small fraction of the total zinc ion content, exist as cytosolic free Zn^{2+} . Since low nanomolar concentration of free Zn^{2+} can be cytotoxic, it is vital to maintain Zn^{2+} homeostasis. If the $[Zn^{2+}]_c$ level is elevated by the influx of Zn^{2+} , the excess is removed by shuffling Zn^{2+} to subcellular stores such as endoplasmic reticulum and mitochondria and by transferring Zn^{2+} to extracellular space.² To visualize such processes in a live tissue, it is crucial to develop TP probes that can simultaneously detect the Zn^{2+} in different organelles.

Simultaneous detection of Zn^{2+} in the two organelles was not yet possible as the TPEF maxima of the available probes were too close to detect independently. We, therefore, have developed TP probes for cytosolic Zn^{2+} (BZn-Cyto) and mitochondrial Zn^{2+} (FZn-Mito), which emit TPEF at widely-separated wavelength regions upon binding with Zn^{2+} . TP fluorophores used to derive BZn-Cyto and FZn-Mito, exhibited significant TP cross section and emitted TPEF at 469 and 529 nm in aqueous buffer, where as the Zn^{2+} chelators utilized of various K_d values are within the range of expected Zn^{2+} concentration in two organelles. Triphenylphosphonium ion was envisioned as the mitochondrial targeting moiety.³

1. Vinkenborg, Ja. L.; Nicolson, T. J.; Bellomo, E. A.; Koay, M. S.; Rutter, G. A.; Merks, M. *Nat. Meth.* 6, 737-740.
2. Colvin, R. A.; Holmes, W. R.; Fontaine, C. P.; Maret, W. *Metallomic*, 2010, 2, 306-317.
3. Dickinson, B. C.; Chang, C. J. *J. Am. Chem. Soc.* 2008, 130, 9638.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-5**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이선우

Highly Environmentally Benign Protocol for Synthesis of Quinazolinones via Aerobic Oxidation in DMSO

김라연 천철홍*

고려대학교 화학과

Quinazolinones are very important scaffolds in biologically and pharmacologically compounds, natural products, and materials science. Consequently, great efforts have been made to develop efficient methods for the synthesis of these important building blocks. However, the methods previously developed have some limitations, such as the need to use stoichiometric or super-stoichiometric amounts of reagents, harsh reaction conditions, production of a considerable amount of waste, and expensive separation process. Thus, it is desired to develop more efficient methods for the preparation of quinazolinones. Herein, we would like to present our recent development for the efficient synthesis of quinazolinones via aerobic oxidation in DMSO without any need of bases and metal co-oxidants. In addition, this protocol was further extended to the synthesis of 2,3-disubstituted quinazolinone derivatives. Since this protocol does not use any other oxidants and metal catalyst and generated water as the only by-product, we further applied the resulting quinazolinones to further transformation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-6**

발표분야: Oral Presentation for Young Organic Chemists

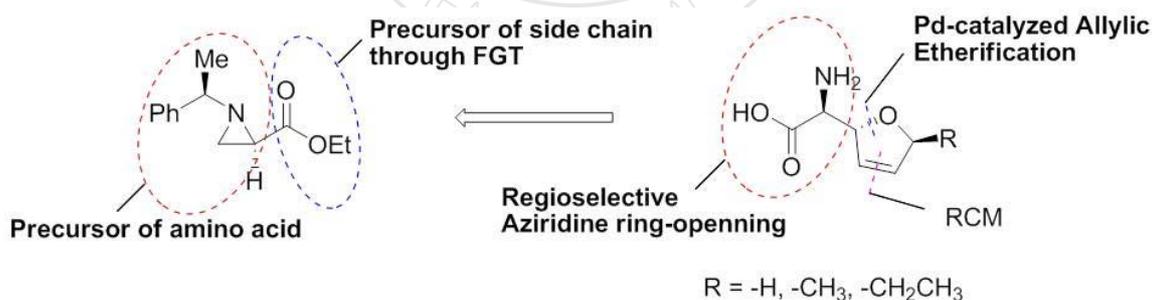
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 이선우

Stereoselective Etherification and Asymmetric Synthesis of Furanomycin from Chiral Aziridines

정재훈 하현준* 이원구^{1,*}

한국의국어대학교 화학과 ¹서강대학교 화학과

The L-(+)-furanomycin as an antibiotic natural amino acid bearing 3,4-dihydrofuran was isolated from the *Streptomyces threomycerius* with antibacterial activity against microorganism such as *E. coli*, *Bacillus subtilis* and several *Salmonella*- and *Shigella* strains. We synthesized furanomycin and its analogues such as norfuranomycin and 5'-ethylnorfuranomycin via the ring-closing metathesis of the diallyl ethers which were generated from the highly stereoselective etherification of branched alkyl part of the requisite ether from chiral aziridine-2-carboxylate.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.O-7**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 이선우

Summary on Development of Acetylcholinesterase Reactivators — antidotes against nerve agents

Kamil Kuca* Kamil Musilek Jiri Kassa Daniel Jun Jana Zdarova-Karasova Ondrej
Soukup Martina Hrabanova Jan Marek Jan Korabecny Vendula Sepsova Rafael Dolezal¹
Martin Kunes¹

*Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech
Republic ¹Biomedical Research Center, University Hospital Hradec Kralove, Czech Republic*

No clinically used acetylcholinesterase (AChE) reactivators (pralidoxime, obidoxime, trimedoxime, MMB-4 and HI-6) can be used as a universal antidote for treatment of nerve agent intoxications. Although oxime HI-6 seems to be the best AChE reactivator, its potency to reactivate tabun and OP-pesticide inhibited AChE is limited. Due to this, hundreds of novel oxime candidates were synthesized and tested for their potency to reactivate nerve agent and OP-pesticide inhibited AChE within last ten years at our department. Two candidates were selected as the most promising reactivators — oxime K027 (against pesticides) and oxime K203 (against tabun). Both compounds together with oxime HI-6 DMS are currently of our high interest and are well investigated in Czech Republic for their potential military and civilian use. In this contribution, summary on results obtained with these compounds will be presented. This work was supported by the grant of Ministry of Health (Czech Republic) No. NT12062 and A long — term organization development plan 1011

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.O-1

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이창연

Hybrid Dielectric Materials for Unconventional Electronic Circuitry

하영근

경기대학교 화학과

Recent advances in semiconductor performance afforded by organic π -electron molecules, carbon-based nanomaterials, and metal oxides have been a central scientific and technological research focus over the past decade for flexible and transparent electronics. However, recent advances in semiconductor require corresponding advances in compatible gate dielectric materials, which exhibit excellent electrical properties such as large capacitance, high breakdown strength, low leakage current density, as well as mechanical flexibility with arbitrary substrates. High-k inorganics such as hafnium dioxide (HfO₂) or zirconium dioxide (ZrO₂) offer some improvements in device performance, but these materials must be very thick to avoid leakage and are difficult to deposit as smooth films on plastics due to high process temperature. Conventional organic/polymeric materials are readily accessible and solution processable. However, these materials exhibit low capacitances, and the corresponding TFTs operate consequently at relatively high voltages. More recently, to combine the desirable properties of high-k metal oxides and organic dielectric processability and mechanical flexibility, a new approach for fabricating gate dielectrics using self-assembled multilayers has emerged. In this presentation, we introduce novel organic-inorganic hybrid gate dielectrics, fabricated by self-assembled multilayer deposition, and its application with unconventional semiconductors. We first present an overview of hybrid dielectric materials for thin-film transistor (TFTs). We next describe the design, fabrication, and applications of solution-deposited organic-inorganic hybrid multilayers, using self-assembly techniques which provide chemical bonding between organic-inorganic layers.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.O-2

발표분야: Current Trends in Materials Chemistry

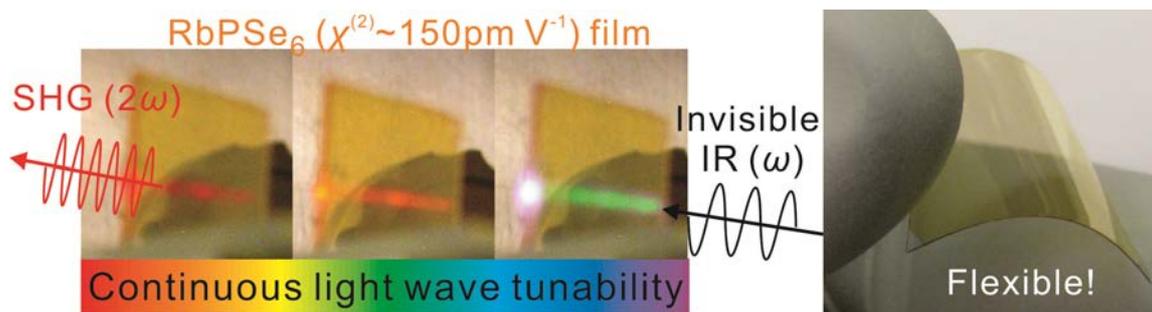
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 이창연

Nonlinear optical glass fibers and thin films for IR applications

정인

한국과학기술원(KAIST) 나노과학기술대학원

Obtaining a new coherent beam of tunable light frequencies is of great importance. Nonlinear optical (NLO) phenomena such as second harmonic and difference frequency generation (SHG and DFG, respectively) are effective at producing a coherent laser in difficult to reach frequency regions of the electromagnetic spectrum. Tunable and coherent IR laser sources in the region of the spectrum between 2-12 μm are especially in high demand. These include remote sensing organic and inorganic molecules for homeland security and environmental monitoring applications as well as minimally invasive medical surgery, and direct imaging of anisotropic biological structures in tissues, cell metabolism and disease states. A main challenge for NLO applications is the costly, lengthy, and labor-intensive process of growing large optical quality single crystals. It is also difficult to fabricate fibers and films of the materials, though many applications require them. Despite excellent formability and inexpensive processing cost, glasses ordinarily lack a second-order optical nonlinearity because of the presence of inversion symmetry at the macroscopic level. In this talk, I will discuss a new concept to prepare strong NLO bulk glasses, fibers, and thin films utilizing noncentrosymmetric phase-change materials without poling. Because of the phase-change behavior of these materials, NLO glass fibers and thin films can convert to crystalline counterparts when annealed, resulting in a huge boost of their NLO properties while maintaining their shape. This approach points to a path that may circumvent some bottlenecks in the practical use of inorganic NLO materials.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.O-3

발표분야: Current Trends in Materials Chemistry

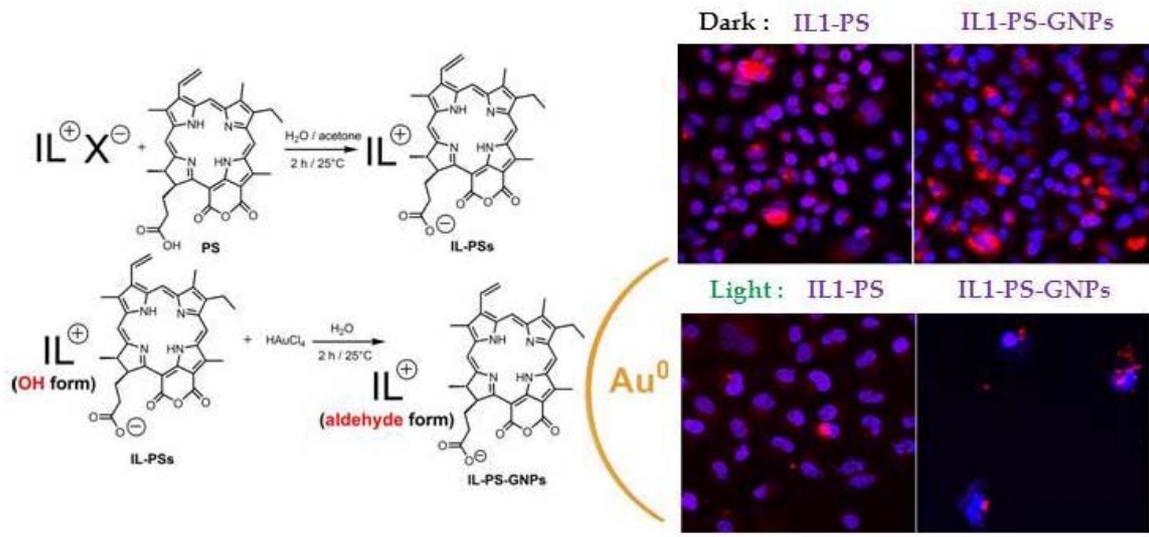
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Gold Nanoparticles of Ionic Liquid Type Purpurin-18 Derivatives for Photodynamic Therapy

윤일* 이태현¹ 심영기¹

인제대학교 PDT 연구소 ¹인제대학교 나노공학부

Photodynamic therapy (PDT) is a promising cancer treatment by using a combination of light, photosensitizer (PS) and oxygen. Generally, most of the PSs are hydrophobic, which may afford disadvantages to make the PSs insoluble under physiological conditions and hinders to reach the accumulation in the tumor sites. For clinical application it is very important to keep suitable hydrophobic/hydrophilic balance of PSs, for which use of gold nanoparticles (GNPs) and ionic liquids type PS (ILPSs) may help PSs capable of increased solubility in aqueous system as well as support attachment of PSs on GNPs surface through stable electrostatic interactions between ILs and PSs. In this work, we used hydrophilic ILPS1 and Au(III) without any additional reducing agents and surfactants. The hydroxyl groups of N-methyl-D-glucamine (NMGA) in ILPS1 have important roles as a reducing agent as well as a stabilizer through the electrically charged functional groups (i.e. carboxylate and amine groups) in forming the PS?GNPs complex 1. Also PS?GNPs complexes 1?5 were prepared from the reaction of different molar ratios between Au(III) and ILPS1 (complex 1, 1:2; 2, 1:4; 3, 1:6; 4, 1:8; 5, 1:10, Au(III):ILPS1) in water to afford different particle sizes and shapes. Finally, different kind of ILs, such as morpholinium, cholinium, imidazolium, and ammonium type, of Pu-18 (ILPSs 2?5) were used to prepare PS?GNPs complexes 6?9 and their PDT effect was investigated. The PS?GNPs complexes showed higher cell viability compared to the corresponding free ILPSs, respectively, due to higher cell penetration based on excellent delivery effect of the GNPs, and relative PDT activity difference among the complexes was depend on the property of the ILPSs (e.g. different reduction strength of Au(III)).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.O-4

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이창연

A design strategy for light-responsive palladium complexes

한민아

Nagoya University, Japan

We report the important determinants of stabilizing azobenzene-based palladium complexes capable of undergoing repeated light-triggered conformation changes. Inspired by highly warped palladium complexes with distorted azobenzene ligands, three different types of azobenzene ligands were chosen to modify both the molecular structure and the solubility of the azobenzenes in organic solvents. Single-crystal X-ray structure analyses were carried out for ortho-alkylated azobenzene (ortho-Az: 1b), meta-alkylated azobenzene (meta-Az: 2b) and PdCl₂(ortho-Az)₂ (1-Pd). Whereas both 2b and 3 had planar structures, ortho-alkylated 1b was highly distorted by 68.06° from planarity. In stark contrast to PdCl₂(meta-Az)₂ (2-Pd) and PdCl₂(Az)₂ (3-Pd), which were quickly dissociated in organic solvents, 1-Pd was very stable in nonpolar solvents. 1-Pd underwent repeated conformation changes under alternating UV and visible light irradiation. The breaking rate of the N:→Pd bond increased in the order of benzene < dichloromethane < acetone < DMF, with more polar solvents inducing faster dissociation. The solvent polarity effect on the stability of azobenzene-based complexes can be interpreted in terms of the degree of polarization of the metal-ligand bond formed as a consequence of interactions between the palladium ion as a soft acid and azobenzene nitrogen as a hard base.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.O-5

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 황윤정

Ultrasmall iron oxide nanoparticles: Synthesis, biomedical application, and characterization by mass spectrometry

김병호 **현택환***

서울대학교 화학생물공학부

Ultrasmall iron oxide nanoparticles exhibited very interesting magnetic properties and investigated as high-resolution blood pool T1 MRI contrast agents. We also proposed the use of MALDI-TOF MS to accurately characterize the sizes and size distributions of < 5 nm iron oxide nanoparticles. We have devised an equation whereby the mass data can be easily converted to size information. The converted size distribution data distinguished size differences as small as 0.1 nm, which is very difficult to achieve with conventional techniques, and the method was successfully applied to study the growth mechanism of nonfluorescent iron oxide nanoparticles.

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장소: 창원CECO

발표코드: MAT.O-6

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 황윤정

Surface Plasmon Induced Enhancement in Förster Resonance Energy Transfer Based Light Emission in Hybrid QDs-Dye Systems

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이화여자대학교 화학나노과학과

Förster resonance energy transfer (FRET) is a nonradiative energy transfer from the excited state donor to the ground state acceptor by dipole-dipole interactions. The advantages of FRET can be effectively used in optoelectronics and photovoltaic devices. FRET efficiency is strongly influenced by spectral overlap and separation distance between donors and acceptors. Quantum dots (QDs) are considered as very useful donors in FRET due to the simplicity to tune their optical properties by changing their size. Nevertheless, due to the distance dependence on FRET, the efficiency of FRET is limited. Presence of plasmonic metals nanoparticles (NPs) in the vicinity of QDs can either quench or enhance the intensity of emission of QDs, which is mainly dependent on the size and distance from the QDs. A close contact between QDs and metal NPs leads to direct energy transfer (DET) from metal to QDs, resulting in the quenching of emission, whereas plasmonic resonance energy transfer (RET) from metal NPs to QDs overweighs the DET if the metal NPs and QDs are separated by a thin insulating layer. This eventually enhances the emission of donor, i.e., QDs, and the improved emission energy of the donor can be transferred to the acceptor via FRET. Therefore, an improved emission from the acceptor induced by RET is expected. Here, we study the RET induced enhancement in FRET between CdSe QDs and Sulforhodamine101 dye using gold (Au) NPs as a probe to study RET. A core-shell type nanostructure was prepared by first coating Au NPs with thin shell of silica followed by decorating the silica surface with CdSe QDs. This core-shell structure was again coated with a second shell of silica, onto which dye molecules are adsorbed. The first shell of silica acts as the spacer between Au and QDs and second as the spacer between QDs and dye. The thickness of both the shells was varied to define the optimum distance for effective RET and FRET. Transmission electron microscopy was used for the structural analysis of core-shell nanostructures. Photoluminescence (PL) spectra and steady-state fluorescence spectra were used to study the enhanced

FRET and change in life time of QDs, respectively. In the first step, RET from Au NPs was studied using PL spectra and it was observed that the emission intensity of CdSe QDs was enhanced in the presence of Au NPs. In the second step, concurrent RET and FRET phenomena in Au@SiO₂@QD@SiO₂@Dye nanostructures were studied. The result was then compared with the QD@SiO₂@Dye core-shell structure. It was observed that efficiency of FRET is significantly improved in the presence of Au NPs, showing the effective transfer of surface plasmon resonance energy from Au NPs to the QDs.



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발표코드: MAT.O-7

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 12:05, 좌장: 황윤정

Fabrication of nanostructured heterophase $\text{Bi}_2\text{Te}_3/\text{Bi}_2\text{O}_5\text{Te}$ and their thermoelectric properties

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We report a facile method for the fabrication of heterophase $\text{Bi}_2\text{Te}_3/\text{Bi}_2\text{O}_5\text{Te}$ nanostructured bulk thermoelectric materials via a simple route involving solution process and spark plasma sintering (SPS). Highly uniform Cu-doped Bi_2Te_3 and undoped Bi_2Te_3 nanostructures are initially synthesized through a simple and fast solution process by using ultrathin Te nanowires as sacrificial templates. Upon SPS consolidation of both types of Bi_2Te_3 nanostructures, only Cu-doped Bi_2Te_3 nanorods are transformed to nanoscale heterostructured phase with Bi_2Te_3 nanograins and $\text{Bi}_2\text{O}_5\text{Te}$ interfaces after sintering. Unlike undoped Bi_2Te_3 , $\text{Bi}_2\text{Te}_3/\text{Bi}_2\text{O}_5\text{Te}$ heterophase nanostructured bulk sample shows drastically reduced thermal conductivity due to the synergetic effect of nanosize and grain boundaries through phonon scattering and energy-barrier scattering. As a result, the ZT value of $\text{Bi}_2\text{Te}_3/\text{Bi}_2\text{O}_5\text{Te}$ heterophase is significantly enhanced (ZT ~ 0.68 at 418K). This approach can be considered as a simple way to manufacture heterostructure in the matrix, thus enhancing thermoelectric figure of merit.

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장소: 창원CECO

발표코드: MAT.O-8

발표분야: Current Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 황윤정

NUV-LED용 Barium-yttrium-orthosilicate 백색 형광체 합성 및 특성 연구

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LED 용 형광체 모체로 새로운 Ba₉Y₂Si₆O₂₄ 를 간단히 고상법으로 합성하였다. X 선 회절 결과를 통해서 orthosilicate 류의 tetrahedral 의 단일상 구조를 확인하였다. Eu³⁺와 Eu²⁺를 성공적으로 Ba₉Y₂Si₆O₂₄ 모체에 치환하였으며, Eu 를 모체의 Ba 와 Y 자리에 치환함으로써 발생하는 특성을 여기와 발광 PL 스펙트럼을 이용하여 관찰 하였다. 합성된 발광재료의 농도에 따른 상대적 발광세기와 CIE 값 계산으로 생성된 밝은 초록색과 붉은색 형광체를 확인되었다. 모체에 Eu²⁺와 Mn²⁺를 공동 치환하여 에너지 이동 특성을 관찰하였으며, NUV 영역의 여기원을 이용한 녹색과 오렌지색이 혼합된 백색 빛을 확인하였다. Eu²⁺로부터 Mn²⁺의 에너지전이 메커니즘에 대한 논의를 하였으며, Eu-Mn 이 공동 치환된 Ba₉Y₂Si₆O₂₄ 형광체는 NUV 영역의 여기원을 가지는 백색 형광체로 NUV-LED 용 형광체로 유용할 것으로 예상된다.

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장소: 창원CECO

발표코드: **ELEC.O-1**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김주훈

Electrochemical Glucose Sensors Based on an Ionic Liquid of a Gold Nanocluster

곽규주 이동일*

연세대학교 화학과

Ionic liquids have found many applications in electrochemical sensors due to their ionic conductivity and electrochemical stability over wide potential window. In particular, Ionic liquids maintain the bioactivity of enzymes and reaction rate that makes them ideally suited for the development of biosensors. In this talk, we present that a stable molten salt of a quantum-sized gold nanocluster can be prepared by ion-pairing of a Au₂₅ nanocluster protected with (3-mercaptopropyl)sulfonate with ionic liquid, 1-decyl-3-methylimidazolium, and its application for the detection of glucose based on its unique electrochemical and biocompatible properties. To prepare electrochemical biosensor, the glucose oxidase (GOx) was immobilized in the Au₂₅ molten salt, which was subsequently cast on a glassy carbon electrode to form modified electrodes. The cyclic voltammogram of the modified electrode exhibited well-defined and reversible redox peaks corresponding to Au₂₅^{0/1-} and Au₂₅^{+1/0}. The electrochemical sensor showed dramatic enhancements in the anodic and cathodic peak currents upon the addition of glucose. The electron transfer dynamics in the modified electrode was investigated as a function of Au₂₅, which manifests the dual role of Au₂₅ as redox mediators as well as electronic conductors controlling the sensing sensitivity. In addition, the fact that redox peak currents were increased as the addition of GOx suggests the Au₂₅ molten salt acts as an excellent support for the enzymatic reaction.

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장소: 창원CECO

발표코드: **ELEC.O-2**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 김주훈

Electrodeposition of Triangular Rod Pd nanostructures and Their Electrocatalytic and SERS Activities

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충북대학교 화학과

Electrocatalytic and surface enhanced Raman scattering (SERS) activity were investigated at palladium nanostructures electrodeposited on Au surfaces. Scanning electron microscopic and transmission electron microscope images show that the Pd nanostructures contain unique triangular rod shape. Triangular rod Pd structures exhibit highly electrocatalytic activity for oxygen reduction reaction (ORR) and methanol oxidation. Cathodic peak potential for ORR on triangular Pd is observed at ~200 mV more positive potential than that on the bare Pd surfaces. It was similar to bare Pt electrode. The anodic peak current for methanol oxidation is greater than bare Pd electrode. Moreover, triangular rod Pd provided efficient SERS activities. The SERS enhancement factor was estimated to be greater than 1600. The unique morphology and surface orientation of triangular Pd demonstrate high electrocatalytic activities and efficient SERS activities. [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. 2012H1B8A2026112)]

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장소: 창원CECO

발표코드: **ELEC.O-3**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 김주훈

Hollow TiN Nanowires Array Prepared via Nanoscale Kirkendall Effect for an Electrode Substrate in Supercapacitor Application

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The development of an electrode substrate with large surface area and high electrical conductivity is of great importance for highly efficient electrochemical devices. We synthesized a noble substrate, hollow TiN nanowires array, which can meet the demand for the ideal substrate. Single crystalline, rutile TiO₂ nanowires integrated on carbon paper were transformed into polycrystalline, hollow TiN during a hot nitridation process. Our in-depth investigation revealed that this transformation took places via nanoscale Kirkendall effect. As the TiN nanowires array had a large surface area, high electrical conductivity and mechanical stability, it would be potentially useful in the electrode substrate for energy storage devices such as supercapacitors. When employed as substrate for Ni(OH)₂ in supercapacitor application, the TiN nanowires array exhibited a superior performance than tis counterparts.

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발표코드: **ELEC.O-4**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김주훈

Photocatalytic Reduction of Azobenzene Using ZnO - Noble Metal Nanoparticles Composites

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연세대학교 화학과

This presentation describes metal effect on the catalytic activities of ZnO nanoparticles coated with noble metal nanoparticles with diameters of 2.4nm (metal = Au, Ag, Pd, and Pt). The ZnO-metal composites were prepared by anchoring glutathione-protected metal nanoparticles on ZnO surface and photocatalytic experiments were conducted with composite colloids under UV-vis light ($\lambda > 320$ nm) in a deaerated 1:1 (v/v) EtOH-H₂O medium. The photocatalytic activity of bare ZnO was found negligible, comparing with ZnO-noble metal composites for reduction of azobenzene. The photolysis time($t_{1/2}$) corresponding to 50% reduction of azobenzene was 1.5 min with ZnO-Pd composites which was at least 10 times higher than that of ZnO-other noble metal composites. Similar metal effects have been found in electrocatalytic measurements. In trifluoroacetic acid medium, current reached to 550 μ A and 450 μ A for ZnO-Pt and ZnO-Pd which are 5 fold higher than that of ZnO-Au and ZnO-Ag. Through product analysis of photocatalytic measurements, it was observed that azobenzene has been reduced to hydrazobenzene, accompanying with 2 electron and 2 proton transfer, which is called hydrogenation reaction. It is known that proton is easy to bind with Pd and Pt, and its bonding strength is proper for catalytic hydrogenation. These results demonstrate that the photolysis activity of the composites can be controlled by metal nanoparticles, and the proton is playing an important role in catalytic reduction of azobenzene using ZnO-noble metal composites.

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장소: 창원CECO

발표코드: **ELEC.O-5**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 장병용

Chitosan based redox polymers for electrochemical sensing platform

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Chitosan is a bio-polymer obtained from the partial deacetylation of the chitin which is major component of the shells of the crustaceans like crabs, shrimps. Chitosan possess plenty of free amine and hydroxyl groups which can be used for immobilization of redox moieties. Chitosan crosslinked osmium polymer (PVP-Os) via glutaraldehyde is prepared and used for the electrode modification. Chitosan-PVP-Os film electrode shows enhanced electrochemical properties. Enzyme immobilized in the chitosan / PVP-OS composite shows enhanced catalytic performance for the glucose sensing. Hydroquinone derivatives linked to free amine of chitosan are synthesized and its nanocomposite with the carbon nanoparticles is prepared. The nanocomposite modified electrode shows selective ascorbic acid detection at lower overpotential. The catechol link chitosan composite shows the NADH detection at lower overpotential with high sensitivity. Metal salen complexes of the Fe, Cu and Ni were linked to chitosan and their composites modified electrode shows hydrogen peroxide sensing. Simple methods of preparations, formation of stable nanocomposite film makes chitosan as an important polymeric biosensing platform.

References

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일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.O-6**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 장병용

Tuning of the electrocatalytic activities of Au electrodes

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부산대학교 화학과

Much effort has been devoted to achieving high activities via morphology or composition control and/or via thermal, cathodic, or chemical treatment. Nevertheless, the dependence of electrocatalytic activities on aging has never been investigated. If electrocatalytic activities of nanomaterials or bulk electrodes change with aging, the activities measured just after their preparation or pretreatment does not represent normal ones. The electrocatalytic activities of Au electrodes are enhanced by NaBH₄ treatment (dipping electrodes in NaBH₄ solution), mechanical polishing or by piranha treatment. However, the enhanced activities slowly decrease with aging. Moreover, Au nanoparticles freshly prepared also show high electrocatalytic activities, but the activities slowly decrease with aging both in air and in solution. This deactivation becomes faster by treatment with Fenton's reagent on gold electrode. The electron-transfer rate and surface roughness of Au electrodes can be decreased simply by ultrasonic treatment. It seems that the hydroxyl radical generated during ultrasonic treatment plays an important role, as in the case of treatment with Fenton's reagent.

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장소: 창원CECO

발표코드: **ELEC.O-7**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 장병용

Spatially Selective Electroplating on Native Oxide-Covered Amorphous Hydrogenated Silicon by Localized Illumination

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서울대학교 화학부

Electrodeposition on photoconductive amorphous hydrogenated silicon (a-Si:H) by localized illumination demonstrated. It is conventionally believed that the electrochemical fabrication of two-dimensional patterns needs pre-patterned electrodes or masks, and that the native oxide layer on Si substrates, which acts as an insulating barrier, should be carefully removed before the electrochemical processes. In this work, we show the electrochemical dot patterning of amorphous MoO_yS_z and nanoparticles of Pt and CdSe, which were stable without any stabilizer and exhibited good adhesion to the oxide surface of a-Si:H. This process required neither pre-patterned electrodes nor masks. Photoelectrochemical measurements and electrochemical impedance spectroscopy revealed that electrochemical reduction in the presence of the native oxide film without etching to remove the oxide layer can be tuned via the potential applied, the duration of the potential pulse, and the pH of the electrolyte.

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장소: 창원CECO

발표코드: **ELEC.O-8**

발표분야: Young Electrochemists Symposium

발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 장병용

Electrochemical investigation of the electrolyte with binary redox couples for high-voltage dye-sensitized solar cells (DSSCs)

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The redox electrolyte is one of the key components of the DSSC and its properties have great influence on both the efficiency and stability of the devices. The difference between the quasi-Fermi level of TiO₂ photoelectrode under illumination and the redox energy level of the electrolyte is considered as the theoretical maximum value of open-circuit voltage (V_{oc}). Since, V_{oc} is highly dependent on the electrochemical potential of redox couple in the electrolyte, a number of redox mediators including bromine, pseudohalogens, organic redox couples, and cobalt-complex redox couples have been studied to replace I⁻/I₃⁻ couple for higher V_{oc}. Meanwhile, a redox couple of more positive potential is expected to offer a larger value of V_{oc}, none of them were successful in rivaling I⁻/I₃⁻ in reaching a higher photovoltaic performance mostly due to the significant retardation of dye regeneration. In this view, we have prepared and characterized a series of novel electrolytes with binary redox couples for high-voltage DSSCs. It was found that the additional interhalogen/pseudo-interhalogen based redox ion, I₂Br⁻, I₂SCN⁻ can be formed by both chemically and electrochemically in I⁻/I₃⁻ based classical system. It was found to produce extra redox pairs, (I⁻,Br⁻)/I₂Br⁻, and (I⁻,SCN⁻)/I₂SCN⁻ with new energy states at a more positive potential than that of I⁻/I₃⁻. The Fermi levels of those electrolytes shifted positively by the weighted-average of the two redox systems. They induced the increase of V_{oc} up to 30, 60, and 50 mV for N719, Ruthenizer 505, and eosin Y dyes, respectively, which, eventually, resulted in the enhancement of the overall power conversion efficiency (η) up to 8, 14, and 13%, respectively. This study offers a very promising strategy to develop a novel electrolyte of which the energy level can be controlled by introducing an additional redox species with more positive potentials without compromising the rate of regeneration of dyes.

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장소: 창원CECO

발표코드: **EDEC.O-1**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 고한중

KSA 2Rs' Experienced-Based Learning Programs for Science-gifted Students

오진호* 천만석¹

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한국과학기술원부설 한국과학영재학교는 2003 학년도부터 미래를 선도하는 과학영재교육기관의 비전을 가지고, 일류에 공헌할 수 있는 있는 창의적인 글로벌 리더를 양성해오고 있는 한국 최초 과학영재학교이다. 한국과학영재학교는 속진 및 심화 중심의 교육과정과 창의 연구활동과 리더쉽 활동을 근간으로 하는 교육과정을 통해 지난 10년간 우수한 수학, 과학영재학생들을 배출해오고 있다. 본 연구에서는 한국과학영재학교에서 미래 세계를 선도해 나갈 우수한 수학자 및 과학자로 성장할 수 있는 잠재력을 가진 과학영재학생들을 위한 한국과학영재학교의 교육과정 프로그램을 소개한다. 특히 한국과학영재학교 학생들이 미래 우수한 과학자로 성장하는데 도움을 줄 수 있는 KSA 2Rs' Experienced-Based Learning Programs for Science-gifted Students 인 KSA Research& Education Program 과 국제공동연구 프로그램의 운영 결과를 설명한다. KSA 2Rs' Experienced-Based Learning Programs for Science-gifted Students 을 통해 한국과학영재학교 학생들은 글로벌 리더로서의 자질을 함양하고 있다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **EDEC.O-2**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 고한중

중학교 일정성분비의 법칙 수업에서 드러난 과학교사의 PCK 연구

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이 연구의 목적은 중학교 일정성분비의 법칙 수업에서 드러난 과학교사의 PCK 와 PCK 형성에 영향을 준 요인에 대해 알아보는 것이었다. 이를 위해 이 연구에 참여한 과학 교사 8 명에 대한 수업 녹화, CoRe 질문지, 면담으로 자료를 수집하였다. 연구 결과, 교사들의 과학교수지향은 탐구적 활동지향, 비탐구적 활동지향, 상호작용 중심 강의지향, 내용전달 중심 강의지향으로 범주화 할 수 있었는데, 이는 수업경험을 통해 얻은 학습자의 내용 이해를 바탕으로 형성된 교사 개인의 고유한 신념임을 알 수 있었다. 교사들은 학습자의 내용 이해에 효과적인 교수전략을 수업목표와 관련지어 교육과정목표를 인식하였으며, 선수학습과의 연계 및 수업내용 재구성은 대체적으로 일정성분비의 법칙에 대한 수업경험이 많은 교사일수록 그 수행수준이 높았다. 이로부터 교사들의 교육과정에 대한 지식은 과학교수지향과 밀접하게 관련된 요소이며, 교수 내용에 대한 수업경험이 많을수록 발달함을 알 수 있었다. 많은 교사들은 교수내용 구성 과정에서 학습자의 학습 가능성을 고려했으며, 학습자의 학습 어려움을 고려하여 수업을 진행한 정도는 선수학습과의 연계 및 수업내용 재구성에 대한 분석 결과와 일치했는데, 이는 선수 학습내용을 본시학습 내용과 연계하고 수업 내용을 재구성하는 것은 학습자의 학습 어려움을 덜고 이해도를 높이기 위한 방안이기 때문으로 판단된다. 또한, 교사들이 활용한 교수전략의 특성으로부터 교수 전략에 대한 지식은 교사의 교수지향을 명시화시켜주는 요소임을 알 수 있었다. 과학교사들의 PCK 형성에 영향을 준 요인은 수업경험을 통한 반성적 사고, 동료교사와의 상호작용, 교육환경에 대한 고려, 학습자로서의 수업 및 연수내용, 교사 자신의 흥미와 호기심으로 나타났다. 그 중에서 가장 큰 영향을 준 요인은 수업 경험을 통한 반성적 사고였으며, 교사 자신의 흥미와 호기심은 비록 부분적으로 나타났다지만 과학교수지향에 매우 강력한 영향을 주는 요인으로 작용하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **EDEC.O-3**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 유미현

멘토링이 멘토의 효능감과 멘티의 만족도에 미치는 영향

이동원 남정희* 이수지 이순덕

부산대학교 화학교육과

멘토링은 교사 교육의 주요한 방법 중 하나로 사용되고 있지만, 실제 멘토링이 교사들에게 미치는 효과는 여러 요인의 영향을 받는다. 멘토와 멘티가 가지고 있는 멘토링에 대한 인식 또한 멘토링의 효과에 영향을 주는 요인 중 하나가 될 수 있으며 이는 세부적으로 멘토가 스스로 멘토로서 역할을 해낼 수 있는지에 대한 효능감 부분과 멘티가 멘토링을 통해서 지원을 받는다고 느끼는 정도에 대한 만족도로 나눌 수 있다. 멘토의 효능감과 멘티의 만족도가 높다면, 멘토링에서 더욱 큰 변화를 기대할 수 있을 것이다. 이 연구에서는 멘토링 사전, 사후에 멘토와 멘티가 각각 효능감과 만족도 검사를 실시하고 여기서 나타나는 변화를 수업동영상, 멘토링 대화, 저널등과 함께 분석하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **EDEC.O-4**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 유미현

페이스북을 활용한 예비 화학교사 대상의 e-멘토링

차정호

대구대학교 과학교육학부

이 연구에서는 소셜 미디어 중 하나인 페이스북을 활용하여 예비 화학교사들이 학교현장실습(구 교육실습) 기간 동안 e-멘토링을 실시하는 방안을 탐색하였다. 학교현장실습이 진행되기 전에 예비 화학교사를 대상으로 페이스북 활용 및 e-멘토링의 취지에 대하여 안내한 뒤 사용방법을 익혔다. 실습이 진행되는 한 달간 실습지도교수 및 선배 교사가 멘토로 활동하였다. 멘토링은 페이스북의 "그룹" 기능을 통해 닫힌 사용자 모임의 형태로 진행되었다. 실습이 끝난 뒤 예비 화학교사 및 선배 교사를 대상으로 페이스북 활용 및 e-멘토링에 대한 인식을 조사하였다. 이번 발표에서는 e-멘토링을 실행하는 시스템으로서의 페이스북에 대한 특징과 활용 경험을 소개할 것이다.

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장소: 창원CECO

발표코드: POLY.P-1

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-dimensional AgX Nanowires/Nanotubes for Sunlight-driven Nanophotocatalysts with High Performance

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Our study proposes a novel strategy for the synthesis of Ag derivatives (AgX@Ag (X = Cl and Br) or Ag nano/microtubes) using the controlled chemical reduction or electron-beam irradiation of AgX nanowires (NWs), which were formed from the controlled dewetting of a AgX thin film on colloidal particles. The size of the AgX@Ag and Ag nano/microtubes can be controlled using the AgCl NWs as templates and varying the concentration of NaX. By controlling the concentration of NaBr, heterojunction-structured AgCl/AgBr NWs (H-AgCl/AgBr NWs) can be produced from the AgCl NWs due to a partial ion-exchange reaction (low concentration), and the AgBr NWs produced after a complete ion-exchange reaction between Cl⁻ and Br⁻ were further grown into micrometer-sized AgBr wires (high concentration). The resulting AgX NWs can be transformed into corresponding AgX@Ag or Ag nano/microtubes via a controlled chemical or physical method. The AgX derivatives (AgX@Ag nanotubes (NTs) and AgX NWs) were tested as visible-light-induced photocatalysts for decomposition of methyl orange.

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장소: 창원CECO

발표코드: POLY.P-2

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rattle-typed hierarchical particles containing multilevel of cores (Ag@AgCl@SiO₂ and Au/Ag@AgCl@SiO₂) for versatile nanocatalysts

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A novel protocol for the synthesis of rattle-typed core@shell particles containing Ag@AgCl or Au/Ag@AgCl core structures has been introduced, and their use as catalysts for decomposing toxic materials has been demonstrated. A monometallic Ag or bimetallic Au/Ag core was incorporated into the interior of SiO₂ capsules via controlled heat treatment of the metal nanoparticle/SiO₂-coated polymer particles and it resulted in the formation of rattle-typed core@shell structures. By appropriate treatment, it was possible to transform the Ag or Au/Ag core into the multilevel of core (Ag@AgCl or Au/Ag@AgCl) within the SiO₂ capsules (Ag@AgCl@SiO₂ or Au/Ag@AgCl@SiO₂). This novel method for rattle-typed core@shell particles is useful for further introducing AgCl fused with plasmonic materials into the capsule structures. The rattle-typed core@shell structures have been firstly used as photocatalysts for decomposition of organic pollutants such as methyl orange. Furthermore, nanocatalyst incorporated semiconductor such as AgX also newly applied for reduction of nitrophenol (NPh) to aminophenol (APh). The Ag@AgCl@SiO₂ or Au/Ag@AgCl@SiO₂ catalysts showed excellent catalytic properties for the decomposition of toxic substances in terms of their activities and reuses.

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장소: 창원CECO

발표코드: **POLY.P-3**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

C5 유분을 활용한 Cyclo Olefin Polymer 의 제조 및 응용

박원진

코오롱유화(주) 석유수지 연구소

과거 원유를 크래킹하여 나온 C5, C9 유분은 활용가치가 떨어져 저가의 연료로 사용되어 지거나 폐기처분하여 버려졌다. 하지만 코오롱은 1980년대 이후 이러한 유분을 원료로 점접착부여수지를 개발하여 현재 국내 1위, 세계 3위의 생산 및 판매량을 기록하고 있다. 또한 이러한 유분을 이용한 고부가가치와에 대한 관심이 증가하고 있으며 특히 C5 유분 중 Dicyclopentadiene (이하 DCPD) 를 이용하여 상업적으로 부가가치가 높은 Cyclo Olefin Polymer (이하 COP) 를 제조하는 연구가 활발히 이루어지고 있다.

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장소: 창원CECO

발표코드: POLY.P-4

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic nonvolatile memory transistors with polymer energy well structure

남성호 김화정 이문호¹ 김영규*

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Organic memory devices have recently attracted keen attention because of their potential for next generation electronic memory that requires ultrathin, lightweight, flexible and diverse shaped features. In addition, organic memory devices are expected to be cost-effectively manufactured if whole fabrication step is carried out using roll-to-roll (R2R) processes at room temperature. Various types of organic memory devices have been reported so far, but two major structures (resistor-type and transistor-type) have been extensively studied. Considering the simplified device structure in the integrated circuits, transistor-type memory devices have attractive merits over the resistor-type devices. Very recently we invented new category of transistor-type memory devices with a polymer energy well structure that is formed by sandwiching high k polymer nanolayer between low k nanolayers for stable storage of charge carriers. The detailed working principle and outstanding retention characteristics will be discussed in this presentation. Organic memory devices have recently attracted keen attention because of their potential for next generation electronic memory that requires ultrathin, lightweight, flexible and diverse shaped features. In addition, organic memory devices are expected to be cost-effectively manufactured if whole fabrication step is carried out using roll-to-roll (R2R) processes at room temperature. Various types of organic memory devices have been reported so far, but two major structures (resistor-type and transistor-type) have been extensively studied. Considering the simplified device structure in the integrated circuits, transistor-type memory devices have attractive merits over the resistor-type devices. Very recently we invented new category of transistor-type memory devices with a polymer energy well structure that is formed by sandwiching high k polymer nanolayer between low k nanolayers for stable storage of charge carriers. The detailed working principle and outstanding retention characteristics will be discussed in this presentation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-5

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Co-Vapors on the Microstructures of Polypyrrole Grown by Vapor-Deposition Polymerization

이지은 윤현석^{1,*}

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시스템공학과

We have investigated the effect of co-vapors on the microstructures of polypyrrole (PPy) obtained via vapor-deposition polymerization. Co-vapors, such as short-chain alcohols and alkanes, were introduced with pyrrole monomer together into a reaction chamber. The resulting polymers were characterized by electron microscopies to obtain information about their microstructures. Interestingly it was found that the microstructures of the PPy were highly influenced by the nature of the co-vapors used. Therefore, it is expected that judicious choice of co-vapors in vapor-deposition polymerization can allow control over the structural properties of polymers.

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장소: 창원CECO

발표코드: POLY.P-6

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Reactive Energetic Plasticizers with Clickable Functionality to Control Processing Properties of Castable PBX's

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Plasticizers are additives widely used in the polymer industry. Generally, they are known to improve processability by lowering the viscosity during the formulation as well as impart low temperature flexibility by lowering the glass transition temperature of the polymers. For specific applications in the field of high energy materials, energetic functional groups such as azido, nitro and difluoramino groups have been introduced in the plasticizers, known as energetic plasticizers. It has been one of major issue, especially in the field of high energy materials, to provide energetic plasticizers with new concepts. Hence, this research focuses on the design, synthesis and characterization of reactive energetic plasticizers and their application to polyurethane binders in the formulations castable plastic bonded explosives(PBXs).The reactive energetic plasticizers are synthesized by using either the aldol condensation reaction of alcohol compounds and formaldehyde catalyzed with Lewis acid, or the esterification between corresponding alcohols and carboxylic acids compounds. Structural integrity of the synthesized reactive energetic plasticizer is identified by using elemental analyzer, GC-Mass, 1H and 13C NMR. Plasticization performance and click reaction using reactive energetic plasticizers are also investigated. These results indicate that these reactive energetic plasticizers work properly as a general plasticizer in the beginning of the formation, preferably, of alkyne groups in the plasticizer and azide groups in the prepolymer.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-7**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The sulfamate-Conjugated pH-Responsive Block Copolymers

김혜미 이형일*

울산대학교 화학과

We successfully synthesized pH-Responsive block copolymers based on sulfamate-derivatized groups. Poly(HEMA-TMS) was extended from PEO macroinitiator via atom transfer radical polymerization (ATRP), resulting in PEO-*b*-PHEMA-TMS. TMS groups were deprotected in the presence of KF, and in situ transformed to amino sulfamate groups. The resulting block copolymer was functionalized with trityl groups. This block copolymer can self-assemble into spherical aggregates under physiological conditions. Due to the unique pH-responsive nature of the sulfamate bond, the spherical aggregates can be formed and dissociated reversibly in response to small pH fluctuations in the physiologically accessible range; this leads to self-assembly and disassembly of the aggregates.

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장소: 창원CECO

발표코드: POLY.P-8

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Thermoresponsive Fluorinated Double-Hydrophilic Poly{[N-(2,2-difluoroethyl)acrylamide]-*b*-[N-(2-fluoroethyl)acrylamide]} Block Copolymers

김혜미 이형일*

울산대학교 화학과

Novel thermoresponsive double-hydrophilic fluorinated block copolymers were successfully synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization. Poly[N-(2,2-difluoroethyl)acrylamide] (P2F) was synthesized via RAFT polymerization of N-(2,2-difluoroethyl)acrylamide (M2F) using 2-dodecylsulfanylthiocarbonylsulfanyl-2-methylpropionic acid (DMP) as the chain transfer agent (CTA) and 2,2'-azobisisobutyronitrile (AIBN) as the initiator. The resulting P2F macroCTA was further chain extended with N-(2-fluoroethyl)acrylamide (M1F) to yield poly{[N-(2,2-difluoroethyl)acrylamide]-*b*-[N-(2-fluoroethyl)acrylamide]} (P2F-*b*-P1F) block copolymers with different lengths of the P1F block. Molecular weight and molecular weight distribution were determined by gel permeation chromatography (GPC). The average molecular weight (M_n) of the resulting polymers ranged from 2.9×10^4 to 5.8×10^4 depending on the length of the P1F block. The molecular weight distribution was low ($M_w / M_n = 1.11 \sim 1.19$). Turbidimetry by UV-vis spectroscopy, dynamic light scattering (DLS), and in situ temperature-dependent $^1\text{H-NMR}$ measurements demonstrated that the P2F block underwent a thermal transition from hydrophilic to hydrophobic, which in turn induced self-assembly from unimers to aggregates. Transmission electron microscopy (TEM) studies demonstrated that polymeric aggregates formed from an aqueous solution of P2F-*b*-P1F at 60°C were disrupted by cooling down to 20°C and regenerated by heating to 60°C . Temperature-triggered release of a model hydrophobic drug, coumarin 102, was also demonstrated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-9

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Compressive Stress Relaxation(CSR)을 이용한 가교 시스템별 EPDM 고무의 압축 응력 완화 및 수명의 변화에 대한 연구

이정기

(주)화승알앤에이 FL 재료팀

고무의 압축 응력 완화는 O-ring 혹은 금구류가 체결되는 자동차 호스 제품의 성능에서 가장 중요한 지표이며, 높은 온도와 압력하에서 변형되지 않고 그 형태를 유지하는 데 매우 중요한 역할을 한다. 동일한 폴리머를 사용할 경우 적절한 가교 시스템의 적용이 압축 응력 완화에 큰 영향을 미치게 되며, 이는 Compressive Stress Relaxation (CSR) test 를 이용하면 가장 정확하게 측정될 수 있고 나아가 고무의 수명 예측도 가능해 진다. 본 연구에서는 EPDM 에 각기 다른 가교 시스템(1. Sulfur, 2. Semi- Peroxide, 3. Peroxide)을 적용하여 고무를 배합하였고, CSR test 을 이용하여 고무의 압축 응력의 변화와 수명을 측정해 보았다. 그 결과 Peroxide 적용 배합에서 압축 응력 변화가 가장 적게 나타내어 장기 수명을 보였으며, 이는 Peroxide 의 가교에 의한 폴리머 사슬간의 높은 결합에너지에 의한 것이라고 추측된다. 끝으로 각기 다른 온도에서 측정한 CSR test 결과를 토대로 Arrhenius Plot 을 구성하여 고무의 수명을 예측 할 수 있었고 이러한 방법은 앞으로 고무 수명 측정을 위한 지표로 활용될 수 있을 것이다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-10

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

약물 전달 시스템(Drug Delivery System)에 적용하기 위한 알지네이트의 화학적 변형(Modification)에 관한 연구

최수경 핑기정*

연세대학교 화학과

알지네이트(Alginate)는 DNA(Deoxyribo Nucleic Acid), Oligonucleotides, Cell, Protein 과 같은 물질의 담지를 위한 담지체로서, 약물 전달 시스템(DDS : Drug Delivery System)에서 많은 응용이 이루어져 온 천연 고분자 물질이다. 하지만 알지네이트는 지용성 약물이나 단백질과 같은 물질을 빠르게 배출한다는 단점이 있다. 이런 소수성 물질의 담지율을 높이기 위하여 약물의 제어방출이 이루어져야 하는데 주로 친수성 알지네이트의 화학적 변형(Chemical modification) 방법을 이용한다. 화학적 변형을 통해 알지네이트에 소수성 작용기를 늘려주게 되면 약물의 담지가 늘어나는 효과가 있게 된다. 본 실험에서는 친수성 알지네이트와 여러 가지 알코올류를 이용해서 에스터화 반응(Esterification reaction)을 진행 시켜 알지네이트의 소수성을 향상 시키고자 하였으며, 합성 여부를 푸리에 변환 적외부 스펙트럼의 측정(FT-IR, Fourier Transform Infrared Spectroscopy)과 핵자기 공명 측정(NMR, Nuclear Magnetic Resonance)을 통해 확인해 보았다. 합성된 알지네이트를 이용하여 DDS 에 적용 했을 경우 변화를 살펴 보기 위하여 In vitro release 실험을 수행하였다. 기존의 알지네이트와 소수성이 향상된 알지네이트를 비교함으로써 지용성 약물의 담지 효율의 변화를 살펴보았다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-11**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cross-linkable Polynorbornene Terpolymer with Carbazole Host, Ir(III) Emitter, and Styrene Side Groups

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울산대학교 화학과

Vinyl addition terpolymerization of norbornene monomers functionalized with 9,9'-(1,1'-biphenyl)-4,4'-diylbis-9H-carbazole (CBP), $(ppy)_2Ir(acac)$, or styrene (NB-SM) side groups has been investigated to produce polynorbornene terpolymers with pendant CBP host, Ir(III) emitter, and SM groups by use of Pd(II) catalyst. The catalytic system efficiently leads to soluble copolymers with a controlled amount of Ir(III) moiety. Depending on the content of Ir(III) moiety, the intensity of phosphorescence band was also changed. When exposed to thermal annealing of the polymer film, almost complete crosslinking of polymer chains through the styrene groups occurred, affording an insoluble film. Details of synthesis, characterization, photophysical property, and thermal crosslinking behavior of the terpolymers will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-12

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Three-Dimensional Carbon Nano-hybrids with an Opened Structure for Energy Storage Application

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시스템공학과

We have explored the effect of nanofibers intercalation on the microstructure of graphene sheets. The nanofibers intercalation was readily achieved in solution phase via van der Waals interactions, and the resulting nano-hybrids were characterized by scanning electron microscopy. It was found that the nanofibers intercalation prevented the irreversible aggregation of graphene sheets and allowed an opened microstructure inside the nano-hybrids. It is expected that these structural characteristics will make the nano-hybrids promising candidates for applications in various fields, such as composites, separation/filtration, and energy devices.

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장소: 창원CECO

발표코드: **POLY.P-13**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Adhesive Chitosan via Catechol Conjugation

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Due to the importance of controlled release in oral drug delivery system, efforts have been made to prolong the drug retention in vivo. Yet, drug adhesion to mucus and mucin present in the inner wall of digestive system for satisfying retention time has been a challenging issue. With an overwhelming library of tissue-adhesive polymers available, one practical way to improve adhesion is chemical modification of the existing polymers. In this report, we synthesized sticky chitosan suitable for biomedical applications via simple tethering of catechol groups which are abundantly found in the wet-resistant mussel adhesive proteins. In vitro residual amount of chitosan-c showed four-fold enhancement compared to unmodified chitosan and in vivo retention of chitosan-c was observed for more than 10 hours in stomach and intestine. Our results indicate that conjugation of catechol moieties might be a facile and universal way to enhance the intrinsic adhesive property of the existing polymers.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-14

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses of Poly(glycidyl tetrazole-co-glycidyl triazole)s

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국방과학연구소 4-2 ¹국방과학연구소 4본부 2부 ²국방과학연구소 4-2-5

Triazoles and tetrazoles are nitrogen-rich compounds which have high heat of formation. So they have used as explosive and gas generator. We designed polymer containing both triazole and tetrazole pendants to obtain a good candidate for high energy density material (HEDM). Poly(glycidyl tetrazole-co-glycidyl triazole)s (PGTTs) are synthesized by three steps reaction. First, poly(epichlorohydrin-co-glycidyl tetrazole)s (PEGTs) are synthesized through reaction of PECH with various tetrazoles using NaOH in DMSO. And then PEGTs are reacted with sodium azide in DMSO to get PGATs. Finally, PGATs converted to PGTTs by click reaction using various alkynes. The structures of PGTTs are confirmed by IR, ¹H and ¹³C NMR spectral analyses. Thermal properties of the PGTTs are evaluated using differential scanning calorimetry(DSC).

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장소: 창원CECO

발표코드: **POLY.P-15**

발표분야: 고분자화학

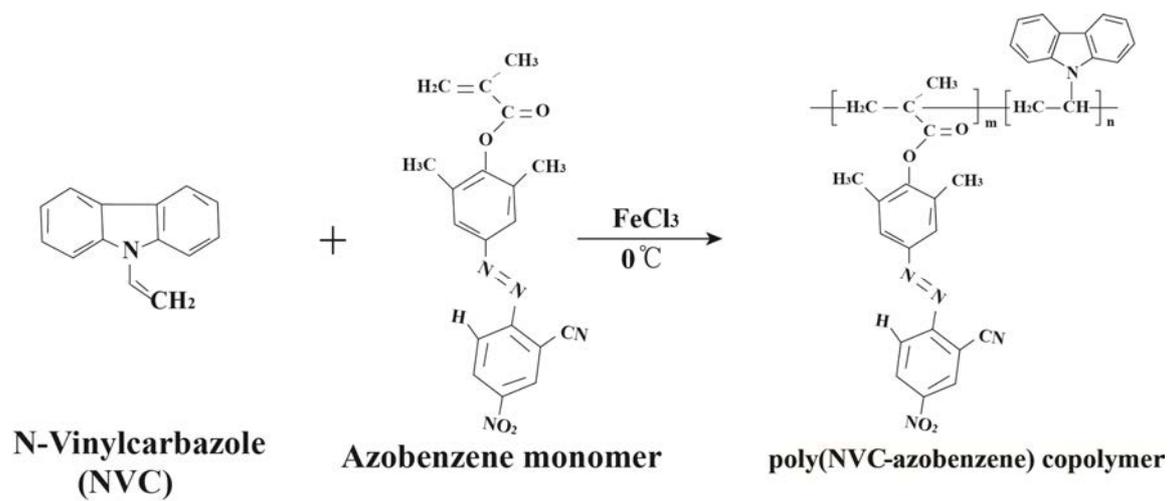
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photo-controlled fabrication of honeycomb-patterned films in poly(N-vinylcarbazole/azobenzene) copolymer

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We have obtained a highly ordered honeycomb-patterned porous film by the help of UV illumination on the fabrication of polymer solution by the breath figure process under humid conditions. For the photo-controlled fabrication, a new type of UV-sensitive polymer that comprises N-vinylcarbazole and azobenzene monomer, poly(N-vinylcarbazole/4-[N'-(2-cyano-4-nitrophenyl)azo]-2,6-dimethylphenol methacrylate, was synthesized and fabricated without addition of an amphiphilic copolymer necessary to hold water droplets on the hydrophobic solution surface as an air-water interface stabilizer. Highly well-ordered regular structure of honeycomb-patterned films was obtained by the illumination of UV light during the fabrication. The effect of UV illumination on the fabrication of the polymer film can be interpreted by the photo-switched isomerization of the azobenzene component in the copolymer from trans- to cis-isomer, which increases the hydrophilicity of the polymer solution inducing the decrease of interfacial tension of the polymer solution for the formation of uniform honeycomb pattern.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-16

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reversible Adsorption-Desorption Oscillations of Silver Nanoparticles on a Patterned P(MMA-EG-NGO) Hydrogel Surface Induced by a pH Oscillator in a Closed Chemical System

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Oscillatory adsorption-desorption of Ag nanoparticles on a pH-responsive hydrogel surface was induced by a pH oscillator in a closed reaction system. The hydrogel surface was prepared as a honeycomb-patterned using a honeycomb-patterned polystyrene as a template to speed up the response time in the stimuli-responsive hydrogel. We composed P(MAA-EG-NGO) Hydrogel, that is pH-responsive Hydrogel. The surface morphology and hydrophobic interaction of the patterned hydrogel surface were significantly altered by the pH change of the aqueous solution that came into contact with the gel. The surface of the hydrogel became hydrophobic for adsorption in a lower-pH solution but became hydrophilic with decreased adsorptivity at higher pH conditions. A closed system chemical pH oscillator composed of Na₂SO₃-K₄Fe(CN)₆-NaHCO₃ at 45 °C was applied to force the periodic adsorption-desorption of Ag nanoparticles on the gel surface. The experimental conditions for the chemical oscillator were optimized to obtain long-lasting high-amplitude pH oscillations in a closed reactor system. The periodic adsorption-desorption was proved to be induced by the periodic pH change in the solution, although the two phenomena synchronized. That is, the periodic time was longer and the number of oscillations was for the adsorption-desorption compared with the pH oscillations that occurred in the solution state. The heterogeneous oscillations obtained in this study clearly suggested that the hydrophobic interaction was reversibly changed in the patterned pH-responsive hydrogel surface, similar to various biological systems in nature.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-17**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly luminescent carbon dots derived from xylitol: Synthetic insights and their biological application

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Fluorescent biological labels including fluorescent organic dyes, engineered proteins and semiconductor quantum dots have received significant attention these days. Carbon dots (CDs) have recently emerged as promising alternatives by virtue of their biocompatibility, low toxicity and high stability retaining excellent optical properties. Herein, we present a facile microwave pyrolysis approach of preparing CDs of controlled photoluminescence using biomass derived sugar alcohol, xylitol. We found that the critical role of both surface passivation agent, ethylenediamine, and HCl additive during the synthesis of CDs in controlling the luminescent properties. Xylitol-derived CDs exhibited bright luminescence and low cytotoxicity in WI-38 cells and HeLa cells, demonstrating their potentials for biological imaging and sensor application.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-18**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of poly(styrene sulfonic acid)-grafted porous PTFE as a substrate of reinforced composite fuel cell membrane

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한국원자력연구원 첨단방사선연구소 공업환경연구부

In this study, poly(styrene sulfonic acid)-grafted porous polytetrafluoroethylene (PTFE) was prepared by a simultaneous irradiation grafting of styrene monomer onto PTFE porous membrane and followed by hydrolysis-condensation and sulfonation to provide hydrophilicity on the super-hydrophobic surface of PTFE. The effects of the degree of grafting and ion exchange capacity of the grafted substrates on the chemical, physical, and morphological properties such as contact angle, gurley number, surface images, and tensile strength were investigated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-19

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of crosslinked SPEEK/1,4-butanediol membrane prepared by an EB-irradiation method

송주명 손준용 신준화*

한국원자력연구원 첨단방사선연구소 공업환경연구부

The crosslinked SPEEK/1,4-butanediol membranes were prepared by the radiation crosslinking of SPEEK with various 1,4-butanediol contents. The crosslinked SPEEK/1,4-butanediol membranes can be used to proton exchange membrane (PEM) for fuel cell applications. The crosslinked SPEEK/1,4-butanediol membrane were investigated by FT-IR, TGA, DMA and SAXS instruments. The FT-IR was used to confirm the sulfonation and crosslinking of the membranes. TGA results indicated that the initial thermal degradation temperature was shifted to lower temperature with increase in the 1,4-butadiol content. With increase in the 1,4-butanediol content, the DMA results observed that the cluster T_g peak area was decreased and SAXS peak maximum position shifted to lower q . It was suggested that the degree of clustering in the crosslinked membrane was reduced with increase in the 1,4-butanediol content. The proton conductivity of all the membrane was more than 10^{-2} S/cm.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-20**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

방사선 그래프팅 기술을 이용한 친수화 다공성 지지체 제조 및 특성연구

박병희 손준용¹ 신준화^{1,*}

한국원자력연구원 공업환경연구부¹ 한국원자력연구원 첨단방사선연구소 공업환경연구부

방사선 그래프팅 방법을 이용하여 PTFE 다공성 지지체에 acrylonitrile(AN)과 친수성 작용기를 가진 sodium allylsulfonate(SAS)를 접목시켜 복합연료전지막의 지지체로 사용되는 친수화 다공성 지지체를 제조하여 물성을 평가하였다. 다양한 물리화학적 분석을 통하여 제조된 지지체에 각 단량체들이 성공적으로 그래프팅 되었음을 확인하였고, 표면의 변화와 친수화 정도를 관찰하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-21**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of crosslinked SPEEK/PVDF membrane using radiation

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한국원자력연구소 첨단방사선연구소 공업환경연구부 ¹한국원자력연구원 첨단방사선연구소
공업환경연구부

Poly(ether ether ketone) [PEEK] has many advantages such as thermal and chemical stability, solvent resistance, high strength, and low cost. It has been widely used for industrial application. In this study, crosslinked SPEEK/PVDF membranes were prepared using an EB-irradiation method with various contents of PVDF. The crosslinked SPEEK/PVDF membrane and non-crosslinked SPEEK/PVDF membrane were investigated by using FT-IR, TGA, DMA, and DSC.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-22

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of Organic/Inorganic Nanocomposite Hybrid Membrane Prepared by Radiation Technology

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In this study, crosslinked nanocomposite SPEEK membranes with various contents of zirconium phosphate [ZrP] particles were prepared using an electron beam. The properties of the prepared membranes such as the morphology, water uptake, and proton conductivity were measured. The SEM-EDX results show that the ZrP particles were well distributed throughout the prepared membrane. The water uptake and swelling ratio of the CSPEEK/ZrP membranes were increased with an increase in the zirconium phosphate [ZrP] particle contents. The proton conductivity results show that the CSPEEK/ZrP membranes exhibit an increased proton conductivity value compared to the CSPEEK membrane.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-23

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ion chelated Polymeric Nanoparticles as a Multifunctional Drug carrier for Cancer Therapy and imaging

박경은 임용택^{1,*}

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In this study, we have produced ion chelated polymeric nanoparticle for cancer imaging and therapy. Ion chelated polymeric nanoparticles were prepared using a solvent emulsion evaporation method to load chlorin e6 (Ce6) and gadolinium (Gd^{+3}). Loaded Ce6 molecules maintained their spectroscopic and functional properties for near infrared fluorescence imaging and photodynamic therapy (PDT). Gadolinium chelated hyaluronic acid coating on the PLGA particle surface and offered the functions of magnetic resonance imaging (MRI). We characterized the physicochemical properties of nanoparticles, efficacy of PDT, fluorescence and MRI imaging performance. These results suggest that ion chelated polymeric nanoparticles have potential for effective cancer treatment and imaging.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-24

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Introduction of sulfonic acid group onto a poly(vinylbenzyl chloride)-grafted poly(ether ether ketone) film for fuel cell application

최지선 손준용¹ 신준화^{1,*}

한국원자력연구소 공업환경연구부 ¹한국원자력연구원 첨단방사선연구소 공업환경연구부

Radiation-induced graft polymerization is known to be a useful method for preparing polymer electrolyte membranes (PEM) for fuel cells. In this work, a poly(vinylbenzyl chloride)-grafted poly(ether ether ketone) film was prepared using a radiation grafting method, and a sulfonic acid group was then incorporated to give a fuel cell membrane. The successful incorporation of a sulfonic acid group was confirmed through FT-IR and SEM-EDX. The physicochemical properties of the prepared membrane for fuel cell application were also investigated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-25

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optofluidic Microcapsulation of Quasi-Amorphous Photonic Materials for Tunable Color Pixels

현진호 서춘희 남지혜 강영종^{1,*}

한양대학교 화학과 ¹한양대학교 자연과학대학 화학과

Self-assembly of colloidal nanoparticles have been extensively investigated not only as fundamental tools for understanding crystallizations but also as building blocks for novel functional materials. Despite their promising optical characteristics such as high reflectivity and broad color expression range, colloidal photonic crystals have not been well investigated for a component of displays because of strong angle dependent hue and poor processibility. Solution-phase colloidal photonic materials can provide ideal solutions for these problems. Our group recently reported that the colloidal solutions exhibit strong photonic colors at certain conditions without forming regular crystalline structure. The colloidal photonic solutions (named with “quasi-amorphous photonic materials”) exhibit unique angle-independent photonic colors, and which are highly tunable by electrochemical stimuli. In terms of the practical applications, the microcapsulation of quasi-amorphous photonic materials are preferred for achieving easy processibility. In this presentation, we report fabrication of the microcapsulated quasi-amorphous photonic materials by using multi-channel microfluidic device, and their applications in photonic display pixels. We showed that nanoparticles modified with conducting polymers are spontaneously assembled into isotropic photonic structures in solution at sufficiently high concentration (15~25 wt%). Furthermore the resulting quasi-amorphous photonic materials can be easily encapsulated into uniform double emulsion type microcapsules by using multi-channel microfluidic device ($d < 500 \mu\text{m}$). The microcapsulated photonic pixels showed vivid photonic colors ($400 \text{ nm} \leq \lambda \leq 650 \text{ nm}$) in response to the external electric field.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-26

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyelectrolyte-Triggered Synthesis of AgBr Nanostructures with Controlled Structures and Sizes

이이슬 이하진¹ 최원산*

한밭대학교 응용화학과 ¹한국기초과학지원연구원 전주센터

Silver/Silver halide (Ag/AgX) has been considered as new visible light-driven photocatalysts owing to good sensitivity to sunlight. The Ag/AgX catalysts display high photocatalytic activity and stability under visible light irradiation due to the SPR of silver nanoparticles produced at the surface of AgX. Recently substantial efforts have been focused on the synthesis of Ag/AgX photocatalysts with high performance using facile and versatile methods. However, most of photocatalysts prepared by reported methods are formlessness or spherical structure with irregular shape. Relatively little attention has been directed to controlling structures of photocatalysts into well-defined structure. It has been well-known that nanomaterials with well-defined structures can exhibit unique properties which are not observed in bulk or nanomaterials with irregular structures. Herein, we report a novel approach for controlling structure and size of AgX structures. We report CTAB-decorated AgBr microplates (MPs) that are obtained by mixing silver precursor with hexadecyltrimethylammonium bromide (CTAB) under controlled conditions. By appropriate polyelectrolytes (PEs) coating, it is able to transform structure of AgBr MPs into submicrometer-sized spherical or cubic shape with controlled sizes. We believe that the PEs which possess certain types of functional groups are the crucial factors that control the structure and size of the AgBr MPs. The size and shape-controlled AgBr cubic NPs can be used as plasmonic photocatalysts for the degradation of methylene orange (MO) dyes that are well known for toxic substances under sunlight irradiation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-27**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thickness effects on the sulfonation of polystyrene-grafted PFA film with a highly cross-linked network

신준화* 손준용

한국원자력연구원 첨단방사선연구소 공업환경연구부

PFA films with various thicknesses were used as a backbone film for the radiation grafting of a styrene/divinylbenzene mixture to give a polystyrene-grafted PFA film with a highly cross-linked network. For sulfonation of the thicker grafted films, it was found that severe sulfonation conditions are needed to provide enough sulfonic acid groups onto the films. The sulfonation process was monitored through IEC and SEM-EDX measurements.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-28

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Physical properties and phase transition of a tetrathiafulvalene molecule

김인수 정광운^{1,*} 이명훈² 송대현³

전북대학교 유연인쇄전자전문대학원 ¹전북대학교 고분자·나노 공학과 ²전북대학교 고분자나노공학과 ³전북대학교 고분자 나노 공학과

As a result of attaching four flexible alkyl chains at the periphery of board-shaped molecule, a symmetric tetrathiafulvalene-base molecule (symTTF11) was newly synthesized. Phase behaviors and physical properties of symTTF11 were further investigated by the thermal, microscopic and scattering experimental techniques. Their phase structures of columnar crystalline phase and a columnar smectic LC phase were indentified. Since the assembled symTTF11 columns were well organized in the ordered layer structures over a macroscopic domain in the columnar smectic LC phase, symTTF11 showed a good charge carrier mobility, which was about two-order of magnitude faster than that in the columnar crystalline phase. This work was mainly supported by Converging Research Center Program (2013K000404), and Human Resource Training Project for Regional Innovation funded by the Ministry of Education, Science, and Technology of Korea.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-29

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dipotassium heteroaryl bis(trifluoroborate)를 단량체로 한 고성능 전자 전달형 유기 및 고분자 트랜지스터 재료의 합성

정석현 이진균*

인하대학교 고분자공학과

본 발표에서는, 쉽고 간편하게 정제가 가능한 monomer 인 heteroatom monomer 의 bis(trifluoroborate)의 합성으로 인해 suzuki polycondensation reaction 에서 높은 분자량의 고분자의 합성을 성공하였다. 그 중, 2-alkylbenzotriazole 의 bis(trifluoroborate)는 Palladium 촉매와 Lithium 계의 염기를 이용하여 다양한 electron-acceptor monomer 와 공중합체를 합성을 진행하였다. 일반적으로 electron-acceptor monomer 와 electron-acceptor 성질을 띄는 2-alkylbenzotriazole 의 합성은 합성이 어렵다고 알려져 있다. 이러한 합성이 어려웠던 electron acceptor 간의 합성을 bis(trifluoroborate)의 도입을 통해 성공하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-30

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photovoltaic Polymer : A Tetrathiafulvalene-based Polymer with Fullerene

김희수 송대현¹ 이명훈 정광운^{2,*}

전북대학교 고분자나노공학과 ¹전북대학교 고분자 나노 공학과 ²전북대학교 고분자 나노 공
학과

A novel photovoltaic polymer (6TTF-polymer) is embedded with electron rich group. Tetrathiofulvalene (TTF) and fullerene (C₆₀) was successfully synthesized and enhanced electrical properties. The chemical structures of 6TTF-polymer and its intermediates were identified by FT-IR and ¹H NMR spectroscopes. Additionally, the electrochemical properties of 6TTF-polymer were observed by cyclic voltammetry, photoluminescence, and ultraviolet spectroscopes. The thermal behavior of 6TTF-polymer was experimented by DSC and TGA. The cast 6TTF-polymer films were flexible and durable, which result notices that its molecular weight is high enough to be entangled. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2013K000404) of Korean government.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-31

발표분야: 고분자화학

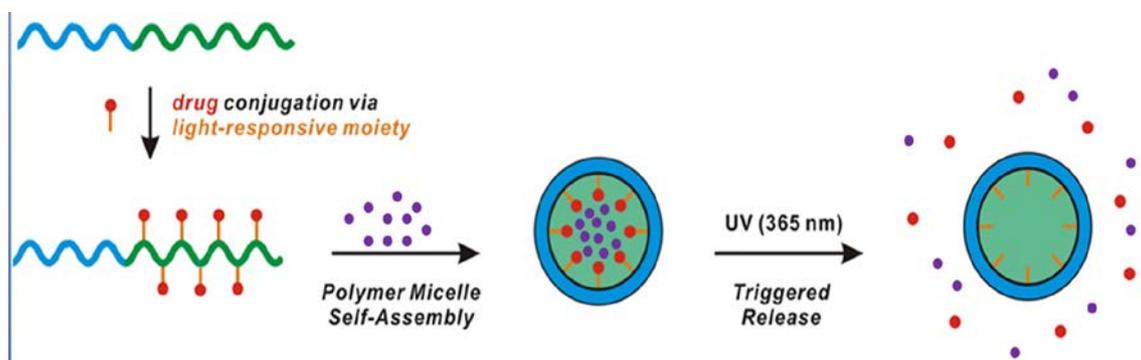
발표종류: 포스터, 발표일시: 수 16:00~19:00

Light responsive polymers for drug delivery

이지은 이형일*

울산대학교 화학과

Stimuli-responsive polymeric micelles are composed of a hydrophilic shell and a responsive hydrophobic core with tunable solubility that depends on external stimuli. If a responsive hydrophobic core contains a covalently attached drug moiety which is labile to external stimuli, one can achieve site-specific and time controlled delivery of therapeutics to improve therapeutic efficacy. For this purpose, we synthesized a diblock copolymer composed of a hydrophilic poly(ethylene oxide)(PEO) block and a drug-containing hydrophobic block by a combination of atom transfer radical polymerization(ATRP) and a copper-catalyzed azide-alkyne click chemistry. In aqueous solution, this block copolymer self-assembled to form micelles in which the drugcontaining hydrophobic block forms the inner core, and the hydrophilic PEO the other shell. Irradiation with UV light (365nm) led to cleavage and subsequent release of the drug moiety.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-32**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel thermoresponsive polymers with upper critical solution temperature properties

이지은 이형일*

울산대학교 화학과

The secondary amine-derivatized thermoresponsive polymers were successfully synthesized by a combination of atom transfer radical polymerization (ATRP) and Cu(I)-catalyzed 1,3-dipolar cycloaddition between azide and alkynes (click chemistry). The resulting polymer (P1) is shown to possess insoluble-soluble transitions (UCST-type phase behavior). P1 was further reacted with chloro ethylalcohol and chloro propylalcohol to lead to P2 and P3, respectively. These polymers were analyzed by cloud point measurements and exhibited different UCST behaviors. These behaviors were carefully characterized using a number of techniques, including percent transmission analysis, UV-Vis spectroscopy and ¹H-NMR spectroscopy, and dynamic light scattering (DLS).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-33

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Large Scale Growth of Hierarchical Metal Oxide Nanoparticles on Hydrophilic and Hydrophobic substrates

신혜진 이하진¹ 최원산*

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Large scale growth of metal oxide nanoparticles was achieved on hydrophilic as well as hydrophobic substrates: needlelike IO nanoparticles were grown on the surface of the glass or Teflon substrate by the addition of a mixed aqueous Fe precursor solution with the potassium persulfate (KPS) solution to be used as initiator. The surface morphology of the IO film was determined by scanning electron microscopy. The length of the IO needles could be controlled by changing the incubation time or cycle of the iron precursor solution. As the reaction time was adjusted from 3 to 12 hours, the average length of the IO needles increased from 300 to 950 nm. In the early stage of growth, the IO needles were sparsely distributed and thus laid parallel to the surface of the substrates. By comparison, as the growth proceeded, overcrowding of the IO needles led them to stand up, forming densely packed IO needles with high surface coverage. It is worth noting that the presence of the oxidant helped to activate the surface of substrates regardless of hydrophilic or hydrophobic nature, thus promoting the growth of IO nanoneedles with uniform distribution on any substrates. Even though the glass substrate has many reaction sites, such as negatively charged hydroxyl groups as well as defects, IO nanoneedles were not formed on the substrate in the absence of oxidant. Only in the presence of oxidant, positively charged iron precursors are more favorable for adsorption on the glass or Teflon substrate activated by oxidant. We expect that other metal oxide films can also be prepared and the resulting films can be utilized as a versatile film for environmental remediation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-34

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface-induced phase structures of the rod-disc liquid crystal

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전북대학교 고분자나노공학과 ¹전북대학교 고분자 나노 공학과

Upon varying the width of the LC cells and their surface chemical and physical states, the RD12 phase transition behavior was dramatically changed. Surface-induced phase transition behaviors of a rod-disc (cyanobiphenyl-triphenyl) liquid crystalline (LC) molecule (RD12) were researched by changing the surface physical and the chemical interactions. The nematic (N) phase of RD12 in the LC cell with a low cell gap and polyimide rubbed surface could be preserved and the crystallization of RD12 was completely suppressed. Based on the systematic experimental investigations, it was concluded that the glassy N phase was formed due to the fact that the surface anchoring force is bigger than the crystallization force. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2013K001428, , 2013K000404) of Korean government.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-35

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of carbon fiber surface treatment on the impact properties of carbon/carbon composites

유성은 박수진^{1,*}

전북대학교 Bin 융합공학과 ¹인하대학교 화학과

In this study, the effect of MoO₃ content on the impact properties of carbon-carbon composites(C/C composites) was investigated in the presence of Mo₃. The content of MoO₃ was varied in 0, 5, 10 wt% on the basis of resin matrix for anti-oxidation properties of the composites under high temperature. The impact properties of the composites were studied in drop-weight impact tester and interlaminar shear strength(ILSS) and critical stress intensity factor(KIC). As a result, the composites made with MoO₃ resulted in an increase of interfacial adhesion between fibers and matrix, which could improve the impact properties of the composites.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-36**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Oxidation Inhibitor on Fracture Toughness of Carbon/Carbon Composites

유성은 박수진^{1,*}

전북대학교 Bin 융합공학과 ¹인하대학교 화학과

In this study, the effect of oxidation inhibitor contents on fracture toughness of unidirectional carbon-carbon composites (C/C composites). MoO₃ used as an oxidation inhibitor was impregnated with phenolic resins to improve the anti-oxidation properties of the composites in different concentrations of 0, 5, and 10 wt%. Based on Wilhelmy equation, the work of adhesion of the C/C composites was calculated by contact angle methods. Fracture toughness and impact strength were examined by three-point bending test for the critical intensity factor (KIC) and Izod impact test method, respectively. As a result, the C/C composites made with MoO₃ resulted in an increasing of both fracture toughness and impact strength.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-37

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction of Newly Synthesized Low Bandgap Polymer with Protic and Aprotic Ionic Liquids

김중일 장원 김인태*

광운대학교 화학과

In this case, we have examined the conductivity and interaction studies of ammonium and imidazolium based ionic liquids (ILs) with the newly synthesized low bandgap polymer(Poly(2-heptadecyl-4-vinylthieno[3,4-d]thiazole) (PHVTT)). Use of low bandgap polymers is the most suitable way to harvest a broader spectrum of solar radiations for solar cells. But, still there is lack of most efficient low bandgap polymer. In order to solve this problem, we have synthesized a new low bandgap polymer and investigated its interaction with the ILs to enhance its conductivity. ILs may undergo almost unlimited structural variations; these structural variations have attracted extensive attention in polymer studies. The aim of present work is to illustrate the state of art progress of implementing the interaction of ILs (protic and aprotic ILs) with newly synthesized low bandgap polymer. In addition to this, our UV-Vis spectroscopy, confocal Raman spectroscopy and FT-IR spectroscopy results have revealed that all studied ILs (tributylmethylammonium methyl sulfate ([N1444][MeSO₄] from ammonium family) and 1-methylimidazolium chloride ([MIM]Cl, and 1-butyl-3-methylimidazolium chloride ([Bmim]Cl from imidazolium family) has potential to interact with polymer. This study provides the combined effect of low bandgap polymer and ILs that may generate many experimental opportunities.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-38**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction of Polyaniline and New Protic Ionic Liquid

김영범 김인태*

광운대학교 화학과

Among the conducting polymers, Polyaniline(PANI) has received greater attention due to cheap and superior stability to air oxidation. Unfortunately, it has rather poor mechanical, general physical properties, and processability. In order to solve this problem, we used to interact ionic liquids(ILs) with PANI for enhance physical properties. ILs may undergo almost unlimited structural variations; these structural variations have attracted extensive attention in polymer studies. The aim of present work is to illustrate the state of art progress of implementing the interaction of ILs with PANI. In addition to our UV-Vis spectroscopy result showed red shift due to interactions of PANI with ILs. This study provides multiple application of PANI and ILs that may generate many experimental opportunities.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-39**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, characterization and photo-responsive behavior of new polymers containing azobenzene

박정호 김성호 김인태*

광운대학교 화학과

Series of polymers containing azobenzene have received much attention in the past years because of their unique properties and potential applications in optical information storage and other areas. In this work, new polymers containing azobenzene functionalized with electron-withdrawing groups have been designed and synthesized. New polymers were successfully characterized by organic spectroscopic methods (^1H NMR, FT-IR, UV-vis and GPC). Their photo-induced surface relief gratings were fabricated on thin glass films of the azobenzene containing polymers by exposure to interferenced two coherent laser beams (532nm) in few minutes. Their properties can be used in optical data storage and other optical devices.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-40

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photo-induced Actuation of Photochromic Liquid Crystalline Polymer

최유진 김대윤¹ 이명훈¹ 정광운^{2,*}

전북대학교 고분자 나노공학과 ¹전북대학교 고분자나노공학과 ²전북대학교 고분자 나노 공학
과

We have newly synthesized a novel photochromic polymer abbreviated as PLCP via the acrylic diene metathesis polymerization. Based on the combined the techniques of DSC, POM and 2D WAXD, it was identified that PLCP formed a nematic (N) LC ordered phase containing the cynclinically tilted SmC-type cybotactic clusters, in which packing structure is related to the head-to-side connected PLCP chemical structure. Additionally, we demonstrated the rewritable micro-patterned PLCP film. Due to the wireless remote controllability of reversible actuating and patterning behaviors of PLCP, it can be applied as materials in opto-electronic devices. This work was mainly supported by Converging Research Center Program (2013K000404), and Human Resource Training Project for Regional Innovation funded by the Ministry of Education, Science, and Technology of Korea.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-41**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Super-Robust Carbon nanotube (CNT) enhanced polymeric nanofibers

김한수 신관우^{1,*}

서강대학교 화학과 ¹서강대학교 화학과 및 바이오융합과정

Well-aligned polymeric nanofibers can be made from electrospinning, which is one of the useful tools for polymer nanofibers fabrication. It is difficult to measure mechanical properties of polystyrene (PS) nanofibers because its intimate properties, such as brittleness and easily frigid characteristic, trigger problems at modulus and tensile strength analysis. It is crucial to achieve high mechanical properties by removing residual solvent, finding an appropriate ratio for PS and CNT composites, cross linking effects from PS, and surface modification of CNT to enhance mixing properties in solvent. Since the deviation of fiber diameters causes fluctuation of its modulus, FE-SEM was used to determine average diameters of fibers, ranging from 200 to 300 nm. Motor-controlled setup, equipped with chemical balance, provided measuring tool for mechanical properties of electrospun nanofibers.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-42**

발표분야: 고분자화학

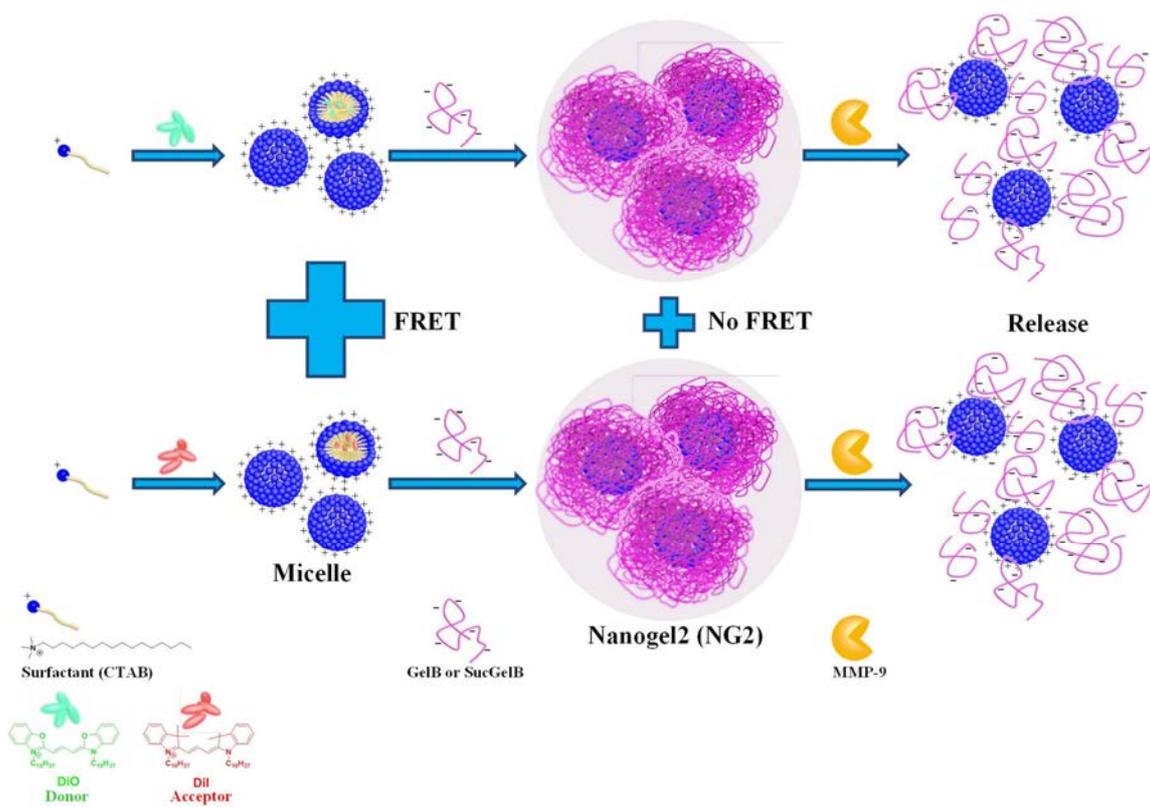
발표종류: 포스터, 발표일시: 수 16:00~19:00

Natural Polypeptide-Based Supramolecular Nanogels for Stable Noncovalent Encapsulation

배보람 유자형*

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Supramolecular nanogel, a physically cross-linked nanosize hydrogel, spontaneously self-assembles in aqueous solution via secondary interactions and is thus of great interest in nanomedicine as a drug carrier. We developed a versatile method for supramolecular nanogel self-assembled by electrostatic interaction between positive surfactant micelles and negative polypeptides. Core-shell-like structures of supramolecular nanogels provide stable hydrophobic pockets that prevent simple diffusion of hydrophobic guest molecules, resulting in high encapsulation stability. The size of the supramolecular nanogels can be systematically controlled by varying the size of the surfactant micelles. Furthermore, noncovalently encapsulated dye molecules can be released in response to matrix metalloproteinases highly overexpressed in tumor tissues, potentially providing tumor-triggered targeting.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-43**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Encapsulation of Polyelectrolytes inside the Halloysite Nanotube

김재현 유정주 손대원*

한양대학교 화학과

Halloysite ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 \cdot n\text{H}_2\text{O}$) is a hollow nanotube, which consists of one alumina octahedron sheet and one silica tetrahedron sheet in a 1:1 stoichiometric ratio. Because of the different chemical constitutions, halloysite in water has negative charge on the outer surface and positive charge on the inner surface at a wide range of pH. We focused on the size of the halloysites' pore, 5-20nm diameter, which is large enough to contain polymers. Therefore, halloysite could capture polystyrene sulfonate, which has negative charge, inside the halloysites' pore by electrostatic interaction between aluminol group of inner surface of halloysite and anionic polymer. DLS (dynamic light scattering) was used to characterize the halloysite-PSS nanocomposites. The morphology and the binding characteristics of halloysite and PSS were confirmed by TEM and IR spectroscopy, respectively.

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발표코드: POLY.P-44

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Characterization of Sheath-Core Structured TiO₂ Nanofiber Mats

김지태 강동규 박민욱 정광운^{1,*}

전북대학교 고분자나노공학과 ¹전북대학교 고분자·나노 공학과

Epitaxially grown titanium dioxide (TiO₂) nanofibers containing single crystalline TiO₂ nanowires with anatase structure were successfully fabricated by electropinning poly(vinylpyrrolidone) solutions mixed with hydrothermally synthesized titanium dioxide nanowires and titanium (IV) isopropoxide Ti(OiPr)₄ precursor. Utilizing SEM and TEM, morphological examination was conducted. Structure and orientation of TiO₂ single crystalline nanowires were also identified by XRD and SAED simultaneously. Improved optoelectronic properties of TiO₂ nanofibers were also identified with UV-Vis spectroscopy experiments. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2013K000404) of Korean government,

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장소: 창원CECO

발표코드: **POLY.P-45**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

이소시아네이트 경화제 (TDI+EG)의 반응경로 추적

김지석 이연정 김성호*

순천향대학교 화학과

우레탄이나 아크릴계 폴리머 제조 시 사용되는 isocyanate 계 경화제는 isocyanate 화합물 단독으로 사용되지 않고, ethylene-glycol 이나 TMP 등의 화합물과 혼합되어 사용된다. 본연구에서는 IR 과 MALDI-MS 만을 이용하여 시간에 따라 변화하는 각 성분(pre polymer)과 각성분의 몰 분률 변화를 실시간으로 분석하였다. 먼저 생성 가능 화합물을 예측하였으며, 질량분석기를 이용하여 반응물의 종류를 확인하고, 피크의 intensity 분석을 통하여 생성물의 몰비를 예측하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **POLY.P-46**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Wood Adhesive Derived from the Milk Protein and the Blocked Isocyanate

이향렬

한국교통대학교 생명공학과

Abstract : To investigate the adhesion effect of sodium bisulfite content in making blocked isocyanate, wood adhesive PB-1, PB-2, PB-3 and PB-4 containing sodium bisulfite content of 15%, 22.5%, 30% and 37.5% were synthesized respectively. As a result, when the amount of sodium bisulfite increased in adhesives, the tensile strength was found to be proportionally increased. The final adhesive mixtures were manufactured using a two-components system which are prepared by mixing two separate protein and BI solutions due to the precipitate in the adhesives. As PVA was added to adhesives to increase tenacity, the plywood dehiscence phenomenon after cold pressing process was declined. By addition of PVA, the tensile strength was improved up to 6.5~7kgf/cm² with BI/protein ratio from 1:6 up to 1:8. Phase separation between milk fat and aqueous layer was disappeared after addition of emulsifier, Tween 20. Addition of Tween 20 showed tensile strength up to 5 ~ 6.5 kgf/cm² at NCO/protein ratio of 1:12 ~ 1:14 without phase separation.

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장소: 창원CECO

발표코드: POLY.P-47

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conducting Binaphthyl Polymer Networks via Ring Opening Metathesis Polymerization

양기석 정동철 최은정 송창식*

성균관대학교 화학과

Electroactive polymers can easily be obtained from electropolymerizable monomers via oxidative coupling. However, mechanical properties of the resulting polymer films are often not satisfactory for practical applications. We designed and synthesized mechanically robust, free-standing, electroactive films from macrocyclic binaphthyl monomers using ring-open metathesis polymerization (ROMP). Without ROMP, electropolymerized polymer films were rather brittle. When the macrocyclic binaphthyl monomer was co-polymerized with cyclooctene via ROMP, mechanically robust elastomers were produced. Subsequent oxidative coupling by electrochemical or chemical methods furnished cross-linked polymer networks that were electroactive without mechanical disintegration. The cross-linked ROMP polymer showed electrochromic and chemochromic properties, which were stable even after repeated cycles under ambient atmosphere. The polymer may find use in applications such as electrochromic or chemochromic devices, electro-stimulated drug delivery systems, and electrically controlled membranes.

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장소: 창원CECO

발표코드: **POLY.P-48**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of carbon nanotube-containing electroconductive hydrogels

최은정 송창식* 정동철 이해경

성균관대학교 화학과

Electroconductive hydrogels are polymeric blends or interpenetrating networks that combine electroactive molecules, including conducting polymers, with hydrogels. These hybrid materials have the electrical properties of electroactive molecules and environmentally responsive properties of hydrogels. In this study, hyaluronic acid based hydrogels crosslinked by a dopamine linker were synthesized, and carbon nanotubes were incorporated to improve their electrical properties. The electrical properties were characterized by electrochemical impedance spectroscopy. Also, the shear modulus of hydrogel materials was measured to investigate whether carbon nanotubes additionally improve the mechanical properties of hydrogels.

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장소: 창원CECO

발표코드: POLY.P-49

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of photoactive self-repair polymer networks based on metal-ligand interactions

정동철 양기석 최은정 송창식*

성균관대학교 화학과

We designed the self-repair photo-active materials using terpyridine (tpy) ligand and its metal complexes. Tpy ligand easily binds to metals (Zn, Fe, Co) and the characteristics of metal-tpy complexes can be changed by various metals and modifying functional groups. In this study, we synthesized tpy-containing polyvinyl alcohols (PVAs) that are attached with photoactive Ru(II) complexes. When Fe(II) added to PVA-tpy solution, the sol-to-gel transition was observed. We confirmed in the UV absorption spectra that the metal-to-ligand charge-transfer (MLCT) band was increased with the growing concentration of Fe(II). This increase demonstrates that the metal Fe(II) interacts with PVA-tpy ligands. We made thin films of metal-PVA-tpy networks on glass substrates by the layer-by-layer (LBL) method. We observed that the MLCT increased as the number of layers increased. We also synthesized Ru(II)-tpy containing polymer networks in a similar method to adopt photoactive properties. Ru(II)-induced photocurrents were observed in the assembled films, which was enhanced by inclusion of methyl viologen.

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장소: 창원CECO

발표코드: POLY.P-50

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Characterization, and properties of a new conducting polymer containing fluorinated quinoxaline derivative

장원 김인태*

광운대학교 화학과

Recently, the incorporation of an electron-withdrawing F atom onto the periphery of acceptor unit is attractive, since its small size is expected to minimize the undesired steric interaction and its strong electron-affinity nature is also expected to stabilize the HOMO and LOMO energy levels. Furthermore, fluorination also causes a decrease in the band gap in solid state, arising from the fact that the improvement in planarization of the conjugated backbone through favorable F-atom-induced intramolecular and/or intermolecular interactions. So we synthesised copolymer using the fluorinated quinoxaline derivative monomer and EDOT monomer. The polymer will be characterized by ¹H NMR, UV-vis spectroscopy.

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장소: 창원CECO

발표코드: **POLY.P-51**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of honeycomb-patterned Polyaniline thin films with high conductivity and mechanical stability

노국태 허도성*

인제대학교 화학과

Honeycomb-patterned polymer thin films have attracted considerable attention because of their potential application in various fields, such as separation membranes, superhydrophobic materials, photonic or optoelectronic devices, cell-culturing substrates, and micropatterning templates. Honeycomb-patterned thin films have been fabricated by a variety of methods such as lithography, the use of colloidal crystals, self-assembly, and the rod-coiled copolymers process. Among them, a simple and useful technique for preparing honeycomb-patterned thin films is the breath-figure method. In this method, the substrate can be completely dispersed in organic solvents, such as chloroform, and films are then fabricated by casting these solutions under humid conditions. However, polyaniline has a great drawback for the fabrication of honeycomb-patterned films, because of its insolubility in organic solvents. In spite of its intrinsically conducting polymer nature. Therefore, we have modified polyaniline for the fabrication by chemically using dichlorodicyanobenzoquinone (DDQ).

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장소: 창원CECO

발표코드: POLY.P-52

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chromonic nanofiber containing the self-assembled nanocolumns

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전북대학교 고분자나노공학과 ¹전북대학교 고분자 나노 공학과

Macroscopically oriented Chromonic electrospun nanofibers with the self-assembled Sunset-Yellow FCF (H-SSY) were fabricated by combination of electrospinning and self-assembling methods. Based on the thermal, scattering and microscopic analyses, it was realized that H-SSY formed a glassy columnar nematic (N) phase in the PVP/H-SSY nanofiber. Utilizing the 2D WAXD and polarized FTIR results, it was achieved that the nanocolumns were aligned parallel to the long axis of the nanofiber. The anisotropically oriented PVP-H-SSY nanofiber mats embedding the self-assembled nanocolumns may develop new ways for the practical applications in electro-optical devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2013K001428) of Korean government

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장소: 창원CECO

발표코드: POLY.P-53

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrospun Nafion/Polymer와 이온성액체를 이용한 이산화탄소 분

리막 연구

방호선 황용하 조정현 원종욱*

세종대학교 화학과

오늘날 지구온난화에 대한 위기의식이 고조됨에 따라 온실가스를 감축하기 위한 노력들이 진행 중이다. 이산화탄소 분리막을 이용하면 이산화탄소를 분리, 회수하는 과정에서의 비용을 줄일 수 있다. Polymer 는 PVP(poly(vinylpyrrolidone))와 PEO(poly(ethylene oxide))를 사용하여 비교 연구하였다. 5wt% Nafion solution 에 PVP 2.5wt%와 PEO 3wt%를 각각 첨가하여 지지체인 polysulfone membrane 위에 electrospinning 기법으로 직접 방사하여 Nafion/PVP fiber 를 얻어냈다. polysulfone 지지체 위에 Nafion/PVP fiber 층을 만든 후 각각의 2 가지 이온성 액체 {(1-hexyl-3-methylimidazolium tetrafluoroborate([hmin][BF₄]), 1-hexyl-3-methylimidazolium hexafluorophosphate([hmin][PF₆])}를 첨가하여 electrospun Nafion/PVP membrane 을 제조하였다. SEM 을 이용하여 electrospun Nafion/PVP membrane 의 단면 및 fiber 의 형태를 확인 할 수 있었고 기체투과도 장치를 이용하여 막을 통과한 기체의 양을 bubble flow meter 를 통해 이산화탄소의 selectivity 를 측정하였다. electrospinning 으로 제조된 Nafion nano fiber 로 만들어진 electrospun membrane 은 Nafion 과 ionic liquid 의 조합으로 selectivity 가 증가하고 electrospun mat 에 생기는 nano size 의 기공을 통해 permeance 가 증가할 것이라 생각했지만 순수한 이온성액체보다 electrospun membrane 의 selectivity 만 약간 증가한 것을 확인하였다.

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발표코드: POLY.P-54

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

TEMPO를 이용하여 산화시킨 셀룰로오스의 특성 연구

김지영 원종욱* 최혜리

세종대학교 화학과

셀룰로오스는 천연 고분자 자원으로써, 지구상에서 가장 풍부한 유기고분자이다. 이는 가장 쉽게 목재로부터 얻을 수 있고 셀룰로오스를 만드는 미생물, 그리고 연체동물의 점액물질로부터 셀룰로오스를 얻을 수 있어, 원료를 대량으로 쉽게 얻을 수 있다는 장점이 있다. 이로 인해 시료의 가격 경쟁성이 있어서 셀룰로오스를 시료로 이용할 경우 경제적이며, 또한 생분해가 가능한 환경친화적인 고분자라는 장점도 있다. 셀룰로오스의 하이드록시기를 라디칼인 2,2,6,6-Tetramethylpiperidine-1-oxyl (TEMPO)와 NaClO, NaBr 를 이용해 카르복시기로 산화시켜서, 산화된 셀룰로오스가 가지는 특성을 연구하였다. 물에 녹지 않는 셀룰로오스의 특성으로 인하여, 셀룰로오스를 산화시키는 단계 전에 팽윤시키는 단계를 추가하여서 실험을 진행하였다. 충분히 팽윤 된 셀룰로오스를 산화시켜서, 산화된 셀룰로오스가 갖는 작용기를 FT-IR 분석을 통해 확인하였고, 산화된 셀룰로오스가 가지는 카르복시기의 특성은 이온전도도 값으로 확인하였다. 산화된 셀룰로오스를 분리막으로 제조하여 Soap Bubble Flowmeter 를 이용한 기체 투과도를 확인하였고, 분리막의 형태는 SEM 이미지를 통해 확인하였다.

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장소: 창원CECO

발표코드: POLY.P-55

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

imidazolium계 이온성 액체를 이용한 이산화탄소 분리 연구

황용하 원종욱*

세종대학교 화학과

이산화탄소의 양이 증가함에 따라 지구온난화가 고조됨으로써 이산화탄소를 분리, 회수, 저장하는 기술의 개발과 적용에 대한 관심이 높아지고 있다. 하지만 이산화탄소를 분리, 회수, 저장 시 많은 에너지가 필요로 한다. 이를 해결하기 위해 에너지 절약 공정인 이온성 액체 분리막을 연구하였다. 이온성 액체의 높은 열적 안정성, 낮은 점도, 낮은 휘발성과 최대 장점인 이산화탄소의 높은 선택성을 이용하여 대기중에 배출된 이산화탄소를 효율적으로 줄일 수 있다. 이산화탄소 흡수량이 큰 이온성 액체를 지지체인 polysulfone 막 위에 이온성 액체를 도포한 후 충분히 스며들 수 있도록 상온에 하루(24 시간)정도 방치한다. 사용된 이온성 액체로는 1-hexyl-3-methylimidazolium hexafluorophosphate, 1-hexyl-3-methylimidazolium tetrafluoroborate, 1-butyl-3-methylimidazolium tetrafluoroborate, 1-butyl-3-methylimidazolium hexafluorophosphate, 1-butyl-3-methylimidazolium tricyanomethanide, 1-hexyl-3-methylimidazolium tricyanomethanide, 1-hexyl-3-methylimidazolium tricyanomethanide 이 사용되었다. 이온성 액체가 도포된 polysulfone 막을 bubble flow meter 를 통해 기체의 투과도를 측정한다. (상온) 또한 양이온과 음이온의 종류에 따라 이산화탄소의 선택성을 비교하였다.

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장소: 창원CECO

발표코드: POLY.P-56

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Biopolymer를 도입한 염료 감응 태양 전지 전해질의 물성 변화로 인한 안정성 향상

송홍규 원종욱* 최혜리 김지영

세종대학교 화학과

기존 염료 감응 태양 전지의 액체상 전해질은 누수와 증발이 가장 큰 약점이었다. 이 약점을 극복하기 위해 염료 감응 태양 전지 내의 전해질 안정성을 향상시키기 위하여 biopolymer를 전해질에 도입하여 준고체형 염료 감응 태양 전지를 제작하였다. Biopolymer의 대표적인 물질인 cellulose는 쉽게 구할 수 있고, 가격이 저렴하다는 장점이 있으며, 전해질에 도입하였을 때 물성을 고체상으로 변화시키면서 효율이 기존 전해질과 비교하여 많이 감소 하지 않았다. 또한, biopolymer를 전해질에 첨가하였을 때에는 액체상을 유지하였다가, 24 시간이 지난 뒤에는 고체상이 되는 것을 확인하였다. 이에 따라 전해질을 제조하여 염료 감응 태양 전지에 도입하여 semiconductor인 TiO_2 층에 액체상으로 스며들게 한 후, 제작이 끝난 뒤에 TiO_2 층 내에서 전해질이 고체상으로 물성이 변하여 기존 고체상 전해질보다 TiO_2 와 접촉하는 부분이 많아질 것을 기대할 수 있다. 이에 따른 효율의 유지를 확인하기 위하여 photovoltaic performance의 측정을 통하여 변환 효율을 측정하고, IPCE (Incident Photon-to-electron Conversion Efficiency)를 통해 J_{sc} 역시 유지되는 것을 확인하였다. 또한, EIS (Electrochemical Impedance Spectroscopy) 및 IMVS (Intensity Modulated Voltage Spectroscopy)를 측정하여 염료 감응 태양 전지에 bio polymer를 포함한 전해질이 미치는 영향을 연구하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-57

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

전자수용체에 따른 Ag나노입자 축진수송 분리막의 올레핀/파라핀 분리 성능 비교 연구

최지영 원종욱* 강용수¹ 이정현¹

세종대학교 화학과 ¹한양대학교 에너지공학과

기존에 정유 단계에는 석유를 분리한 후 남은 물질을 아스팔트로 사용하였다. 그러나 아스팔트의 수요가 적어져 최근에는 분별증류 탑을 이용하여 C₈ 이하의 탄소물질을 분리하게 되었다. 이러한 분리 방법에는 많은 에너지가 소비되게 된다. 최근 많이 대두 되고 있는 에너지 고갈 문제로 인해 에너지 절약을 위하여 분별증류 방법을 대신할 올레핀과 파라핀을 분리 할 수 있는 분리막을 제작하였다. 올레핀 운반체(carrier)로는 Silver tetrafluoroborate (AgBF₄)를 사용하였다. Ag의 안정성을 높이고 또 표면에 δ⁺로 올레핀과의 상호작용을 높이기 위해 안정제인 Polyvinylpyrrolidone (PVP)를 사용하여 Ag를 나노 크기의 입자로 만들었다. Ag 나노 입자의 생성을 확인하기 위하여 UV를 측정하였다. Ag 나노 입자 표면의 δ⁺를 상승 시키기 위하여 전자수용체로서 각각 7,7,8,8-Tetracyanoquinodimethane (TCNQ), Tetracyanoethylene (TCNE), Fluorescein (Flu), Rhodamine6G (Rho)를 도입하였다. 각 전자수용체와 Ag 나노 입자간의 binding energy를 확인하기 위하여 XPS를 측정하였다. 위 용액을 Polysulfon support membrane에 코팅하여 올레핀/파라핀 분리막을 제조하였다. 기체크로마토그램을 이용하여 각 전자수용체에 따른 올레핀/파라핀 분리 성능을 확인하고 비교하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-58

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cellulose와 conductive polymer의 composite을 전극으로 적용하기 위한 성능 연구

최혜리 송홍규 원종욱* 김지영

세종대학교 화학과

보편적으로 염료 감응 태양 전지는 counter electrode 에 redox couple regeneration 을 촉진하는 물질로 Pt-layer 를 적용하고 있다. Pt 가 코팅된 전극은 좋은 성능을 나타내는 반면 몇 가지 단점을 갖고 있다. Pt 는 한정된 자원이며 가격이 비싸고, Pt 를 코팅하기 위해 thermal decomposition 과 vacuum sputtering 을 하는 과정은 고온에서 수행되기 때문에 large scale 로 응용하는데 있어서 제한적이다. 이러한 단점을 보완할 수 있는 물질로 cellulose-poly(pyrrole) composite 을 제조하였다. Poly(pyrrole)은 대표적인 전도성 고분자로 제조가 간편하고 전도성이 높고, 열적으로 안정하나 기계적인 강도가 좋지 못하기 때문에 주로 복합체로 응용된다. Cellulose 는 natural polymer 로 물리·화학적 처리를 하여 다양한 물성을 갖게 할 수 있고 기계적 강도가 좋다. 따라서 본 연구는 poly(pyrrole)을 cellulose 표면에 deposition 시켰다. poly(pyrrole)이 잘 deposition 될 수 있도록 cellulose 를 TEMPO 로 산화한 후, FeCl₃ 를 넣어서 pyrrole 을 oxidative chemical polymerization 시켰다. Cellulose 에 poly (pyrrole)이 잘 deposition 되었는지 확인 하기 위해 SEM 을 측정하였고, electrical resistance 는 Digital Multimeter 로 확인하였다. 그리고 또 다른 전도성 고분자인 poly(aniline)과 cellulose composite 에 대한 연구가 진행 중이다.

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장소: 창원CECO

발표코드: **POLY.P-59**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

CATALYST COMPONENTS FOR THE POLYMERIZATION OF OLEFINS

주천익

롯데케미칼 연구5팀

ziegler-natta polymerization is one of most important catalytic industrial process. ziegler-natta catalyst research is progressing to improve high activity and stereospecificity of polyolefin. we designed and synthesized novel donors. The behavior of the donors in modifying the productivity and stereospecificity of Ziegler-natta catalysts in the polymerization of propene was investigated. Some correlation between the structure of the modifiers, the type of supported catalyst, and the polymerization results can be observed.

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장소: 창원CECO

발표코드: **POLY.P-60**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the preparation of crosslinked perfluorosulfonic acid membrane for direct methanol fuel cell

서승희 조창기*

한양대학교 유기나노공학과

Polymer electrolyte membrane(PEM) fuel cells are considered to be a very promising alternative power source. Perfluorosulfonic acid membranes with the trade name Nafion are 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, resistance to water transport from cathode to anode. For improvement of these defects, we studied crosslinking of nafion membranes. crosslinked-Nafion membranes were prepared by reaction of sulfonyl fluoride groups in Nafion 112(SO₂F form) with diamine crosslinkers. Membranes were dipped in swelling solvent for high reactivity of sulfonyl fluoride groups in Nafion 112 (SO₂F form) with crosslinker. The formation of sulfonamide linkages was confirmed by ATR-FTIR and UV-vis spectroscopy. The performance of the membranes was measured in terms of IEC (ion exchange capacity), water uptake, proton conductivity, and methanol permeability.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-61

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Encapsulation of Living Yeast Cells with Degradable Polymeric Shells, using Chitosan and Poly-L-Glutamic Acid

양성호* 최인성^{1,*}

한국교원대학교 화학교육과 ¹한국과학기술원(KAIST) 화학과

Living cells have been individually encapsulated within artificial materials, including silica, titania, calcium carbonate, calcium phosphate, as well as, synthetic/bio-polymers.¹ It was found that the encapsulation was beneficial for maintaining cellular viability, controlling cell division, functionalizing cell surface. However, degradation of artificial shells with external stimuli has not achieved yet, presumably because of a harsh condition for degradation, which would be harmful to the living cells. In this work, living yeast cells were encapsulated within degradable polymer (chitosan and poly-L-glutamic acid) through layer-by-layer self-assembly. Moreover, it was demonstrated that the artificial shell was removable by external stimuli while maintaining viability of the cells. References 1. Yang, S. H.; Hong, D.; Lee, J.; Ko, E. H.; Choi, I. S. *Small* 2013, 9, 178-186.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-62

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stimuli-responsive hydrogel microfibers produced by alginate-templating method and photopolymerization

임다운 윤진환*

동아대학교 화학과

Stimuli-responsive microfibers were prepared by alginate-templating method with simple microcapillary device. In this method, sodium alginate aqueous containing hydrogel monomers and calcium chloride aqueous were continuously injected into separated microcapillaries by syringe pump, and crosslinked alginate microfibers were formed at the junction point of capillaries. After photopolymerization of monomers in alginate microfibers, hydrogel microfibers could be obtained by removing alginate template.

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장소: 창원CECO

발표코드: **POLY.P-63**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Characterization of Polyhedral Oligomeric Silsesquioxane(POSS)-based Composite Film

박덕삼 오신석 김지은 김경민 임정혁*

한국교통대학교 나노고분자공학과

Polyhedral oligomeric silsesquioxane(POSS) as an enhancement of polymer nanocomposite has great characteristics like heat revolution reducer, flammability enhancer, mechanical property transformer, thermal property improver, and viscosity reducer. Multiwall carbon nanotubes(MWNTs) also have unique mechanical, thermal, and optical properties. Conductive polymers have been applied for electrical paper, OLED display, flexible display, touch panel and antistatic film. In this study, POSSS-based nanocomposite film was fabricated with MWNTs and conductive polymers including binder material via coating methods such as bar coating and doctor blade. The improved properties of the coating solution and the film were investigated by FT-IR, FE-SEM, EDS, AFM, UV-Vis and contact angle.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-64

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Remote control for volume phase transition of hydrogel beads incorporating iron oxide nanoparticles by visible light

이현진 윤진환*

동아대학교 화학과

Stimuli-responsive polymers can be responded to external stimuli, such as temperature, pH, and visible irradiation. For stimuli-responsive hydrogels, volume phase transition can be induced by external stimuli. In this work, we have prepared spherical hydrogel beads incorporating iron oxide nanoparticles using alginate-templating method by spray injection of monomer aqueous. Volume change of hydrogel beads could be controlled by both temperature and visible light irradiation. Furthermore, local control for volume change of specific hydrogel beads in selected region was successfully performed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: POLY.P-65

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

방향족 탄화수소 고분자 전해질의 가교를 위한 새로운 라디칼 가교제의 합성과 특성 고찰

이은별 이연식^{1,*}

전북대학교 화학공학과 ¹전북대학교 화학공학부

고온 연료전지용 고분자 전해질 막은 고온가습 조건에서 과도한 팽윤으로 인하여 기계적 물성과 치수 안정성이 저하되는 문제점이 발생하는데, 현재 이러한 현상을 해결하기 위한 연구들이 다양하게 진행되고 있다. 방사선 가교는 광개시제와 같은 첨가제가 필요하지 않고 전해질 막의 내부까지 가교가 가능하며, 막 표면의 산소에 민감하지 않고 동시에 기존의 가교 공정에 비하여 매우 간편하고 신속하다는 장점이 있다. 그러나 현재 공업적으로 많이 사용되고 있는 가교제들은 산성 조건에서 가수분해 되거나 물성을 저하 시키는 문제점 등을 안고 있다. 따라서 본 연구에서는 기존 가교제들의 문제점을 완화시키기 위하여 방사선용 가교제로서 1,1'-4,4'-bisacryloyl biphenyl ether 를 합성하고, 합성된 가교제가 혼합된 sulfonated poly(ether ether ketone) (SPEEK) 막(membrane)에 전자빔(electron beam)을 조사하여 가교 고분자막(C-SPEEK)을 제조하였으며, 제반특성 (예: 수소이온 전도도, 팽윤 특성, 열 안정성 등)을 고찰하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-66

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Redistribution Reaction of Trichlorosilane to Dichlorosilane

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연세대학교 화학과 ¹한국과학기술연구원(KIST) 물질구조제어연구단 ²연세대학교 화학및의화학
학과

Silane (SiH₄) is one of the most important starting materials used for producing high pure polycrystalline silicon. The quality of semiconducting silicon is mainly determined by the purity of silane. The best method to prepare ultra-high grade silane is distillation, because the boiling point of silane is lower than those of all chlorosilanes and impurities such as chlorides and hydrides of boron, phosphorus, and arsenic. The silane can be obtained by redistribution of trichlorosilane in promising method for it.??According to the literature?the best catalyst for the disproportionation of trichlorosilane are ion-exchange resins combining catalytic active functional group such as tertiary amine or quaternary ammonium group. New type catalyst system containing a heterocyclic base, such as pyrrolidine, piperidine, as functional group at polystyrene resin were synthesized. And then the redistribution activity of the synthesized catalysts was tested under various conditions (reaction temperature, contact time) and compared with five commercial ion-exchange resins, such as amberlyst A21, amberlite IRA-400. Among the commercial catalysts, the Amberlyst A21 catalyst in the best catalyst for the redistribution. In the presentation we will discuss about catalytic activity of several commercial ion-exchange resins and new catalyst system.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-67**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mechanistic consideration of synthetic 1,3-disubstituted urea using K₃PO₄ catalyst

김희환 김영진 김훈식* 정민석*

경희대학교 화학과

K₃PO₄ was found to effectively catalyze the carboxylation of amines by CO₂, producing corresponding 1,3-disubstituted ureas in high yields and selectivities. X-ray diffraction and FT-IR spectroscopic analysis of the solid mixture, recovered from the carboxylation of n-butylamine, revealed that K₃PO₄ was completely transformed into KH₂PO₄ and KHCO₃. Mechanistic and computational studies suggested that the high activity of K₃PO₄ could be attributed to the synergy effect exerted by the co-presence of KHCO₃ and KH₂PO₄, generated from the interaction of K₃PO₄ with CO₂ and water.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-68

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

UV/TiO₂ Pretreatment System for copper recovery device applied rated copper recovery

장다영* 김종부 서항복

HAEDONG TECHNOLOGY Co.,Ltd.

PCB etching and stripping processes in the manufacturing process after the cleaning process that occurs in low concentrations of copper etching and stripping processes compared to the concentration of copper is low emissions. So, because of the low recovery rate of waste water treatment plant is fed with a high concentration. In this study, in the manufacture of PCB cleaning wastewater generated in the cleaning process by analyzing the chemical properties of cleaning wastewater to understand. Also, cleaning the copper contained in the wastewater are effectively recovered and are looking for a way to resource recycling. PCB etching occurs on-site cleaning wastewater generated in the primary, the first detachment Sampling cleaning wastewater TOC, conductivity, Cu were analyzed. As a result, etching and stripping wastewater cleaned when comparing cleaning wastewater containing copper was higher in etching. Also ablation etching and cleaning of waste water cleaning wastewater TOC and Conductivity is measured higher load of wastewater treatment and inhibits copper absorption was considered to be a factor. Thus, the degradation of the compounds contained in wastewater pretreatment for was to use the facility. Using the photocatalytic pretreatment facility UV/TiO₂ System was selected. Gel state by hydrolysis of TiCl₄ prepared and coated on the quartz tube. Four times a coating is found to have the highest efficiency was applied to study the adsorption of metal ions copper selective chelating resin was used as the adsorption. As a result, copper is far short of the expected standard of 85% of its yield was about 60%. This equipment is UV/TiO₂ Pretreatment System is not operating normally in the decomposition of the compound that is expected as a result. After recovery through research to find ways to increase will have to see. Acknowledgement : This research was supported by the Program for the Construction of Eco Industrial Park(EIP) which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-69

발표분야: 공업화학

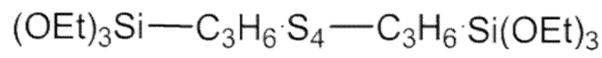
발표종류: 포스터, 발표일시: 수 16:00~19:00

Modification of Inorganic Oxide Nanoparticles with Organosilanepolyol for Organic-Inorganic Hybrid Materials

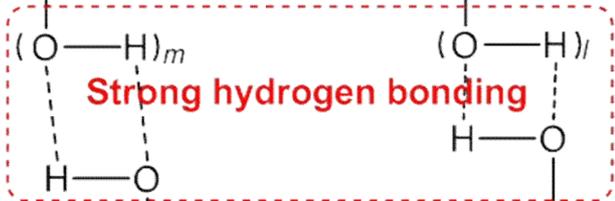
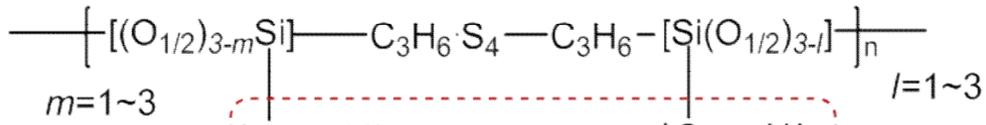
정동의 한준수 이광렬¹ 유복렬*

한국과학기술연구원(KIST) 물질구조제어연구단 ¹고려대학교 화학과

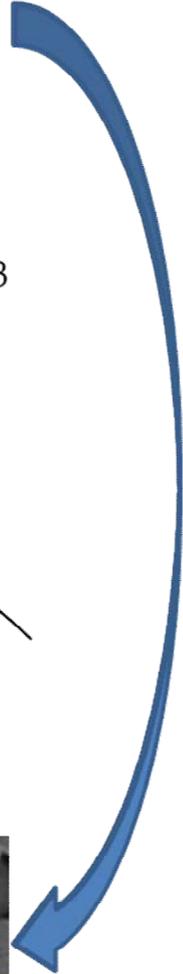
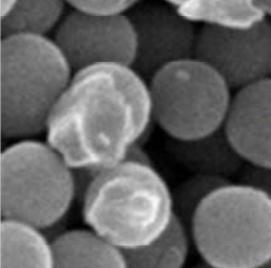
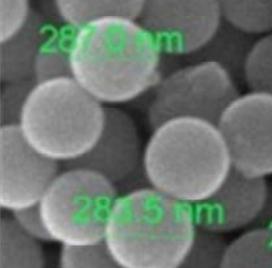
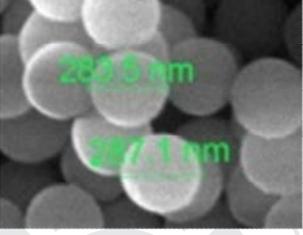
Organosilanepolyols were obtained in 70-98 % isolated yields as white powders by the hydrolysis reaction of organopolyalkoxysilanes under weak acidic condition. These organosilanepolyols were applied as surface modifiers for inorganic oxide particles such as silica, Zinc oxide, and titania. This process relatively good modified route for hydrophobic inorganic oxide particles by two step reactions: 1) organosilanepolyol interact with hydroxyl group on inorganic oxide particles through strong hydrogen bonding to make thin layered coating on the surface of inorganic oxide particles, 2) then can undergo condensation by heating. When ca. 50 nm silica particles treated with 5 wt % organosilanepolyol, all silica particles were floated on water, indicating that such organosilanepolyols are good surface modifiers for silica particles. This way to modify surface of silica should be applied for preparation of organic-inorganic hybrid materials. When organosilanepolyol-treated silica particles were used for hybrid material (composites) with organic rubber such as styrene butadiene rubber (SBR), the composites exhibit increased bound rubber contents and improved mechanical properties. SEM images of the prepared composites clearly show that organosilanepolyol-modified silica particles are well hybridized with SBR. The results of dynamic mechanical analyzer show that composites prepared with organosilanepolyol-modified silica particles have lower $\tan \delta$ values at 60 °C and higher $\tan \delta$ values at 0 °C than a composite obtained by conventional composition process.



Organosilanepolyol



Silica particle



CHEMICAL

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-70

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of purify and high value-production from MFB that is generated during the DMT manufacturing process

김경덕* 김석찬 정효진 박규순

국민대학교 화학과

본 포스트 발표의 주된 내용은 DMT 생성과정에서 필연적으로 발생하는 부산물인 MFB 를 순수하게 정제하여 이를 이용해 합성할 수 있는 4 종의 화합물에 관한 연구이다. 본 포스트에서 제시되는 4 종의 화합물로는 AMCA, PABA, OB-1, MFB-F 가 있으며 각각의 화합물은 기존의 방법과는 다른 경로의 합성법을 이용하여 합성을 완료하였다. 포스트에서 제시되는 각각의 합성방법 저가의 원료를 사용한다는 장점과 폐기물을 다시 재활용 한다는 환경적 이점의에 의해 충분히 기존의 방법을 대체할 수 있다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-71

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic oxidation of copper-containing wastewater in the removal of organic matter investigated the influence of radical scavenger

김종부 장다영* 서항복

HAEDONG TECHNOLOGY Co.,Ltd.

PCB industry occurring in process wastewater contains a large quantity of copper. Copper to form complexes with organic matter removed from the wastewater treatment plant has been fraught with difficulty. In addition, the concentration of copper is more than 1ppm of microorganisms in biological wastewater treatment has been reported that toxic effects. Therefore, in order to efficiently recover the copper complexes formed with pretreatment equipment to remove the organic matter should be focused. Photocatalytic oxidation process factors affecting the reactivity of the factors that have inhibited the formation of radicals. This is called Radical scavenger. Carbonate ions in the water that causes alkalinity (CO_3^{2-}) and bicarbonate ion (HCO_3^-) to exist, these ions trap the OH radical is that acts as a scavenger. OH radicals to produce UV/TiO₂ and UV/H₂O₂ AOP process with respect to the system after the addition of carbonate decomposition characteristics of wastewater DOC reduction was observed. The concentration of carbonate Na₂CO₃ using 0, 0.1, 0.5, 1mM changing with the decomposition of wastewater DOC removal was observed characteristics. Radical scavenger was worked effect parameter on the photo-oxidation of wastewater. Removal rate of TOC and absorbance was decreased by addition of carbonate ions and TOC removal was more sensitive. Acknowledgement : This research was supported by the Program for the Construction of Eco Industrial Park(EIP) which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-72

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and photocatalytic activity of TiO₂-reduced graphene oxide/CNF nano-composite under visible-spectra

김창효 김보혜^{1,*} 양갑승^{2,*}

전남대학교 고분자공학과 ¹대구대학교 과학교육학부 ²전남대학교 고분자 섬유 시스템공학
과

In this work, we prepared high efficient and visible sensitive TiO₂-reduced graphene oxide(RGO)/CNF photocatalyst nano-composite by using electro-spinning and sol-gel method. As-prepared photocatalyst nano-composite were characterized by transmission electron microscopy(TEM), X-ray diffraction(XRD), field-emission scanning electron microscopy(FE-SEM), Raman spectroscopy, X-ray photoelectron spectroscopy(XPS) and PL spectrometer. The photocatalytic activities were evaluated by degradation of methylene blue under visible light irradiation in the aqueous solution. The photocatalytic activities of TiO₂-RGO/CNF was shown highest efficiency than other control samples of RGO/CNF and TiO₂/CNF. The excellent enhancing effect of TiO₂-RGO/CNF was attributed to high migration efficiency of photoinduced electrons and the inhibition of charge/carrier recombination due to the electronic interaction between TiO₂ and graphene. The catalyst efficiency of the TiO₂-RGO/CNF was sustained after 5 cycles.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-73

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Mesophase Pitch Based Carbon Fibers from Fluidized Catalytic Cracking Decant Oils

이동훈 양갑승^{1,*}

전남대학교 고분자공학과 ¹전남대학교 고분자 섬유 시스템공학과

Pitch precursors for carbon fibers were synthesized from fluidized catalytic cracking-decant oils (FCC-DO). The low molecular weight fraction of FCC-DO was separated using the vacuum pump during 240 minutes at 150°C. After separation, they which were called VR were pressurized-heat treated with tetrahydronaphthalene (THN) at 300°C, and then synthesized mesophase pitches from them which were called VR-THN. The pressurized-heat treatment with THN reduced the viscosity of VR from 292.5 to 30.1 cP at 25°C and the elemental analysis of C/H mol% of 0.99 of VR to 0.94 of VR-THN. Optical texture of synthesized pitch were observed using polarized microscopy. During the further heat treatment at 380°C, anisotropic spheres combined in a large domain. The synthesized pitches showed about 15% yield and the softening point was about 290°C. The synthesized pitch was melt-spun through a circular nozzle by pressurized nitrogen gas, stabilized at 300°C, carbonized at 800°C and finally graphitized at 2800°C. The graphitized fiber exhibited anisotropic morphological structures in cross section of the fibers.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-74**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reverse osmosis unit to be concentrated in developing algorithms for recovery

김종부 장다영* 서항복 이장훈

SEC Co., Ltd.

This study of the reverse osmosis unit concentration water circulating in the raw water tank is a device for recycling concentrated. This study concentrated on the reverse osmosis unit effectively and will look for ways to recycle. Today, many techniques have been proposed, but its utilization is infancy. So make the most concentrated and focused to allow. In particular, in the case of concentrated pollution is high. Therefore, if the water is recycled in the system can handle the load on the device is a struggle to do matters. Recycling of the device in the reverse osmosis concentrate concentrated several times to accommodate the drain line automatic drain valve and concentrated automatic valve system was adopted to mount. Recycling of the device in the reverse osmosis concentrated time to accommodate the automatic valve and drain lines concentrated drainage system that is equipped with automatic valves. Reverse osmosis unit can concentrate on how to recycle purified water storage tank is filled with water from the recovery tank after the reverse osmosis purified water circulation device can concentrate is introduced into the recovery tank. Reverse osmosis unit once concentrated in the drain line valve opens automatically when acceptable in determining the control panel to set the relay time was to work. In this study, concentrate water through the reverse osmosis unit brings savings by recycling water. Concentrated for recycling does not occur in a separate investment. Acknowledgement :This research was supported by the Program for the Competitiveness Reinforcement Construction of Industrial Cluster which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-75

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reverse osmosis membrane to extend the life-time of the device for changes in cleaning technology

장다영* 김종부 서항복 이장훈

SEC Co., Ltd.

This research in the field of water treatment method using the reverse osmosis membrane cleaning formulations by changing technology just extend the lifespan occurs. Currently, almost all of the water used in the field of reverse osmosis membrane technology, the impact of this will be very large. This research will be applied to the present case that the existing device efficiency and lower costs in the economic aspects are judged very good technology. In this study, when membrane fouling by running effective membrane cleaning aims to maximize the effect. To this end, focusing on pressure changes in the initial pressure rise was 10% if the membrane cleaning is carried out. In this case, the amount of acid and alkali can be minimized should find a way. RO membrane in the present invention generally after the initial pressure 10bar pressure compared to just 11.5 ~ 12.0bar initial cleaning when carried out in acid solution below pH 2, pH 12 alkaline solution is carried out in more than 30 minutes each. In this case, the more conduct problems membrane cleaning treatment efficiency of the membrane tends to decrease. Initial production flow decreases and eventually just wash shorter jugido membrane should be replaced. The main reason for replacing the membrane just inside the source is not removed through cleaning. 11bar pressure at the membrane surface when conducting membrane cleaning one of the external contamination by removing the source of contamination inside the membrane prior to the initial state variable is able to keep. In addition, these results in order to reach an appropriate control logic is required. Acknowledgement :This research was supported by the Program for the Competitiveness Reinforcement Construction of Industrial Cluster which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-76

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mercury ion adsorption on chemically modified Activated Carbon and Activated Carbon Fiber in aqueous solution

김두원 김대호¹ 김보혜^{2,*} 양갑승^{3,*} 임용균⁴ 박은남⁵

전남대학교 고분자공학과 ¹전남대학교 신화학소재공학과 ²대구대학교 과학교육학부 ³전남대학교 고분자 섬유 시스템공학과 ⁴마이크로필터 ⁵(주)마이크로필터

Adsorption of Hg(II) was studied on four carbon adsorbent: granular activated carbon (GAC), chemically modified GAC (NaGAC), activated carbon fiber (ACF), and chemically modified ACF (NaACF). The surface properties, such as morphology, surface functional group, and composition of two adsorbents were determined by using Elemental analysis, X-ray photoelectron spectroscopy (XPS) and scanning electron micrograph (SEM) measurements. The specific surface area, total pore volume, and pore size distribution were investigated by using nitrogen adsorption, Brunauer-Emmett-Teller (BET), and Barrett-Joyner-Halenda (BJH) methods. In this study, the NaGAC and NaACF showed high adsorption capacity and adsorption rate for the Hg(II), due to the improved ion-exchange capabilities by more oxygen functional groups.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-77

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Manufacture of Low Cost Carbon Fiber through melt-spinning of residual oil/lignin blends

김무성 양갑승^{1,*} 김보혜^{2,*}

전남대학교 고분자공학과 ¹전남대학교 고분자 섬유 시스템공학과 ²대구대학교 과학교육학

부

Carbon fiber (CF), alternatively graphite fiber, carbon graphite or CF, is a material consisting of fibers about 5-10 μm in diameter and composed mostly of carbon atoms. The carbon atoms are bonded together in crystals that are more or less aligned parallel to the long axis of the fiber. and one of the most important materials to develop the eco-friendly society, to apply light weight vehicles and effective adsorbent materials. The low cost is the most important factor to expand applications. We prepared lignin-based graphite fibers from melt spinning of the blends of hardwood lignin and pyrolyzed fuel oil (PFO), byproduct of naphtha cracking process (NCC). We investigated multi-functions through Elemental analysis, Solid C13 NMR, Raman, X-ray diffraction, SEM, and Tensile strength. The CFs have strong potential to apply to reinforce material for carbon fiber composite and adsorbent of toxic gases at low cost.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-78**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aqueous phase adsorption of bisphenol-A over metal-organic frameworks, a porouschromium-benzenedicarboxylate

박은영 정성화*

경북대학교 화학과

Bisphenol-A (BPA) has been adsorbed over a MOF, Cr-benzenedicarboxylate (MIL-53) to understand the applicability of MOFs for the adsorptive removal of hazardous endocrine disturbing chemicals from water. MIL-53 shows very fast adsorption in an hour and the maximum adsorption capacity of MIL-53 is higher than that of commercial activated carbon adsorbent. Moreover, unlike the carbon adsorbents, MIL-53 showed very high efficiency over the adsorption especially at very low concentrations of BPA. Therefore, porous MOFs such as MIL-53 can be one the potential class of adsorbents for efficient decontamination of water. References[1] E. Y. Park, Z. Hasan, N. A. Khan, S. H. Jung, J. Nanosci. Nanotechnol. 2013, 13, 2789-2794.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-79**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic production of styrene through liquid-phase dehydration of 1-phenylethanol over sulfonated D-glucose

HASAN ZUBAIR 정성화^{1,*}

경북대학교 대학원 화학과 ¹경북대학교 화학과

Dehydration of 1-phenylethanol to produce styrene has been studied in liquid phase without any solvent with carbon-based solid acid catalysts prepared from renewable resources like d-glucose for the first time. The catalysts were obtained facily in one-step or carbonization and sulfonation were done simultaneously in one-pot synthesis. The carbon-based catalyst shows higher styrene selectivity and lower activation energy than other solid acid catalysts that have been used so far, demonstrating that a carbon-based catalyst is very effective in producing styrene from 1-phenylethanol. References[1] Z. Hasan, J.-S Hwang, S.H. Jhung, Catal. Commun. 2012, 26, 30-33.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-80**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Denitrogenation of a model fuel by liquid phase adsorption using phosphotungstic acid impregnated-metal organic framework MIL-101

imteaz ahmed 정성화*

경북대학교 화학과

Liquid phase adsorption of nitrogen-containing compounds (NCCs) from a model fuel was carried by metal-organic framework (MOF) MIL-101 impregnated with phosphotungstic acid (PWA) [1]. The model fuel contained one sulfur-containing compound (SCC), benzothiophene (BT); one basic NCC, quinoline (QUI); and one neutral NCC, indole (IND). NCC adsorption selectivity was very high compared to the SCC selectivity in both MIL-101 and PWA-impregnated MIL-101s. Additionally, the adsorption capacity of basic QUI increased by 20% with only 1% PWA impregnation in MIL-101. The adsorption of a neutral compound, IND, was slightly reduced with PWA impregnation in the MOF. The adsorption capacity/selectivity can be remarkably improved by a slight modification of MOFs, for example, to impart acidity [2]. So, it could be concluded that the MOF impregnated with PWA may be very interesting in commercial denitrogenation, especially for coal-derived fuels which contain mainly basic NCCs, by adsorption since the selectivity for NCCs (compared to SCCs) over the adsorbent is very high and the adsorbent can be reused many times. References [1] I. Ahmed, N. A. Khan, Z. Hasan, S. H. Jung, J. Hazard Mater. 2013, 250-251, 37 ? 44. [2] I. Ahmed, N. A. Khan, Z. Hasan, S. H. Jung, Appl. Catal. B: Environ. 2013, 129, 123 ? 129.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-81**

발표분야: 공업화학

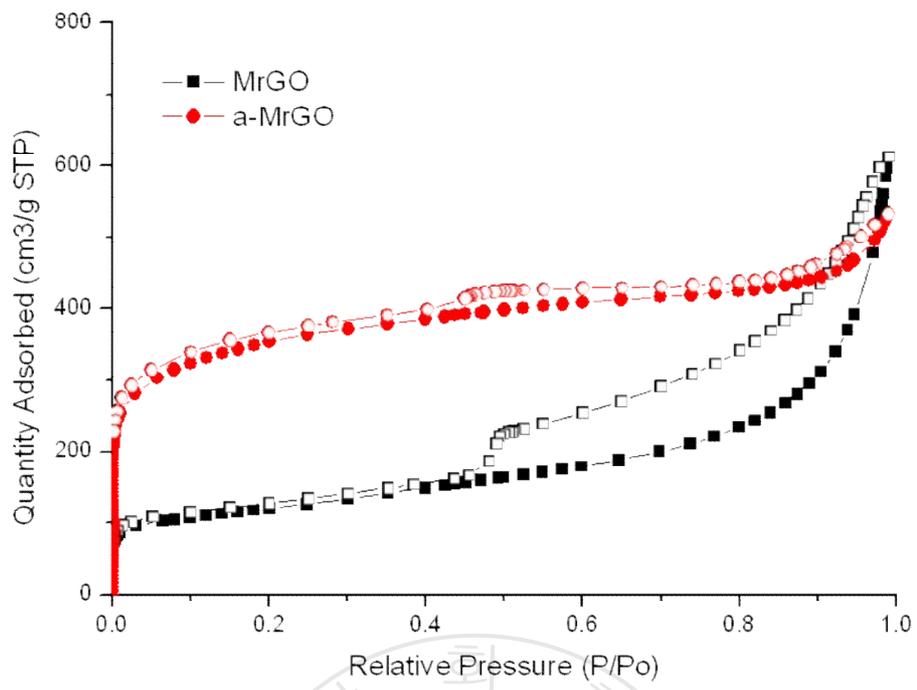
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gas adsorption properties of modified GO by chemical activation

이상문 홍원기 이진배*

한국기초과학지원연구원 물성과학연구부

Activated carbon adsorbents are one of the most extensively used materials for gas adsorption. Carbon dioxide and hydrogen gas storage technology based on physisorption of gases has gained considerable interest in recent years. While most of the recent study focuses on enhancing the adsorption capacity, there is still a insufficiency of understanding of the fundamentals involved in such gas adsorption process. Graphene has a theoretical Surface area of $2630\text{m}^2/\text{g}$ and a very high intrinsic electrical conductivity in plane as well as high mechanical strength and chemical stability. Graphene-based material derived from graphite oxide(GO) is now being manufactured in ton quantities at low cost. Here, we report a simple activation with KOH of microwave reduced GO(MrGO). We prepared MrGO powders by irradiating GO in microwave oven. The as-made MrGO powder was then placed in KOH solution, followed by filtration and drying, to form a MrGO/KOH mixtures for chemical activation. MrGO/KOH mixture was put in a tube furnace under flowing nitrogen and heated at 800°C for 1hr. KOH activation has been extensively used to obtain porous carbons and improved porosity and enhanced adsorption performance were reported. Gas adsorption study of modified GO was performed with the observation of adsorption-desorption isotherms of nitrogen, hydrogen, carbon dioxide, oxygen gases.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-82**

발표분야: 공업화학

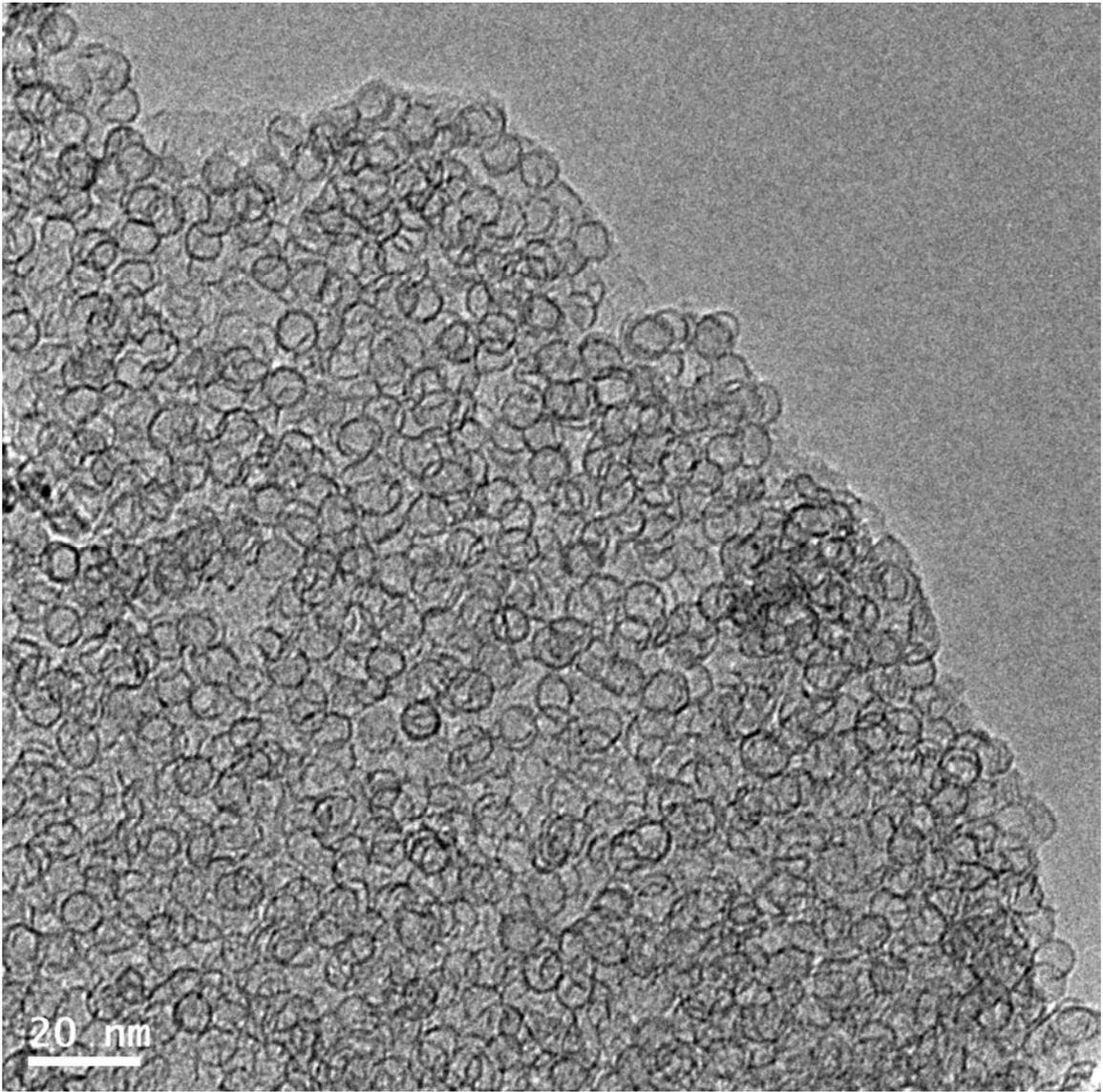
발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphene oxide/manganese silicate composites for hydrogen storage

홍원기 이상문 이진배*

한국기초과학지원연구원 물성과학연구부

Graphene oxide/manganese silicate composites (GO/Mnsilicate) have been prepared by surfactant-free hydrothermal method. Transmission electron microscope (TEM) study of the GO/Mnsilicate shows that hollow spherical manganese silicates are deposited on GO sheets. The hollow manganese silicate nanospheres are approximately uniform in size (~ 8 nm) and the hollow spherical morphology is clearly confirmed. The high pressure H₂ sorption isotherms of GO/Mnsilicate have been performed at liquid nitrogen temperature. GO/Mnsilicate composite exhibits a surface area of 368 m²g⁻¹ and hydrogen storage capacity of 2.9 wt% at 30 bar.



TEAN CHEMICAL

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: IND.P-83

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective extraction of aromatics from aliphatic hydrocarbon mixtures using pyridinium-based Ionic Liquids bearing a thiocyanate anion

신승훈 정민석 김훈식*

경희대학교 화학과

The performance of N-alkylpyridinium-based ionic liquids with a SCN anion (PyILs) was evaluated for the selective extraction of aromatics from aliphatic hydrocarbons. The aromatic extraction ability of PyILs was greatly enhanced by the presence of a methyl group on the pyridinium ring at the 3- or 4-position, whereas the solubility of the aromatics in the PyILs decreased with increasing number of methyl groups on the benzene ring. The computational calculations on the dispersion interactions between aromatics and PyILs demonstrated that the anion-aromatic interaction is much more important than the cation-aromatic interaction in determining the aromatic solubility in PyILs, and such anion-aromatic interaction can be enhanced by introducing a methyl group at the carbon atom of the pyridinium ring.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **IND.P-84**

발표분야: 공업화학

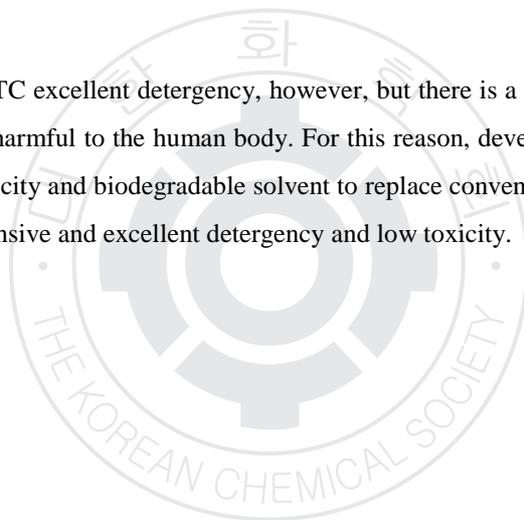
발표종류: 포스터, 발표일시: 수 16:00~19:00

The development of eco-friendly biodegradable detergent

김아나 김종천¹ 김석찬*

국민대학교 화학과 ¹국민대학교 생명나노화학과

1,1,1-TCE and CFC-113 CTC excellent detergency, however, but there is a risk, destruction of the ozone layer, global warming and harmful to the human body. For this reason, developed countries have already been developing of low toxicity and biodegradable solvent to replace conventional cleaners. Hydrocarbon-based detergents are inexpensive and excellent detergency and low toxicity.



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발표분야: 공업화학

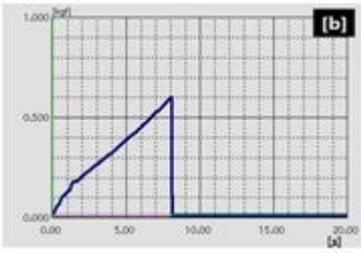
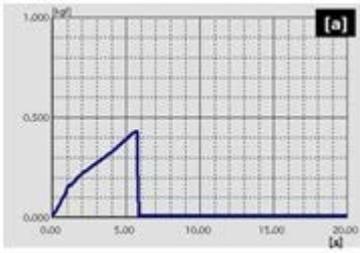
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Ophthalmic Lenses Containing 4-vinylanisole in the presence of nanodiamond particles

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The major physical characteristics of macromolecules used in hydrogel ophthalmic contact lenses include tensile strength, refractive index, optical transmittance, surface hydrophilic or wettability, water content, permeability to oxygen and carbon dioxide, physical and chemical stability, biocompatibility and mechanical properties. High functional ophthalmic lens materials, poly(HEMA-co-MMA)s was prepared by the copolymerization of HEMA, MMA, NVP and 4-vinylanisole in the presence of nanodiamond particles. Nanodiamond particles have high tensile strength and 4-vinylanisole has high refractive index and UV block effect of ophthalmic hydrogel lenses. Ophthalmic lenses of all combinations showed flexible and soft characteristics after being hydrated for 24 hrs in standard saline solution. For 4VA-1~10ND samples to which 4-vinylanisole and nanodiamond particles were added to the Ref._ combination, the transmittance for visible ray, UV-B and UV-A were in the range of 85.4~86.0%, 58.2~76.8%, and 25.0~68.4%, respectively. The pale grey transparent macromolecules exhibited low optical transmittance for wavelengths between 320 nm and 380 nm. The water contents were in the range of 27.80~37.29%, and the refractive index was measured to be in the range of 1.440~1.481. Meanwhile, the tensile strength ranged from 0.4210 to 1.1815 Kgf increased with increasing the addition ratio of nanodiamond. (Fig.1) The polymeric materials satisfied the basic characteristics required for ophthalmic hydrogel lenses. The produced polymers have excellent tensile strength, indicating that the material can be used to fabricate high durability hydrogel ophthalmic lenses with UV blocking effect.



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A study of triglyceride synthesis using 2-O-alkylglycerol

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화학및생물학 ²과학기술연합대학원대학교(UST) 청정화학및 생물학전공 ³한국화학연구원 신
화학연구단

Triglycerides are synthesized with various fatty acid and glycerol. Triglycerides with long chain esters would then be used as transformer oil. There has been increasing researches that focus on the development of triglycerides having outstanding features and biodegradability. In this study, transformer oil substitute was obtained via condensation reaction between 2-alkoxyglycerol and fatty acyl derivatives. Those are characterized by ¹H-NMR, FT-IR and HR/MS. The yields of the products were about 35~50% according to the alkyl chain length.

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장소: 창원CECO

발표코드: **INOR.P-87**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and magnetic properties of Co(II)-terpyridine complexes with ter- and quater-phenyl substituents

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Terpyridine ligands with ter- and quater-phenyl substituents at the 4' position provide bis(ligand)Co(II) complexes showing very different magnetic properties to those of their analogues with long-chain aliphatic substituents, with no evidence of "re-entrant" behaviour. Structure determinations of $[\text{Co}(\text{tpty})_2](\text{BF}_4)_2 \cdot 2\text{CH}_3\text{OH}$ and $[\text{Co}(\text{qtpy})_2](\text{BPh}_4)_2 \cdot 3.5\text{dmf} \cdot 2\text{H}_2\text{O}$ (dmf=N,N-dimethylformamide) show the metal ion centres in both to be relatively distant and that the "terpyridine embrace" observed to be partially retained in their analogues is completely lost. Consideration of available structural and magnetic data for these and other Co(II) complexes of functionalised terpyridines and terpyridine itself provides evidence that spin crossover behaviour may be regulated by face-to-face contacts of the pyridyl units of the head groups.

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장소: 창원CECO

발표코드: **INOR.P-88**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Multi-Layered Core-Shell Microspheres Generated from Multi-Step Growth of Coordination Polymers

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The management of the chemical composition of nano- or micro-scale particles is a quite convenient way to adjust their properties. Currently, the conjunction of coordination polymers (CPs) with other functional materials in core-shell or film forms in order to extend the utilization range of coordination polymer materials has received extensive attention. Herein, the construction of well-defined multi-layered core-shell structures is demonstrated via a multi-step growth of various coordination polymers. Furthermore, the compositions of multi-layered core-shell microspheres are easily controlled by changing the order of the multi-step growth process.

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발표코드: **INOR.P-89**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Microporous organic networks bearing metal-salen species for mild CO₂ fixation

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Carbon dioxide can be chemically transformed to organic compounds by reaction with various coupling reagents. For example, carbon dioxide is fixed to cyclic carbonates by reaction with a variety of epoxides. The resultant cyclic carbonates have been used both as electrolytes in electrochemical devices such as lithium ion batteries and as raw materials for polymer synthesis. Although liquid-phase catalytic systems for transformation of CO₂ to cyclic carbonates have been extensively reported, it needs relatively high temperatures (110~160 °C) and high pressure of CO₂ (1-8 MPa) for achieving the fixation of carbon dioxide with 1-50 h⁻¹ TOF. This work shows that porous heterogeneous catalytic systems for catalytic CO₂ fixation can be developed by a direct assembly of metal-salen containing building blocks with organic connectors through a carbon-carbon bond formation reaction. For use as a dihalo building block, Al, Cr, Co-salen building blocks with two iodo groups were prepared. Sonogashira coupling of these building blocks with tetra(4-ethynylphenyl)methane resulted in microporous organic networks (MONs) bearing Al, Cr, and Co-salen species (Al-MON, Cr-MON, Co-MON). Chemical conversion of carbon dioxide with epoxide to cyclic carbonates under mild conditions (60 °C and 1 MPa CO₂). Among the M-MONs, the Co-MON showed the best reactivity for carbon dioxide conversion to cyclic carbonates with 1400~1860 TON and 117~155h⁻¹ TOF. The size effect of epoxides in CO₂ fixation was observed due to the microporosity of Co-MON.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Iridium(III) complexes bearing imidazoline thione and selone ligands: visible light responsive photocatalysts

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In this work, we report the preparation of iridium complexes containing bis(N-heterocyclic carbene), bis(imidazoline thione), and bis(imidazoline selone) ligands and their properties in photoinduced oxidative coupling of benzylamines to imines in the presence of oxygen. The iridium complexes showed the significant absorption of visible light with maximum intensity at ~460 nm. Especially, Bis(2-(2'-benzothienyl)pyridinato)iridium(III) complexes (Ir-6) with bis(imidazoline selone) showed the highest performance as a photosensitizer in the visible-light-induced oxidative coupling of benzylamine to imine. A 0.25 mol % amount of Ir-6 showed 94% conversion of benzylamine to the corresponding imine in 5 h at room temperature under blue LED irradiation. Through mechanistic studies, it was suggested that the photo-induced oxidative coupling of benzylamine by Ir-6 follows a singlet oxygen pathway. The superior performance of Ir-6 results from the efficient visible light absorption at 460 nm and the enhanced triplet state due to the heavy-atom effect of bis(imidazoline selone). This work shows that bis(imidazoline thione) and bis(imidazoline selone) can be efficient ligands for designing the optical properties of iridium(III) complexes.

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발표코드: **INOR.P-91**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrathin Sn/CoOx nanohollows as anode materials in lithium ion batteries

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성균관대학교 화학과 ¹성균관대학교 에너지과학과

This presentation will introduce the synthesis of tin containing hollow nanomaterials with ultrathin shells using a multi-component single precursor and their performance as an anode material in lithium ion batteries. First, organometallic precursor was designed for the preparation of Sn²⁺Co hetero-component anode materials because both Sn and cobalt oxide are active as anode materials. To confer nucleophilicity on cobalt, Co₂(CO)₈ was reduced to Co(-1) species using sodium naphthalenide. The resultant NaCo(CO)₄ was reacted with a tin electrophile (Ph₃SnCl) to form the target precursor, Ph₃SnCo(CO)₄. Its elemental confirmed the high purity of the obtained precursor. For the synthesis of ultrathin Sn/CoOx hollow nanospheres, the Sn²⁺Co heterobimetallic precursor was dissolved in well-dried oleylamine and injected into a hot oleylamine solution at 260 °C. The reaction mixture was heated for additional 12 hours. After cooling to room temperature, excess methanol was added to form precipitates which were retrieved by centrifugation. Transmission electron microscopy (TEM) analysis of the obtained materials showed nanospheres with empty inner space. The Sn/CoOx nanohollows with 6.1 nm diameter and ~1.5 nm shell thickness showed excellent lithium storage capacity of up to 857 mAh/g after 30 cycles.

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발표코드: **INOR.P-92**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Zn(II)-Ti(IV) heterometallic approach toward porous metal-organic frameworks with highly symmetric (6,8)-connected topology

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한양대학교 응용화학과

Different methods have been adopted to expand the structural diversity of MOFs, and a heterometallic approach is a powerful complement to methods that rely on the extension or derivatization of organic linkers. We have recently reported the first case of zinc-titanium-organic framework (ZTOF) obtained using an asymmetrically substituted dicarboxylate. This synthetic method has been further refined in order to obtain new MOF based on two different building units within the same structure. As a result, we were able to synthesize another ZTOF having a highly symmetric (6,8)-connected topology that is unprecedented in MOFs or other network solids. The new material also possesses a high percentage of solvent-accessible voids. The open framework can sustain the full evacuation of included solvents and displays high surface areas.

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발표코드: **INOR.P-93**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent chemosensor based-on the combination of julolidine and furan for selective detection of zinc ion

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A new sensor 1-[[2-(furan-2-ylmethyl)imino]methyl]-2-hydroxyjulolidine (1) based on the combination of julolidine and furan groups was designed and synthesized as a Zn²⁺ selective fluorescent chemosensor. Upon treatment with zinc ions, the complexation of 1 with Zn²⁺ exhibited a pronounced enhancement in the fluorescence emission in methanol, while many other ions such as Mn²⁺, Co²⁺, Ni²⁺, Cd²⁺, Hg²⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺, Al³⁺ and Ag⁺ had no influence. Notably, this chemosensor could distinguish clearly Zn²⁺ from Cd²⁺. The 1:1 binding mode of the 1-Zn²⁺ complex was drawn, based on UV-vis titration, fluorescence titration, Job plot and ESI-mass spectrometry analysis.

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A Selective Colorimetric and Fluorescent Chemosensor Based-on Naphthol for Detection of Al³⁺ and Cu²⁺

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A simple and easily synthesized colorimetric and fluorescent chemosensor 1, based on naphthol moieties as a binding and signaling unit, has been synthesized in a one step procedure. Chemosensor 1 exhibited a color change from yellow to orange and fluorescence enhancement with a red shift upon binding to Al³⁺ in acetonitrile. Moreover, it can selectively detect Cu²⁺ ions via an ion-promoted oxidation reaction in acetonitrile, resulting in a selective color change from yellow to dark blue and a fluorescence quenching effect. Furthermore, chemosensor 1 showed colorimetric and fluorescence selectivity for Cu²⁺ in aqueous acetonitrile solution.

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폴리머기반 BN White Graphene

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니켈 나노입자(NiNPs)를 테트라글라이머(Tetraglyme) 용매상에서 사용하여 효율적인 촉매반응으로 암모니아 보란에서 보라진으로 합성하였다. 최적의 조건은 3mol%의 니켈 나노입자를 테트라글라이머에 암모니아 보란을 녹인 1.5 M 의 용액에 넣고 80 °C 온도에서 6 시간동안 반응한 후 30 Torr 로 유지한 진공을 유지하여 합성을 진행한 것이다. 보라진은 -45 °C, -78 °C, -196 °C 트랩을 이용하여 분리하였으며 -78 °C 트랩에 순수한 보라진이 53 % 수율로 얻어졌다. 생성된 보라진은 저압화학증착법(Low pressure chemical vapor deposition: LPCVD)을 이용한 고품질의 h-BN (white graphene) 과 대면적의 h-BN sheet 를 형성하는 분자전구체로 활용하였다. Ultra-thin h-BN(단막부터 다막층)은 니켈 호일(Ni foil)위에서 보라진과 암모니아의 최적의 비율로 합성하였고 암모니아의 다양한 부분압을 이용하여 막의 수를 조절하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

유무기 혼성소재 기반 새로운 광전기적 특성의 유기전자 소재

조양진 강상욱*

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세가지 구조이성질체(ortho-, meta-, para-)와 뛰어난 화학적 물리적 안정성을 가지는 카보란을 기반으로 새로운 청색인광 OLED 용 호스트 물질을 개발하였다. 카보란을 중심으로 광특성이 뛰어난 두개의 카바졸이 치환되어 있으며, bis[4-(N-carbazolyl)phenyl] carboranes (o-Cb, m-Cb, p-Cb)으로 명명된다. 구조이성질체에 따라 o-Cb < m-Cb < p-Cb 순서로 경향성 있는 열적 안정성과 전하 이동도를 가진다는 것을 증명 할 수가 있었다. 특히 p-Cb 는 높은 삼중항 에너지($T_1 = 3.1$ eV)와 뛰어난 열적 안정성($T_g = 164$ °C) 뿐만 아니라 1.1×10^3 cm²/(V s)의 뛰어난 정공 이동도를 가지는 것을 실험적으로 확인 하였다. 또한 분자계산을 통하여 카보란 물질이 분자내에서 어떤 전자적 역할을 하는지 확인 하였고, 그 결과 기존에 알려진 청색인광용 호스트 물질에서는 완전하지 않았던 삼중항 에너지가 완전히 한곳에만 갇금되어 있음을 확인함으로써 기존 물질들 보다 카보란 기반 물질이 뛰어난 특성을 가지는 것을 이론적으로 증명하였다. 이 결과들을 바탕으로 p-Cb 물질을 청색인광 소자에 적용하였고, 단순 소자구조에서 15.3%의 높은 외부양자효율을 얻었다.

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장소: 창원CECO

발표코드: **INOR.P-97**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

분자전자용 카바졸 기반물질의 비정질박막에서 원자가전자상태의 에너지분포에 의한 분자들간의 상호작용 효과

조양진 강상욱*

고려대학교 소재화학과

카바졸 기반 물질에서 비정질 고체의 occupied 전자 구조에 대한 분자간 상호작용 효과에 관한 계산은 유기 고체의 이합체들이 무질서한 방향으로 구성되어 있는 가정하에 조사되었다. 전자적 에너지 상태는 많은 수의 이합체들이 무질서하게 분포된 상태에서 계산되었으며 이러한 분포는 semiempirical van der Waals density functional theory 를 이용하여 계산하였다. 에너지레벨 분할과 같은 분자들간의 상호작용은 분자들의 무질서한 분포에 의해 일어난다. 결과적으로, frontier occupied energy 상태는 Gaussian distributions 에 의해 다음을 묘사하고 있다. 1) 주된 분포의 전체 너피를 half maximum 80~110 meV 에서 relaxation 하였고 2) 중심으로부터 150 meV 의 를 벗어나는 부분을 shoulder 로 분리하였다. 이러한 shoulder 들이 나타나는 이유는 더 많은 단단한 구조의 이합체들의 집합에 기인한 것이다.

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발표코드: INOR.P-98

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A NBD-based selective colorimetric and fluorescent chemosensor for Hg^{2+}

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A new NBD-based sensor bearing a dipicolylamine derivative, (2-pyridylmethyl)(2-quinolylmethyl)amine (1), was synthesized, and its chromogenic and fluorogenic behaviors toward various metal ions were investigated in methanol solution. Chemosensor 1 selectively detected Hg^{2+} ions through color change from yellow to colorless. In addition, chemosensor 1 exhibited highly Hg^{2+} -selective ON-OFF fluorescence quenching behavior and was shown to discriminate various competing metal ions, particularly, such as Cu^{2+} , Ag^+ and Pb^{2+} . The binding mode of 1- Hg^{2+} was found to be a 1:2 complex formation, based on Job plot and ^1H NMR titration.

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장소: 창원CECO

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

제1세대인공광합성: Dye/TiO₂/Pt Hybrid Systems 에서 친수성기의 변화를 통한 가시광에서의 수소발생과 Charge-Separate 상태의 동 역학적 연구

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(E)-3-(5'-(4-[bis(4-R1-phenyl)amino]phenyl)-4,4'-(R2)2-2,2'-bithiophen-5-yl)-2-cyanoacrylic acid 염료를 이용하여 Dye/TiO₂/Pt hybrid 기반의 가시광에서의 수소발생에 대한 연구를 진행하였다. 수소발생은 EDTA 를 전자주개로 사용하고 $\lambda > 420$ nm 빛을 조사한 수용액에서 진행하였다. MOD/TiO₂/Pt 의 경우, 광여기 수소발생 양자효율이 0.27 ± 0.03 으로 나타났다. 두 염료(MOD, PD)가 TiO₂ 나노입자에 흡착된 투명필름의 Transient absorption 결과 염료의 라디칼 양이온이 빠르게 (< 100 fs) 생성된 것을 관측 하였다. 염료의 라디칼 양이온의 소광은 두 성분으로 이루어져 있었으며, 치환체 R 에 의존하지 않는(5 ps) 작은 성분과 두 염료 사이에 차이를 보이는 주된 성분으로 되어 있었다. 두 염료는 다음과 같은 두가지 차이를 보였다 : 1) MOD 의 소광이 PD 보다 2.5 배 느리게 진행, 2) MOD 의 transient 스펙트럼이 17 ps 장과장이동 하는 동안 PD 는 변화를 보이지 않음. 수소발생의 치환체 효과는 치환체의 다른 solvent reorganization 에 의해 염료의 라디칼 양이온 전하 재결합 (CR) 에 의존함을 관측하였다.

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장소: 창원CECO

발표코드: INOR.P-100

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Transesterification Reactions of One-dimensional Coordination Polymers Containing Paddle-wheel Type Cu_2 Units Connected by Various Bridging Ligands

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서울과학기술대학교 정밀화학과 ¹이화여자대학교 화학과 ²이화여자대학교 화학-나노과학과 ³
서울과학기술대학교 정밀화학과 친환경소재제품센터

The paddle-wheel dinuclear unit consists of two Cu^{II} ions bridged by four benzoate ligands, and these paddle-wheel $[\text{Cu}_2(\text{O}_2\text{CPh})_4]$ units are connected by various bridging ligands to form one-dimensional chain compounds formulated as $[\text{Cu}_2(\text{O}_2\text{CPh})_4(\mu\text{-L})]$ ($\text{L} = 2,4\text{-bpe}$ (1), $3,3'\text{-dipicam}$ (3), $2,5\text{-Me}_2\text{pyz}$ (4), pyz (5), $4,4'\text{-bpy}$ (6), and 4pds (7)). The compound 2 formulated as $[[\text{Cu}_2(\text{O}_2\text{CPh})_4](\mu\text{-bpp})[\text{Cu}(\text{O}_2\text{CPh})_2]]_n$ consists of $[\text{Cu}_2(\text{O}_2\text{CPh})_4]$ units and $[\text{Cu}(\text{O}_2\text{CPh})_2]$ units connected by bpp alternatively. Compounds 1-5 and 7 catalyzed efficiently the transesterification of a variety of esters. Among them, 2 was most effective for the transesterification reactivity. It has been proposed that a paddle-wheel unit for all compounds except for 2 might be a possible reactive species for the transesterification reaction in solution, while a mononuclear type of Cu complex might exist as a major species of compound 2.

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장소: 창원CECO

발표코드: **INOR.P-101**

발표분야: 무기화학

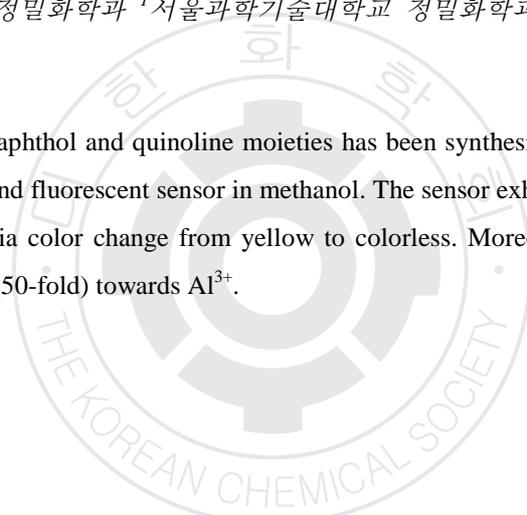
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Colorimetric and Fluorescent Chemosensor for Selective Detection of Cr³⁺ and Al³⁺

송은주 이슬아 조현용 김 철^{1,*}

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A chemosensor based on naphthol and quinoline moieties has been synthesized for the detection of Cr³⁺ and Al³⁺ as a colorimetric and fluorescent sensor in methanol. The sensor exhibited selective and sensitive recognition towards Cr³⁺ via color change from yellow to colorless. Moreover, it showed a significant fluorescence enhancement (50-fold) towards Al³⁺.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-102

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

***In-situ* Observation of Structural Transformation of a Flexible Metal-Organic Framework upon CO₂ sorption**

현성민 김태경 문도현^{1,*} 문희리^{*}

울산과학기술대학교(UNIST) 친환경에너지공학부 ¹포항가속기연구소 빔라인부

A Metal-Organic framework (MOF), $\{[(NiL)_2(BPTC)]_2 \cdot 4DMF \cdot 2H_2O\}$ (1-DMF) ($[NiL]^{2+} = [Ni(C_{14}H_{34}N_6)]^{2+}$, BPTC⁴⁻ = 2,2',5,5'- biphenyltetracarboxylate, DMF = N,N-dimethylformamide) was prepared by self-assembly of $[NiL](ClO_4)_2$ and H₄BPTC in DMF/H₂O mixture solution. Single crystal X-ray diffraction data revealed that 1-DMF has three-dimensional structure with accessible pore occupied by guest molecules. Due to flexibility, the structure of 1-DMF was changed into that of 1 with shrunk and closed pores upon elimination of guest molecules. Gas sorption experiments with N₂ and H₂ confirmed that 1 has closed pore structure because of small adsorption amount. However, CO₂ isotherm at 195 K appeared in two-step adsorption with much larger amount of uptake than N₂ and H₂, which means that CO₂ gas triggered a structural transformation of 1 into open and expanded structure. In addition, the desorption isotherm shows three-steps with hysteresis, which suggests that structural changes of opening and closing experience different process from each other. *In-situ* X-ray powder diffraction (XRPD) experiment confirms that there were different structural phases at each steps. In addition, with comparing XRPD results with X-ray structures of single crystals different kinds of guests, such as water and acetonitrile, structural transformation occurs in two steps by pore-opening through rotation of macrocycles with breaking hydrogen bonds between amines of macrocycles and carboxylates and by expanding the cell volume with increasing uptake of CO₂.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-103**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Reactions of a 14-Membered Tetraaza Macrocycle Bearing *N*-Cyanomethyl Pendant Arms and Its Complexes

장보우 강신결*

대구대학교 화학과

The di-*N*-cyanomethylated macrocycle 1,8-bis(cyanomethyl)-3,5,7,7,10,12,14,14-octamethyl-1,4,8,11-tetraazacyclodecane (L^2) has been prepared by the reaction of 2,5,5,7,9,12,12,14-octamethyl-1,4,8,11-tetraazacyclodecane (L^1) with bromoacetonitrile. The copper(II) complex $[CuL^2]^{2+}$ could be prepared by the reaction of L^2 with Copper(II) nitrate. All our attempts to prepare $[NiL^2]^{2+}$ by the reaction of Ni^{2+} ion were unsuccessful. However, L^2 reacts with water or methanol in the presence of the metal ion to yield macrocyclic nickel(II) or copper(II) complexes bearing various types of functional pendant arms. Synthesis and reactions of L^2 and its complexes are presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-104

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Reaction of C-*meso* and C-*racemic* Isomers of a Tetraaza Macrocycle Bearing N-Propargyl Pendant Arms and Their Complexes

김주영 강신결*

대구대학교 화학과

Two isomers of 1,8-bis(propargyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane(L²), C-*meso*-L² and C-*racemic*-L², have been prepared by the reaction of C-*meso* or C-*racemic*-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane(L¹) with propargyl bromide. Nickel(II) and/or copper(II) of the macrocycles have been prepared and characterised. The N-propargyl pendant arms on [M(C-*meso*-L²)]²⁺ and [M(C-*racemic*-L²)]²⁺ (M = Ni(II) or Cu(II)) react with various nucleophilic reagents. Synthesis and reactions of C-*meso*-L² and C-*racemic*-L² and their complexes are presented.

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장소: 창원CECO

발표코드: INOR.P-105

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of a Macrocyclic Nickel(II) Complex Bearing Two *N*-CH₂C≡CH Pendant Arms and Its Intramolecular Hydroamination

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The macrocycle 2,13-bis(propargyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.^{1.18}0^{7.12}]docosane (L²) bearing two *N*-CH₂C≡CH pendant arms can be prepared by the reaction of 3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.^{1.18}0^{7.12}]docosane (L¹) with propargyl bromide. The complex [NiL²]²⁺ has been prepared by the reaction of L² with Ni²⁺ ion. Interestingly, [NiL²]²⁺ readily undergoes intramolecular hydroamination in the presence of a 14-membered tetraaza macrocycle to give the topologically constrained macropolycyclic complex [NiL³]²⁺, in which two nitrogen atoms of each six-membered chelate ring are linked together by the -CH₂-CH=CH- bridge. Synthesis and chemical properties of the compounds are presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-106

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hard and Soft Metal Complexes of Calix[4]-bis-monothiacrown-5: X-ray and NMR Studies of Homodinuclear Species and Heteromultinuclear Network Complexes

김자연 이심성*

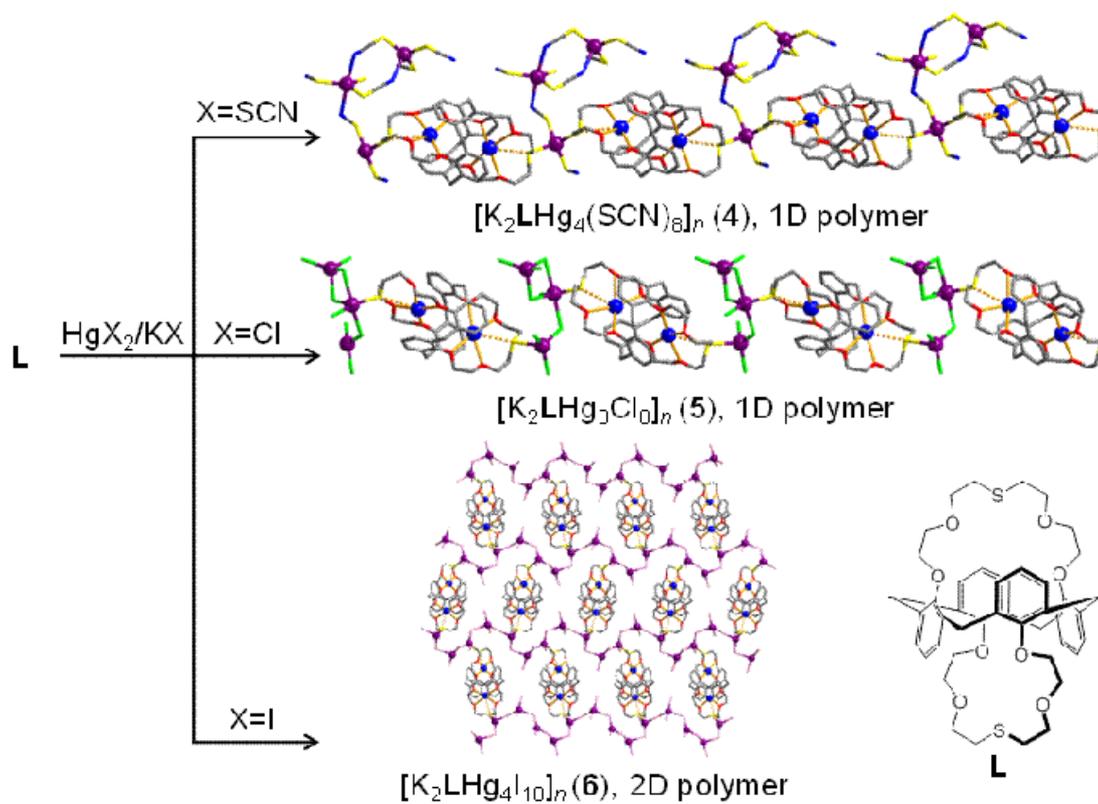
경상대학교 화학과

In the extension of our previous work on the exocyclic coordination polymers of calix[4]-bis-monothiacrown (L) exhibiting a photoluminescence switching behavior,^{1,2} its new networking patterns via homo- and heteronuclear system are reported.³ Also, dipotassium(I) and disilver(I) complexes of L were isolated and their solid state structures characterized. In the reactions of L with Hg(SCN)₂, HgCl₂, and HgI₂ gave commonly 1D coordination polymers [Hg₂L(SCN)₄]_n (1), [Hg₂LCl₄]_n (2), and {[Hg₂LL₄]-CH₂Cl₂]_n (3) with a similar network pattern, in which Ls are linked by -X-Hg-X₂-Hg-X- (X=SCN for 1, X=Cl for 2 and X=I for 3). The reaction of L with KSCN in the presence of Hg(SCN)₂ afforded an endo/exocyclic heteronuclear complex [K₂LHg₃(SCN)₈]_n (4) with a 1D polymeric structure. Also, the reaction of L with KCl in the presence of HgCl₂ afforded an endo/exocyclic heteronuclear complex [K₂LHg₃Cl₈]_n (5) with a 1D polymeric structure. In addition, the reaction of L with KI in the presence of HgI₂ afforded a 2D coordination polymer [K₂LHg₄I₁₀]_n (6) with the endocyclic dipotassium(I) complex linked by exocyclic mercury(II) iodide cluster backbone. Treatment of L with KI in the presence of CdI₂ afforded a discrete endocyclic dipotassium(I) complex [K₂L][Cd₂I₆]-CH₂Cl₂ (7) in which the square-type dicadmium(II) hexaiodide cluster [Cd₂I₆]²⁻ exists in a separated form. In the reaction of L with AgClO₄ afforded an endocyclic dinuclear complex [Ag₂L](ClO₄)₂·2CH₃OH·H₂O (8). To probe the complexation behavior for these same systems in solution, the competition between potassium(I) and silver(I) for L was monitored by ¹H NMR. Potassium(I) forms a more stable dinuclear complex with L than silver(I) both in the solid and solution states.

1. J. Y. Lee, H. J. Kim, J. H. Jung, W. Sim, S. S. Lee, *J. Am. Chem. Soc.* 2008, 130, 13838.

2. J. Y. Lee, S. Y. Lee, W. Sim, K.-M. Park, J. Kim, S. S. Lee, *J. Am. Chem. Soc.* 2008, *130*, 6902.

3. J.-Y. Kim, I.-H. Park, J. Y. Lee, J.-H. Lee, K.-M. Park, S. S. Lee, *Inorg. Chem.* 2013, *52*, 10176.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-107

발표분야: 무기화학

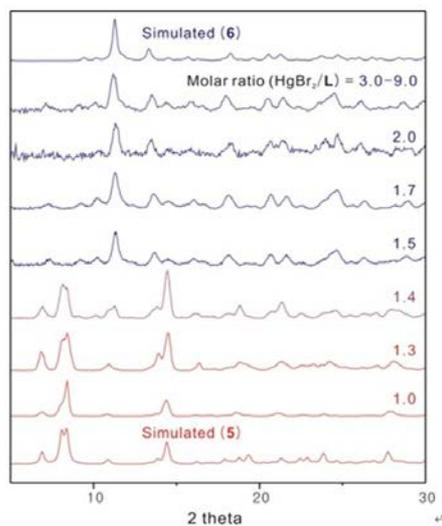
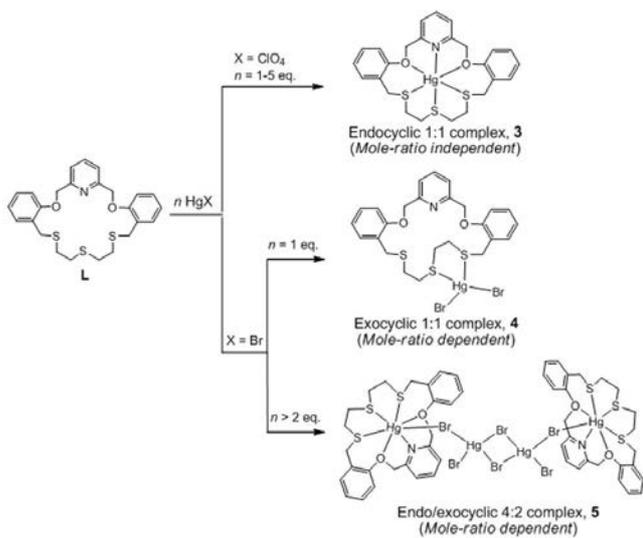
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cooperative Effect of Anion and Mole Ratio on the Soft Metal Complexation of an NO₂S₃-Macrocyclic

이형환 박인혁 이심성*

경상대학교 화학과

The pyridine-containing thioxaaza-macrocyclic L was synthesized by dithiol-dichloride coupling reaction using Cs₂CO₃ in DMF under high dilution condition. Comparative investigation of the coordination behavior of L with Ag(I), Cu(I), and Hg(II) is reported. The X-ray structures of five complexes (1-5) were determined, and a range of structural types and coordination modes including mono- to multinuclear and discrete to continuous ones, is shown to occur. In the reaction with AgNO₃, L forms a rare example of a 1D coordination polymer 1, {[Ag₂L(NO₃)₂]CH₃CN}_n incorporating an endo/exocyclic coordination. In the reaction with CuI, L forms an exocyclic 1D coordination polymer 2, [(Cu₂I₂)L]_n linked by Cu₂I₂-rhomboid giving a zigzag chain. The reaction of L with mercury(II) anion complexes (3 and 4 see below) with different coordination modes, depending on the anions used (ClO₄⁻ and Br⁻). On varying the mole ratio (*n*) of two reactants (HgBr₂/L), two products with an exocyclic 4 and an endo/exocyclic coordination 5 were isolated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-108

발표분야: 무기화학

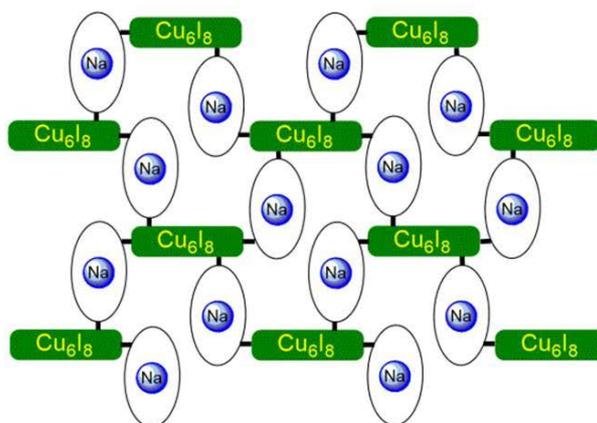
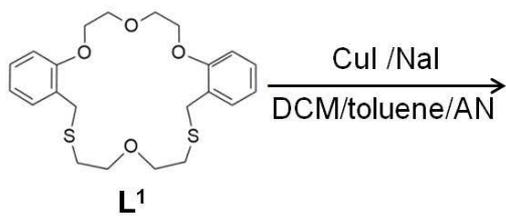
발표종류: 포스터, 발표일시: 수 16:00~19:00

Soft and Soft/Hard Metal Supramolecular Complexes of an O_xS_2 -Macrocycles ($x=3$ or 4) with Discrete Monomer, Dimer, and Polymer Structures

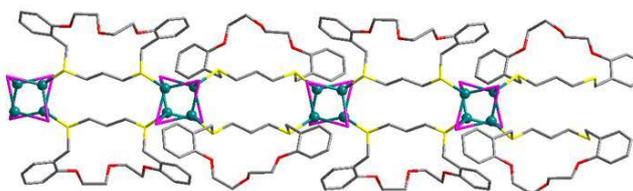
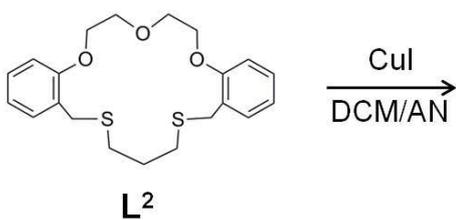
류현수 박기민 이심성*

경상대학교 화학과

An O_4S_2 -macrocyclic L^1 and an O_3S_2 -macrocyclic L^2 were synthesized and structurally characterized by X-ray analysis. The X-ray crystal structures of seven complexes (1-7) have been determined, and a range of structural types and coordination modes, including discrete to continuous forms, mono- to multinuclear, and endo- to exocyclic structures involving M-S and M'-O bonds are presented. Reactions of L^1 with HgI_2 afforded the exocyclic mononuclear complex $[HgL^1I_2]$ (1). Reactions of L^1 with $Pb(ClO_4)_2$ yielded the endocyclic mononuclear complex $[PbL^1(ClO_4)_2]$ (2). Furthermore, the reaction of L^1 with CuI gave a mixture of an exocyclic monomer $[CuL^1I]$ (3, brick-shape) and an exocyclic dimer $[(Cu_2I_2)L^1_2]$ (4, rhomboid-shape) with two different shapes. From the mixture, 3 and 4 were separated under the microscope and confirmed the separation with PXRD patterns. The straightforward one-pot reaction of L^1 with CuI in the presence of NaI resulted in the heteronuclear endo/exocyclic complex $[Na_2(\mu_2-Cu_6I_8)L^1_2(CH_3CN)_4]_n$ (5). In 5, the endocyclic macrocyclic Na^+ complex units are linked by the twisted ribbon-type cluster $[Cu_6I_8]^{2+}$ resulting in the unique 2D network. Reactions of L^2 with HgI_2 afforded the one-dimensional exocyclic polymer $[HgL^2I_2]_n$ (6). Reactions of L^2 with CuI afforded an emissive 1D looped coordination polymer $[Cu_4I_4L^2_2]_n$ (7) linked with a cubane-type copper iodide cluster.



Na/Cu heteronuclear endo/exocyclic complex linked by cluster $[\text{Cu}_6\text{I}_8]^{2+}$ (**5**)



1-D coordination polymer linked by a cubane-type Cu_4I_4 cluster (**7**)



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-109

발표분야: 무기화학

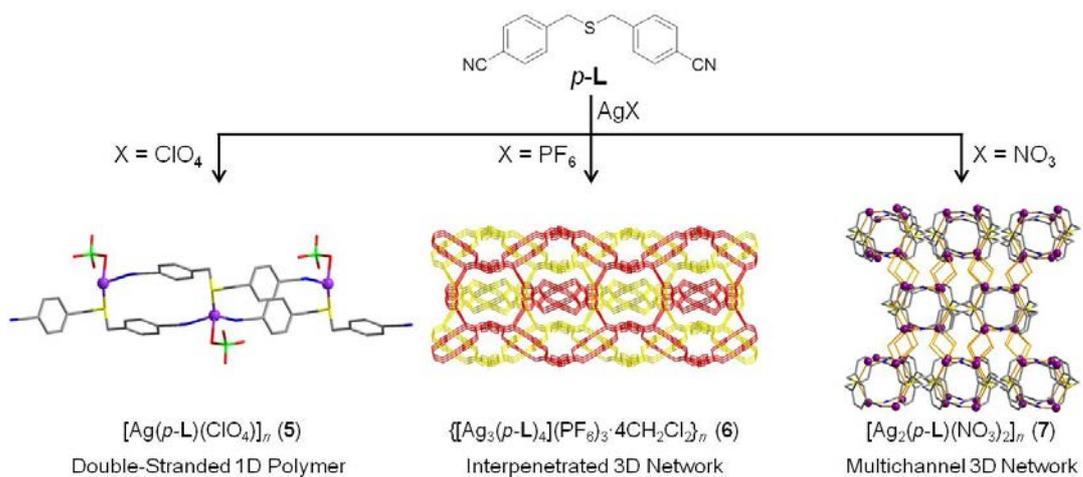
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anion Effects on Supramolecular Silver(I) Coordination Polymers of Bis(cyanobenzyl)sulfide

이은지 이심성* 박기민*

경상대학교 화학과

Regioisomers (*m*-L and *p*-L) of bis(cyanobenzyl)sulfide were employed as building blocks and their supramolecular silver(I) complexes are reported.¹ The reactions of *m*-L and *p*-L with silver(I) salts (X = ClO₄⁻, PF₆⁻, or NO₃⁻) afforded the respective anion-dependent complexes 1-6 with different topologies. For examples, the reactions of *m*-L with AgClO₄ and AgPF₆ yielded isostructural 1D zigzag polymers of type [Ag(*m*-L)(X)]_n (1; X= ClO₄⁻ and 2; X= PF₆⁻). The reaction of *m*-L with AgNO₃, supramolecular isomers 3 and 4 of type [Ag₂(*m*-L)(NO₃)₂]_n with different 2D network structures were obtained depending on the molar ratios of reactants. Meanwhile, the reaction of *p*-L with AgClO₄ afforded a double-stranded 1D polymeric array of formula [Ag(*p*-L)(ClO₄)]_n (5). Treatment of *p*-L with AgPF₆ afforded a 2-fold interpenetrated 3D polymeric array of formula {[Ag₃(*p*-L)₄](PF₆)₃·4CH₂Cl₂]_n (6). In addition, The reaction of *p*-L with AgNO₃ also gave a multichannel type 3D polymeric array of formula [Ag₂(*p*-L)(NO₃)₂]_n (7). The formations of such 1-3D supramolecular complexes are discussed in terms of anion effect. Reference 1. E. Lee, J.-Y. Kim, S. S. Lee, K.-M. Park, *Chem. Eur. J.* In press.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-110

발표분야: 무기화학

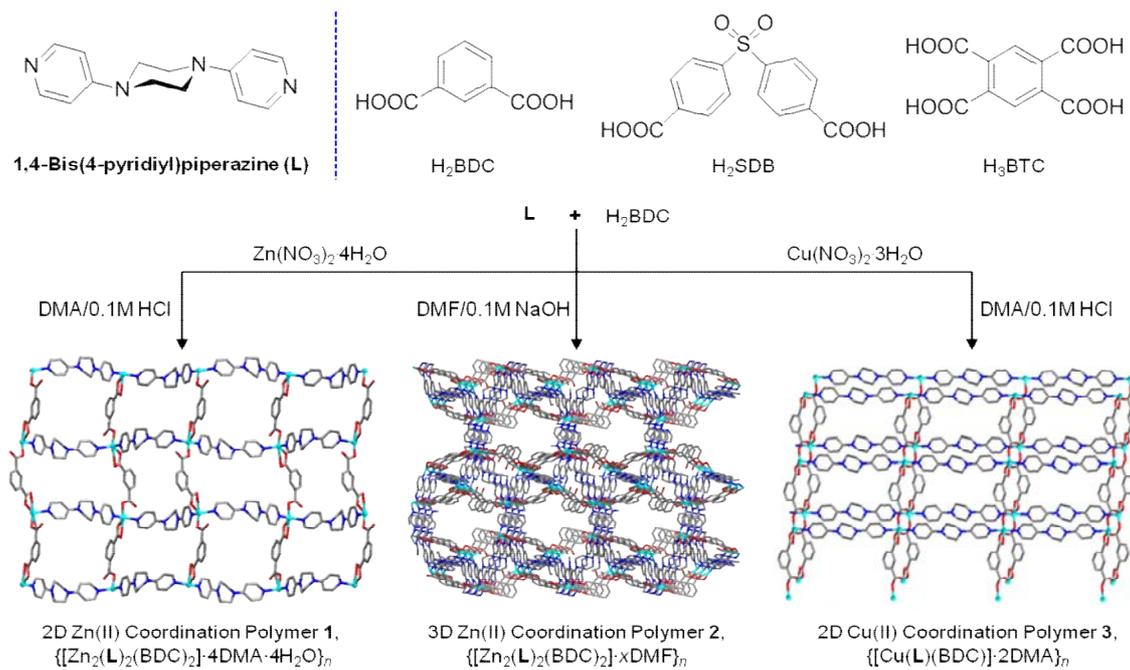
발표종류: 포스터, 발표일시: 수 16:00~19:00

Metallosupramolecules based on 1,4-Bis(4-pyridyl)piperazine and Aromatic Carboxylic Acid with Transition Metal Ions

주희영 박기민* 이심성*

경상대학교 화학과

Binary ligand system of bipyridine derivative and aromatic carboxylic acid was employed to prepare metal-organic frameworks (MOFs 1-6). First, the reaction of 1,4-bis(4-pyridyl)piperazine (L), $Zn(NO_3)_2 \cdot 4H_2O$, and H_2BDC in DMA yielded a grid-type 2D network $\{[Zn_2(L)_2(BDC)_2] \cdot 4DMA \cdot 4H_2O\}_n$ (1). Interestingly, when DMF was used instead of DMA, $\{[Zn_2(L)_2(BDC)_2] \cdot xDMF\}_n$ (2) adopting a 3D channel structure was isolated as a supramolecular isomer of 1. In the reaction of L with $Cu(NO_3)_2 \cdot 3H_2O$ in the presence of H_2BDC , a 2D network $\{[Cu(L)(BDC)] \cdot 2DMA\}_n$ (3) in which the Cu(II) and BDC form a 1D double chain and further doubly linked by L in the axial positions. The reaction of L with $Co(NO_3)_2 \cdot 6H_2O$ in the presence of H_2SDB gave a 2D network $\{[Co_3(HL)_2(SDB)_4(H_2O)_2] \cdot 4H_2O\}_n$ (4) containing a paddle-wheel secondary building unit as a node. In the reaction of L with $Co(NO_3)_2 \cdot 6H_2O$ in the presence of H_4BTEC gave a 3D square channel structure $\{[Co_2(BTEC)(H_2BTEC)(H_2O)](H_2L)\}_n$ (5). When 0.1 M NaOH solution was added, $\{[Co(BTEC)(H_2O)_4](H_2L)\}_n$ (6) adopting a 1D zig-zag polymer was isolated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-111

발표분야: 무기화학

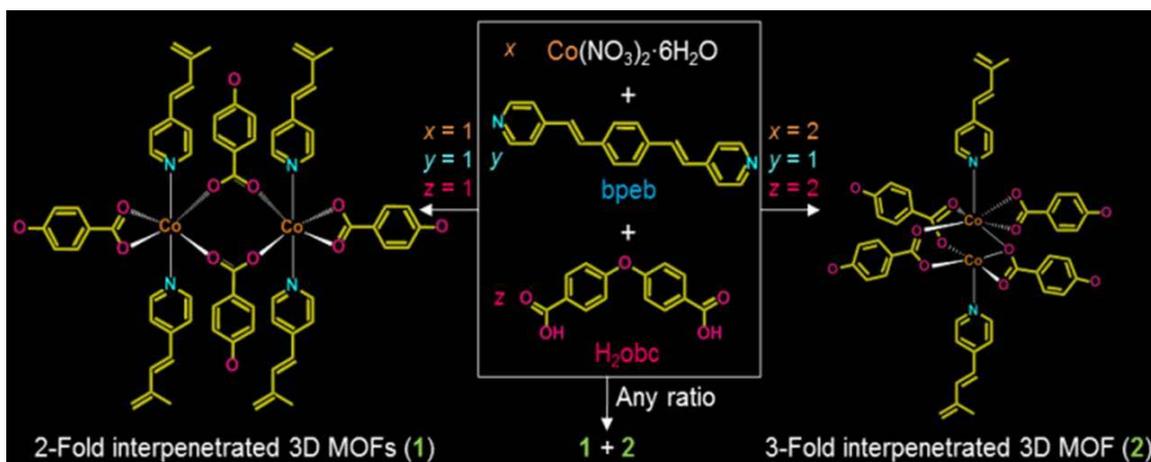
발표종류: 포스터, 발표일시: 수 16:00~19:00

Mole-Ratio Dependent Porous Co(II) Coordination Polymers based on Dipyridyl Ligand and Dicarboxylic Acid

박인혁 김자연 Raghavender Medishetty¹ 이심성* Jagadese J. Vittal^{1,*}

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

Two Co(II) MOFs (1 and 2, see the Scheme below) based on an olefinic dipyridyl ligand (bpeb) and 4,4'-oxybisbenzoic acid (H₂obc) showing different secondary building units (SBUs) are reported. The orange block single-crystals of [Co(obc)(bpeb)]·5H₂O (1) adopting a 2-fold 3D structure were obtained from the solvothermal reaction of Co(NO₃)₂·6H₂O, H₂obc, and bpeb in the equimolar ratio. When two equivalents of Co(NO₃)₂·6H₂O and H₂obc were reacted with bpeb, the dark violet block single-crystals of [Co₂(obc)₂(bpeb)]·2DMF·H₂O (2) showing 3-fold 3D structure was isolated. Although the two 3D MOFs prepared satisfy the conditions for the photo-dimerization but, to our surprise, they were found to be photo-inactive. The details of our investigations will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-112

발표분야: 무기화학

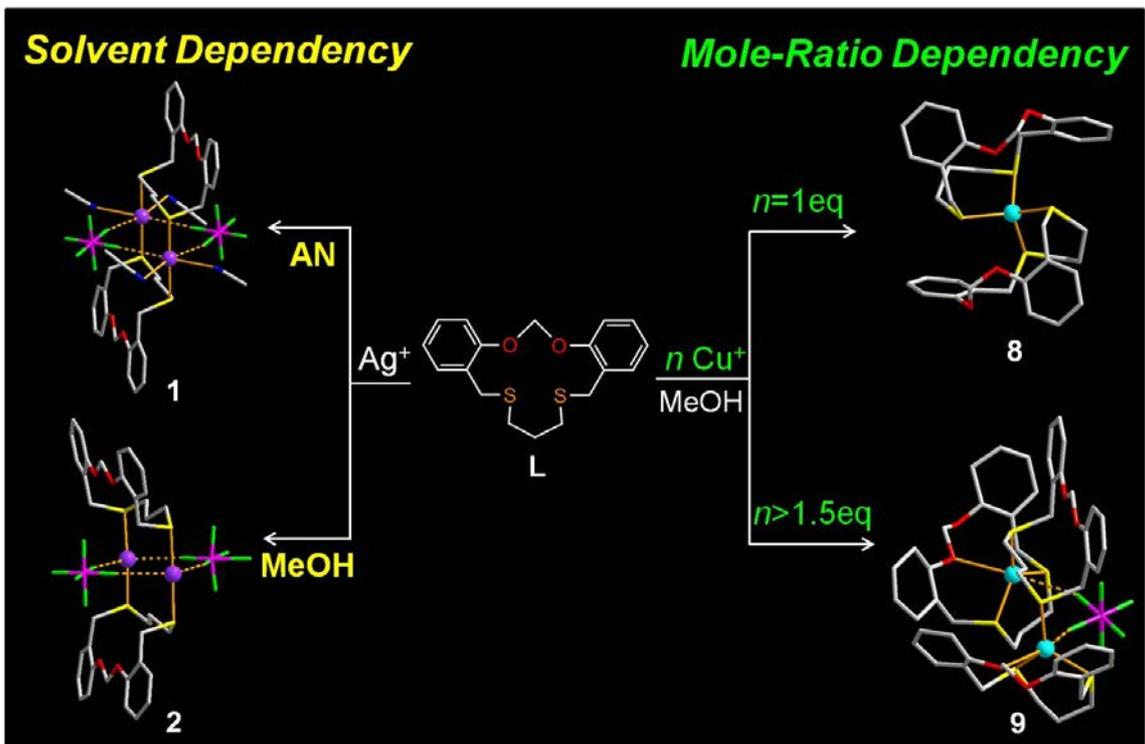
발표종류: 포스터, 발표일시: 수 16:00~19:00

Exocyclic coordination based supramolecular assemblies of discrete and polymeric complexes of a 14-membered O₂S₂-macrocycle

김슬기 Leonard F. Lindoy^{1,*} 이심성*

경상대학교 화학과 ¹The University of Sydney

The preparation and structures of the exocyclic coordination¹ based supramolecular complexes of a 14-membered O₂S₂-macrocycle (L)² with thiophilic metal ions are reported.³ Reactions of L with AgPF₆ in acetonitrile afforded a bicyclic dimer complex [Ag₂L₂(CH₃CN)₄](PF₆)₂ (1), in which two PF₆⁻ bridge two Ag atoms in a bidentate manner to form a 3D bicycle. In methanol, however, the above reaction afforded a bicyclic dimer complex [Ag₂L₂](PF₆)₂ (2). Reactions of L with AgCF₃SO₃ in acetonitrile afforded a propeller-like complex [Ag₂L₂(CF₃SO₃)₂].2CH₃CN (3). L reacts with copper(I) halides and afforded an isostructural complexes [(Cu₂X₂)L]_n (4: X = Cl, 5: X = Br) adopting a 2D network linked by square-type Cu₂X₂ cluster, while CuI gave a yellow emissive complex {[(Cu₄I₄)L₂].2.5H₂O}_n (6). Treatment of L with copper(I) thiocyanate gave a 2D network [CuLSCN]_n (7) in which Cu atoms are linked by SCN⁻ forming a 1D backbone, then further cross-linked by L resulting in a grid structure. Reactions of L with equimolar amount of Cu(CH₃CN)₄PF₆ gave a 1:2 (metal-to-ligand) complex [CuL₂](PF₆)₂ (8) and a 2:3 complex [Cu₂L₃](PF₆)₂ (9) depending on the mole-ratio of the reactants. Reactions of L with HgX₂ (X = Br and I) resulted in the formation of an interesting “ivy-leaves” shaped complex [HgLBr₂]_n (10) and a single-stranded complex [(Hg₂I₄)L]_n (11), respectively, adopting an infinite 1D structure. The reactions of L with Pd(NO₃)₂ gave a 1:1 complex [PdL(NO₃)₂] (12) and a 1:2 complex [PdL₂](NO₃)₂ (13) depending on the mole-ratio of the reactants. A one-pot reaction of Pd(NO₃)₂ with two equivalents of L also resulted in the isolation of the bis(macrocycle) complex 13.1.S. Park, S. Y. Lee, K.-M. Park, S. S. Lee, Acc. Chem. Res. 2012, 45, 391.2.S. Y. Lee, J. Seo, I. Yoon, C.-S. Kim, K. S. Choi, J. S. Kim, S. S. Lee, Eur. J. Inorg. Chem. 2006, 3525.3.S. Kim, E. Lee, K.-M. Park, S. S. Lee, CrysEngComm 2013, ASAP.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-113

발표분야: 무기화학

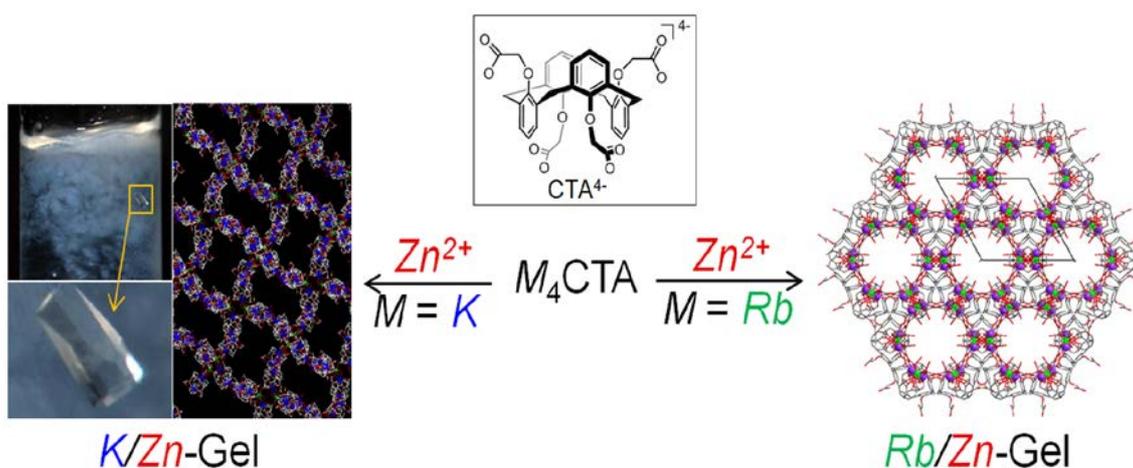
발표종류: 포스터, 발표일시: 수 16:00~19:00

Calix[4]arene-based Supramolecular Heterometallogels

황두미 이심성* 박기민*

경상대학교 화학과

Supramolecular gels constructed by the self-assembly of stimuli responsive low-molecular-mass gelators have attracted particular interest because of their potential applications in many fields. To investigate the structure-property relationships for the supramolecular heterometallogels, we have prepared two calixarene-based gelators. Gelators 1 and 2 form heterometallogels *K/Zn-gel* and *Rb/Zn-gel*, respectively, in the presence of Zn^{2+} . We were successful in growing corresponding single crystals suitable for X-ray structure analysis from the *K/Zn-gel* and the *Rb/Zn-gel*. The single crystal derived from the *K/Zn-gel* shows an interpenetrating 3-D network structure and that derived from the *Rb/Zn-gel* exhibits a 3-D network with the honeycomb-type channel (see below). Basis on the crystal structures of the heterometallogels obtained, the formation and physical properties of the heterometallogels are discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-114**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Similarities and differences in the properties of heterometallic and porous MOFs with the flexible acs topology

홍근일 전형필*

한양대학교 응용화학과

Heterometallic approaches in the synthesis of metal-organic frameworks provide new opportunities to discover porous materials with properties that are both academically interesting and practically appealing. We have adopted this approach to successfully introduce Ti(IV) into Co(II)-based open frameworks with simple dicarboxylate ligands. In this presentation we focus on the gas sorption properties of the cobalt-titanium-organic frameworks with the emphasis on the adsorption of carbon dioxide. Also reported are the synthesis of new mixed-metal analogues based on cobalt-vanadium systems. Preliminary results indicate that both similarities and differences exist in the structures and gas sorption behavior of Co-Ti and Co-V MOFs that share a common network topology based on trigonal prism nodes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-115**

발표분야: 무기화학

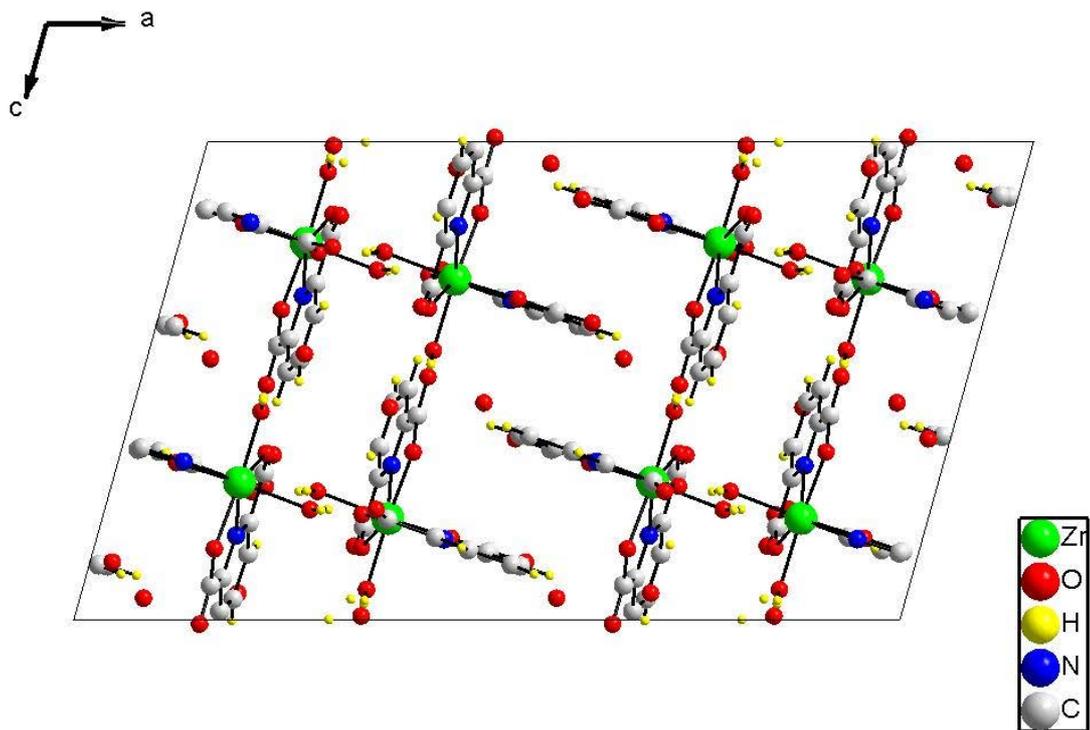
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, structure, and characterization of a new Zirconium-organic framework, [Zr(PDC)₂(H₂O)₂]₂·2H₂O [PDC=2,6-NC₅H₃(CO₂)₂]

이남희 옥강민*

중앙대학교 화학과

A new zirconium-organic framework material [Zr(PDC)₂(H₂O)₂]₂·2H₂O has been synthesized by a hydrothermal reaction method. Single crystal X-ray diffraction was used to determine the crystal structure of the reported material. [Zr(PDC)₂(H₂O)₂]₂·2H₂O exhibits a pseudo-three-dimensional open-framework structure containing a complicated network of hydrogen bonds. [Zr(PDC)₂(H₂O)₂]₂·2H₂O shows a reversible dehydration/rehydration reaction, which is confirmed by powder X-ray diffraction. Activated [Zr(PDC)₂(H₂O)₂]₂·2H₂O reveals a selective CO₂ adsorption over N₂ or H₂. Full characterization including powder X-ray diffraction, elemental analysis, thermogravimetric analysis, spectroscopic analyses (IR, UV-Vis, and NMR) and DFT calculations for the reported material is also presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-116

발표분야: 무기화학

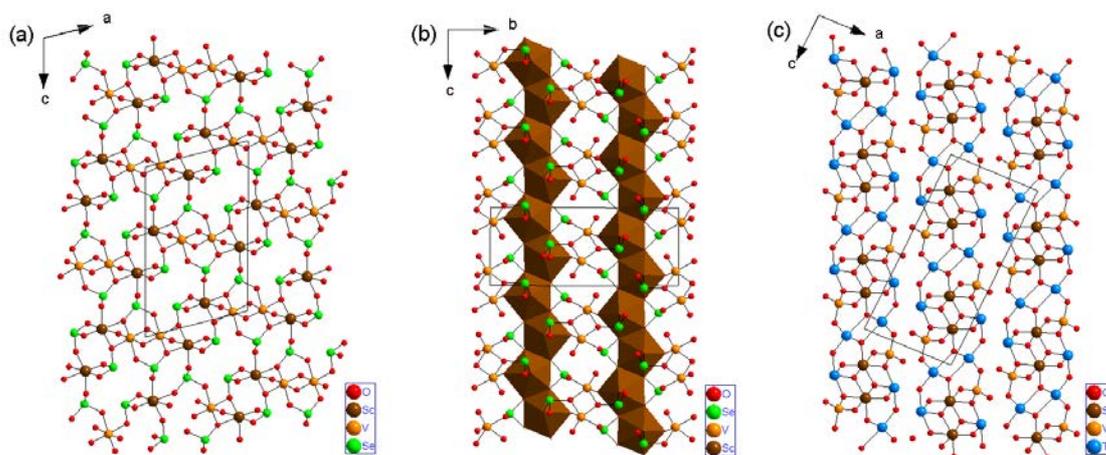
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Quaternary Scandium Vanadium Oxide material: Synthesis, Structure, and Characterization of α -ScVSe₂O₈, β -ScVSe₂O₈, and ScVTe₂O₈

김영훈 옥강민*

중앙대학교 화학과

Three new quaternary mixed metal oxide materials, α -ScVSe₂O₈, β -ScVSe₂O₈, and ScVTe₂O₈, have been synthesized by standard solid-state and hydrothermal reactions using Sc₂O₃, V₂O₅, and SeO₂ (or TeO₂) as reagents. Although α -ScVSe₂O₈ and β -ScVSe₂O₈ exhibit three-dimensional (3D) frameworks, they have different framework geometries: while α -ScVSe₂O₈ is composed of VO₆, ScO₆ octahedra, and SeO₃ polyhedra, β -ScVSe₂O₈ consists of VO₅ trigonal bipyramids, ScO₇ pentagonal bipyramids, and SeO₃ polyhedra. In addition, ScVTe₂O₈ shows a two-dimensional (2D) layered structure composed of ScO₆ octahedra, VO₄ tetrahedra, and TeO₄ polyhedra. The reported materials were fully characterized by Infrared spectroscopy, thermogravimetric analysis, and SEM-EDX. Bond valence sum (BVS) calculations and magnitude of distortion for octahedra of d⁰ cations are also presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-117

발표분야: 무기화학

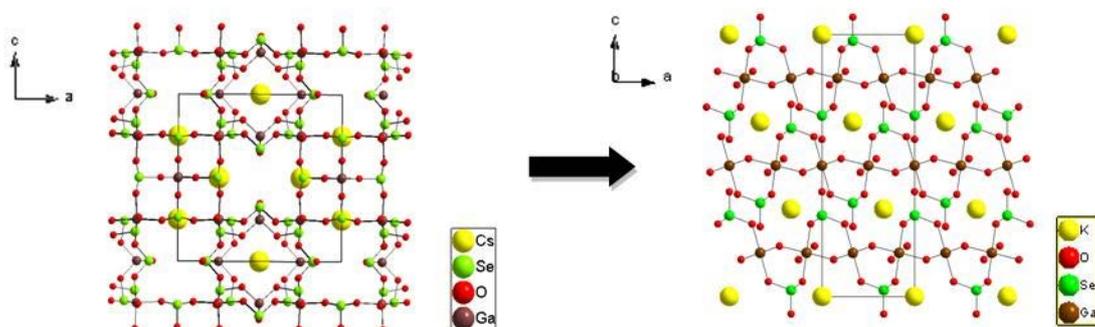
발표종류: 포스터, 발표일시: 수 16:00~19:00

Transformation of an Open-Framework $\text{Cs}_3\text{Ga}_7(\text{SeO}_3)_{12}$ to a Layered Hexagonal Tungsten Oxide (HTO) $\text{KGa}_3(\text{SeO}_4)_2(\text{OH})_6$

안현선 옥강민*

중앙대학교 화학과

Open-framework materials have been of great interest attributable to important applications such as catalysis, gas adsorption, energy storage, and ion exchange. At the same time, hexagonal tungsten oxide (HTO) materials have drawn a great attention attributed to photocatalytic, electrocatalytic, optical, and adsorption properties. A three-dimensional (3D) open-framework material, $\text{Cs}_3\text{Ga}_7(\text{SeO}_3)_{12}$ has been successfully synthesized through a standard solid-state reaction using Cs_2CO_3 , Ga_2O_3 , and SeO_2 as reagents. The reaction between polycrystalline $\text{Cs}_3\text{Ga}_7(\text{SeO}_3)_{12}$ sample and 1 M KNO_3 at 230 °C resulted in a HTO-like $\text{KGa}_3(\text{SeO}_4)_2(\text{OH})_6$. $\text{KGa}_3(\text{SeO}_4)_2(\text{OH})_6$ is the first layered HTO structure containing SeO_4 tetrahedra. We found that an open-framework structure successfully transforms to a layered structure. Single-crystal X-ray diffraction, infrared spectroscopy as well as thermogravimetric analyses have been used to investigate the structures and characteristics of the reported materials.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-118

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Tris-tetrazolyl Iron Scorpionates with Dual Binding Sites

박가현 고민정 이준승*

전남대학교 화학과

Reaction of three equivalents of 5-(2-hydroxyphenyl)-1H-tetrazolyl (TzH₂) with iron perchlorate in the presence of three equivalents of metal hydroxide affords noble Fe metal framework [FeTz₃]³⁻. By X-ray crystallography, their formulas in solid were confirmed as [LiFeTz₃(H₂O)]₂[Li(H₂O)₄]₂[Li₂(H₂O)₇](H₂O)_{4.5}]_n(1), [Na₃FeTz₃(H₂O)₃]_n(2), [K₃FeTz₃(H₂O)₇]_n(3), and [Ca(FeTz₃)₂(H₂O)(DMF){Ca(H₂O)}{Ca(DMF)(H₂O)}]_n(4). [FeTz₃]³⁻ fragment has two binding sites and its binding mode to metal ions highly depends on the used metal, which were studied by solid state structure analysis. In complex 3 using potassium, both of binding sites were tightly connected to metal center with κ³ modes, forming a coordination sequence of K(κ³-N₃)FeTz₃(κ³-O₃)K(κ³-O₃)FeTz₃(κ³-N₃)K. Simple addition of zinc perchlorate to complex 3 forms trimetallic coordination polymer 5, which has honeycomb porous structure. Novel one dimensional metallic sequence of K-Fe-Zn-Fe-K was observed. It was found that hetero bimetallic complexes [NaFeTz₃]²⁻ and [K₂FeTz₃]⁻ could be good chemical sensors for the detection of bidentate electron donating ligands.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-119**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Zinc and Aluminum SALEN Complexes for Luminescent Polylactide

강이영 고민정 이준승*

전남대학교 화학과

Poly lactone polymers (PLA) are biodegradable, biocompatible and non-toxic materials and thus they are important, for example, in the area of the controlled drug-release devices, absorbable sutures, medical implants for orthopedic use, disposable degradable plastic articles and scaffolds for tissue engineering. Many elements of metal and non-metal such as Aluminum and Zinc have been used as catalytic centers for the lactone polymerization. Recently, PLA having specific color have received a great attention for the industrial propose. However we found that there is no example of PLA containing chromophores which are very important in the electronic device application and selective sensing. In this context, we prepared old-fashioned but new SALEN ligand having a hydroxy group, which is a good initiator in the ring opening polymerization of lactide. By the reaction of SALEN ligand with Zn and Al metal precursor, novel metal SALEN complexes have been synthesized easily. Their detailed properties and catalytic performances in ring opening polymerization of lactide will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-120

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High Activity Titanium Catalysts Containing Tetrazolyl Ligand for Cyclo-Addition of CO₂ to Epoxides

고민정 강이영 김영조¹ 이준승*

전남대학교 화학과 ¹충북대학교 화학과

A series of new half-sandwich titanocene $[(\eta^5\text{-C}_5\text{H}_5)\text{TiLCl}_2]$ (1) and non-organometallic titanium complexes $[\text{TiLCl}_3(\text{THF})]$ (2) and $[\text{TiL}_2\text{Cl}_2]$ (3) containing 5-(2-hydroxyphenyl)tetrazole (LH) were synthesized in high yield and fully characterized by various spectroscopic methods and X-ray crystallography. In all complexes, ligand L acted as a monoanionic bidentate ligand and the hydrogen bonding between the oxygen of the tetrahydrofuran and hydrogen of the tetrazolyl unit was observed. In the cycloaddition of CO₂ to propylene oxide, complex 3 showed highest activity among reported Ti complexes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-121**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Supramolecular M4L2 Cages From Tetrapyridyl Metalloligands

류지연 이준승*

전남대학교 화학과

Three dimensional M4L2 supramolecular cages have been synthesized with quantitative yields by the simple combination of 4 equiv of flexible di-platinum or di-ruthenium accepters with 2 equiv of star connector, tetrakis(4-pyridyl)cyclobutadienecyclopentadienyl metalloligand. (metal: Co and Fe). These cages were characterized with multinuclear NMR spectroscopy(^1H and ^{31}P) and high-resolution electrospray ionization mass spectrometry. The structure of tetragonal-prismatic cage, self-assembled from a ruthenium metalloligand and tetrapopic iron metalloligand, was confirmed by X-ray crystallography. These complexes represented novel D4 cages systems.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-122

발표분야: 무기화학

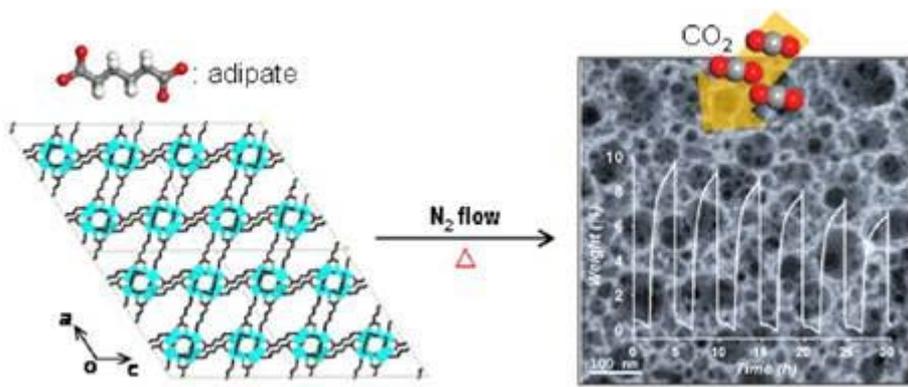
발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoporous Metal Oxides with Tunable and Nanocrystalline Frameworks via Conversion of Metal-Organic Frameworks

이경주 김태경 천재영¹ 이재화 주상훈^{1,*} 문희리^{*}

울산과학기술대학교(UNIST) 친환경에너지공학부 ¹울산과학기술대학교(UNIST) 나노생명화학
공학부

Nanoporous metal oxide materials are ubiquitous in the material sciences because of their numerous potential applications in various areas, including adsorption, catalysis, energy conversion and storage, optoelectronics, and drug delivery. While synthetic strategies for the preparation of siliceous nanoporous materials are well-established, nonsiliceous metal oxide-based nanoporous materials still present challenges. Herein, we report a novel synthetic strategy that exploits a metal-organic framework (MOF)-driven, self-templated route toward nanoporous metal oxides via thermolysis under inert atmosphere. In this approach, an aliphatic ligand-based MOF is thermally converted to nanoporous metal oxides with highly nanocrystalline frameworks, in which aliphatic ligands act as the self-templates that are afterward evaporated to generate nanopores. We demonstrate this concept with hierarchically nanoporous magnesia (MgO) and ceria (CeO₂), which have potential applicability for adsorption, catalysis, and energy storage. The pore size of these nanoporous metal oxides can be readily tuned by simple control of experimental parameters. Significantly, nanoporous MgO exhibits exceptional CO₂ adsorption capacity (9.2 wt %) under conditions mimicking flue gas. This MOF-driven strategy can be expanded to other nanoporous monometallic and multimetallic oxides with a multitude of potential applications.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-123**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Confined synthesis of Metal-Organic Frameworks (MOFs) in three-dimensionally ordered macroporous (3DOM) carbon templates

박우정 유원철* 전형필*

한양대학교 응용화학과

A variety of choices for combination of metals and ligands makes MOFs being widely used as gas storage/separation, catalytic and sensing materials. However, researches on MOFs have been facing many challenges for their industrial applications due to the lower chemical and mechanical stability. To resolve these issues, incorporation of MOFs into a hard template that offers intrinsic porosity and mechanical stability has been suggested. Here, we propose a strategy to fabricate MOFs inside 3DOM carbon materials with pore sizes ranged from sub-hundred to several hundreds of nanometers. Confined synthesis of MOFs inside 3DOM carbon templates could produce a composite material that could maintain the advantages of MOFs as well as mechanical strength and intrinsic porosity of 3DOM carbon materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-124

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

CO₂ Selective 3-D Cu-MOFs with Catalytic Activity

황인홍 김하영¹ 김 철² 여철현³ 김성진^{1,*} 김영미^{4,*}

서울과학기술대학교 정밀화학과 ¹이화여자대학교 화학과 ²서울과학기술대학교 정밀화학과
친환경소재제품센터 ³KISTI ReSEAT Program, Senior Fellow ⁴이화여자대학교 나노바이오 기술
연구소, 화학-나노과학과

Two new bifunctional 3-D Cu-MOFs were prepared, and both Cu-MOFs exhibited high selectivity of CO₂ over N₂ and H₂ as well as high catalytic activity for transesterification of esters. The Cu-MOFs containing Cu₂ dinuclear units connected by glutarates and bipyridyl ligands are formulated as $[\{Cu_2(Glu)_2(?-bpa)\}(CH_3CN)]_n$ (1) and $[\{Cu_2(Glu)_2(?-bpp)\}(C_3H_6O)]_n$ (2) (Glu = glutarate, bpa = 1,2-bis(4-pyridyl)ethane, bpp = 1,3-bis(4-pyridyl)propane). Two new 3-D Cu-MOFs possess very similar pore shape with different pore dimensions, and both MOFs exhibited good CO₂ selectivity over N₂ and H₂. The MOF 2 exhibited more enhanced CO₂ uptake ability than the MOF 1. Heterogeneous catalytic activities of the MOFs were also investigated, and only the MOF 1 appeared to be an efficient, mild, and easily recyclable heterogeneous catalyst for the transesterification of esters.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-125

발표분야: 무기화학

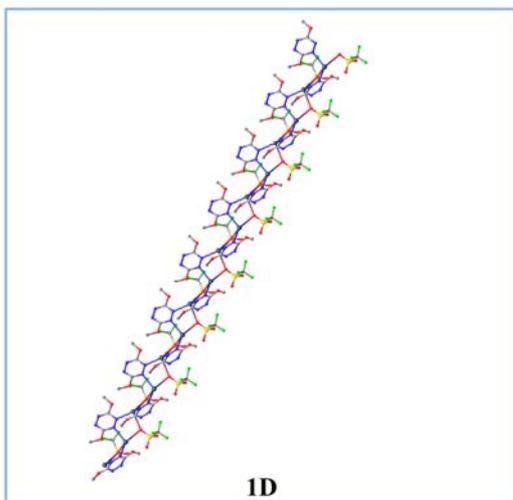
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Structure Studies of 3,6-diethoxy-*s*-Tetrazine Ag(I) Complexes

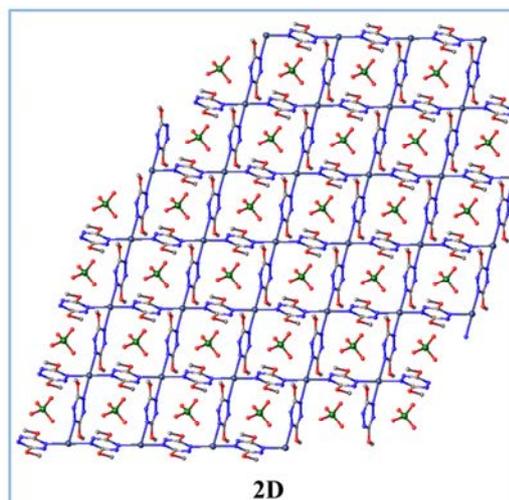
오한솔 강필재 최문근*

연세대학교 화학과

The unique properties of 1,2,4,5-tetrazines the extreme electron deficiency originate in their most nitrogen-rich six-membered aromatic heterocycle. The electron deficiency of the π -system enable to sustain efficient attraction for negatively polarized atoms or anions. Another important property of tetrazines is that since it has the multiple metal binding sites, it makes transition metal complexes easily with multinuclear coordination complexes. The silver(I) coordination polymers containing 3,6-dimethoxy-*s*-tetrazine with novel topology are synthesized and their X-ray crystal structural features will be presented. Especially taking into account the influence of anion- π interaction with various anions to generate new supramolecular architectures.



1D
 $\text{Ag}((\text{MeO})_2\text{ttz})(\text{Otf})$



2D
 $[\text{Ag}((\text{MeO})_2\text{ttz})_2][\text{ClO}_4]$

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-126**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Topology Control over Homochiral Salen Metal Organic Frameworks

김영훈 허정석*

충남대학교 화학과

Homochiral porous coordination polymers are of great interest because of their utility in enantioselective molecular recognitions and asymmetric catalyses of organic reactions. Especially, salen type of building blocks have been employed to construct porous coordination polymer and resulted totally different topologies of network structures depending on substituents on the salen building blocks.¹⁻² We prepared an intermediate bulkiness of salen building unit and used it to build a distinct topology of homochiral MOF. In the poster presentation, X-ray structure of the intermediate salen MOF and compared with two other extreme cases.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-127**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of the single crystal structures on $(\text{CH}_3)_2\text{NH}_2\text{CuCl}_3$

박가람 오인환^{1,*} 박승일²

고려대학교 화학과 ¹한국원자력연구소 중성자과학연구부 ²한국원자력연구원 중성자과학연구

부

$(\text{CH}_3)_2\text{NH}_2\text{CuCl}_3$ belongs to an organic-inorganic hybrid magnetic system with a quasi-one-dimensional alternating antiferromagnetic-ferromagnetic Heisenberg chain ($S = 1/2$). Through inelastic neutron scattering, significant dispersion along the b-axis was found, contrary to the previous proposed model. To verify the crystal structures at room temperature and lower, and to investigate further magnetic behaviors, we decided to synthesize single crystals suitable for neutron diffraction and neutron scattering experiments. In this work, we present crystal structure investigations on Cu-DMA at room temperature and at 173K using X-ray single crystal diffraction, and show preliminary neutron diffraction results at room temperature. Cu-DMA crystallizes in the monoclinic space group $C12/a1$ with $a = 17.44 \text{ \AA}$, $b = 8.65 \text{ \AA}$, $c = 12 \text{ \AA}$, $\beta = 125.2^\circ$ at room temperature. This compound shows a phase transition at 286K. The crystal structure at 173K from X-ray single-crystal data was described with a triclinic space group P-1. The obtained lattice parameters are $a = 8.5522 \text{ \AA}$, $b = 9.6140 \text{ \AA}$, $c = 10.5676 \text{ \AA}$, $\alpha = 73.089^\circ$, $\beta = 68.389^\circ$, and $\gamma = 64.459^\circ$. The disordered $\text{Cu}_2\text{Cl}_6^{2-}$ dimers which are surrounded by 5 Cl^- ions, are completely ordered at low temperature. As a result, two symmetry distinct copper ions exist in the 173K phase. Its mechanism is thought to be driven by the ordering process in the hydrogen bonds. It is difficult to keep the sample in air owing to its hygroscopic nature. To solve this problem, we used the mixture of methanol and ethanol as a solvent. Evaporating this solvent at 307K, we obtained large crystals with good quality. After a week, however, the quality of the crystal deteriorated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-128

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High surface area SnO₂ nanohollows as photocatalysts and anode materials in lithium ion batteries

한승용¹ 손성욱^{1,*} 진재원¹ 천지슬¹ 김경열¹

성균관대학교 에너지과학과 ¹성균관대학교 화학과

A high surface area of nanomaterials influences photocatalytic activity and energy storage capacity. Also, the shape-dependent structural flexibility of nano-electrode materials in lithium ion batteries can enhance the stability of the storage performance. In this regards, the nanoparticulate hollow materials are promising for high performance catalysts and energy storage materials. This presentation will show that a chemical bottom-up and successive top-down approach is a good synthetic strategy for microporous hollow materials. The heating of 3 eq. nickel chloride and 2 eq. tin chloride at 280 oC in the presence of oleylamine resulted in the formation of intermetallic Ni₃Sn₂ alloy materials. When the Ni₃Sn₂ nanoparticles were treated with 1% nitric acid for 48 hours, the nickel component was completely etched. The resultant materials were nanoporous SnO₂ hollow materials which were characterized by TEM, PXRD and XPS. This SnO₂ hollows showed nanoporosity and a high surface area of 101 m²/g. Also, the hollow SnO₂ materials showed excellent photocatalytic activities in the decomposition of Rhodamine B. And these showed promising electrochemical performances with 560 mAh/g discharge capacity after 30 cycles and stabilities as anode materials in lithium ion batteries. The preparation of intermetallic alloy and the selective etching strategy can be further expanded to other intermetallic alloy systems for the development of functional materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-129**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Control over Topologies of Luminescent Metal-Organic Frameworks

김성민 허정석*

충남대학교 화학과

Since porous coordination polymers exhibit high surface area and selective adsorption properties, they allow us promising applications. One big problem in a design of this type of coordination polymer is how to avoid interpenetration which dramatically reduces their void volume. We obtained two distinct topologies of 3-D network structures depending on a metal cluster's coordination geometry in each case. In the first case, its cavity size is very large but prepared as undesirable interpenetrated structure. In the other case, interpenetration problem was prevented owing to its topological requirement. We will present and compare X-ray structures of the two intriguing Metal-Organic-Frameworks.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-130**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

청색 소자를 기반으로한 안트라센 계열의 유기 EL 물질연구

안상원 이승희*

홍익대학교 화학시스템공학과

현재 OLEDs(Organic Light Emitting Diodes)의 물질과 소자에 대한 연구가 활발히 진행되고있다. 이 OLED 의 장점은 빠른 반응속도와 우수한 선명도, 시야각이 넓고, 투명하게 만들수 있으며 , 그 외에 자체발광 하고 온도에 강하고 낮은 전력에서도 구동가능하다는 장점이 있다. 하지만 RGB 물질 중 청색 물질은 큰 밴드갭 때문에 , 녹색과 적색에 비해 효율과 수명 그리고 선명도에 대한 문제점을 보이고 있다. 이러한 문제점을 해결하기 위해 본 실험에서는 새로운 청색 발광 물질을 합성하였다. 기존의 실험에서 사용한 Anthracene 과 Carvazole 에 치환기를 붙여 전기적인 특성과 입체 장애에 의한 OLED 소자의 성질을 살펴 보았다

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-131**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Emission Color Tuning Properties of Di-*o*-carborane Substituted Benzene Compounds

NGUYEN VAN NGHIA 김태원 이민형*

울산대학교 화학과

A series of 1,4-di-(1-Ar-*o*-carborane-2-yl)benzene (Ar = 3,5-bis(trifluoromethyl)phenyl (1), phenyl (2), 4-n-butylphenyl (3), 4-*N,N*-dimethylaniline (4)) compounds that are electronically modulated at the C1-position of *o*-carborane with the electron-withdrawing or -donating aryl groups were prepared and characterized by X-ray crystallography. UV—vis absorption spectra exhibit small low-energy absorption bands at around 275—300 nm for 1—3 while 4 shows a broad absorption tail at 350—400 nm. Although 1—4 show virtually no emission in solution, an intense aggregation-induced emission over the region ranging from 400—700 nm is observed in the solid state. The emission wavelengths of 1—4 exhibit an apparent red-shift upon changing the aryl substituent from CF₃ to NMe₂ group (from 1 to 4). Details of synthesis and emission color tuning property of compounds will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-132

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photophysical Properties of Heteroleptic Tris-cyclometalated Ir(III) Complexes Supported by *ortho*-Carboranyl-pyridine Ligand

박지현 김예진 이민형*

울산대학교 화학과

Heteroleptic tris-cyclometalated Ir(III) complexes, $(C^{\wedge}N)_2 Ir(CBpy)$ ($C^{\wedge}N = ppy$ and $dfppy$; $ppy = 2$ -phenylpyridinato- C^2,N (1); $dfppy = 2$ -(4,6-difluorophenyl)pyridinato- C^2,N (2); $CBpy = (2$ -pyridyl)-1,2-closo-carboran-1-yl) supported by the *ortho*-carboranyl-pyridine ($CBpy$) as a novel $C^{\wedge}N$ chelating ligand were synthesized and characterized. UV-vis absorption and PL experiments indicated that the electronic transition is mixed $ML(C^{\wedge}N)CT$ and $ML'(CBpy)CT$ in character. While both complexes are almost non-emissive in fluidic solution at 298 K, but are luminescent at 77 K and in the solid state, such as film (5 wt% in PMMA) and powder. Electrochemical properties and DFT calculation further showed that the $CBpy$ ligand contributes to the electronic stabilization of complexes, while the photophysical properties are dominated by 2-arylpyridine ligands, such as ppy and $dfppy$. Details of synthesis, characterization, and photophysical properties will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-133

발표분야: 무기화학

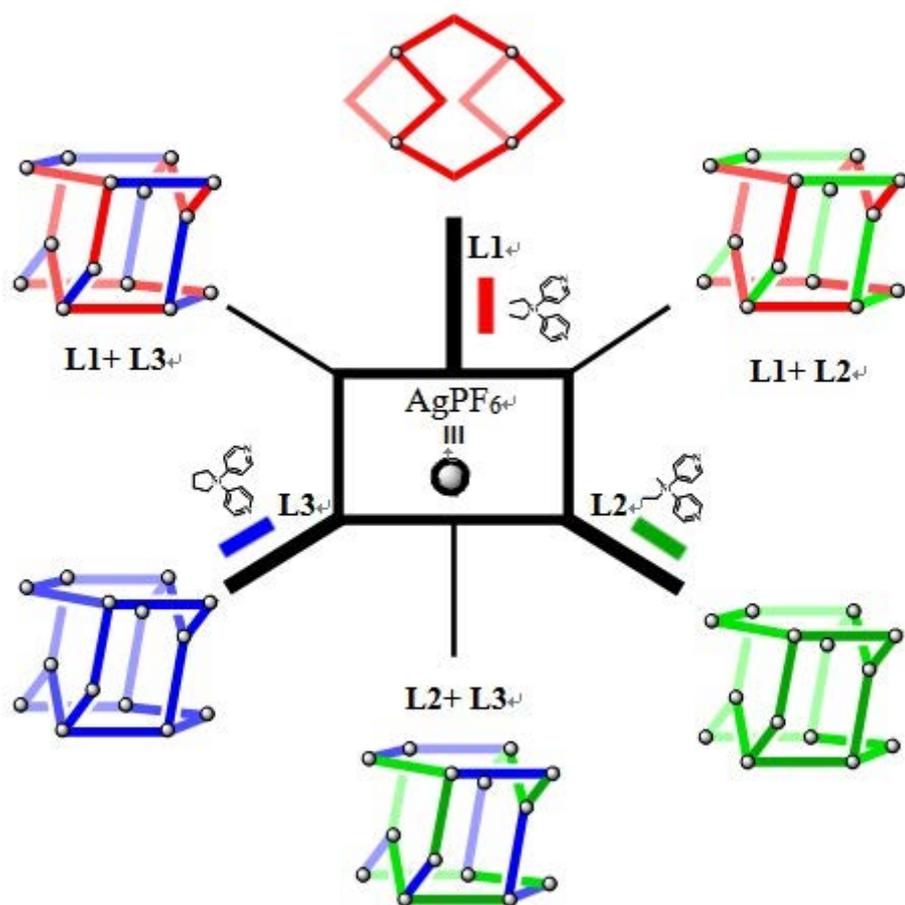
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ligand Spacer Effect on the Molecular Construction of Silver(I) with a Series of L₁, L₂, and L₃

박민우 정옥상*

부산대학교 화학과

Self-assembly of silver(I) hexafluorophosphate (AgPF₆) with L₁, L₂, and L₃ (L₁=bis(4-pyridyl)diethylsilane, L₂= bis(4-pyridyl)ethylmethylsilane, L₃=bis(4-pyridyl)cyclotetramethylsilane) in a mixture of water and methanol produces [Ag₂(L₁)₄](PF₆)₂, [Ag(L₂)₂](PF₆)₂·CH₃OH, and [Ag(L₃)₂](PF₆)₂·CH₃OH, respectively. Furthermore, self-assembly of AgPF₆ with a mixed ligand system of L₁+L₂, L₁+L₃, and L₂+L₃ produces [Ag₂(L₁)₂(L₂)₂](PF₆)₂·CH₃OH, [Ag₂(L₁)₂(L₃)₂](PF₆)₂·H₂O, and [Ag(L₂)(L₃)](PF₆)₂·H₂O, respectively. The crystal structure of [Ag₂(L₁)₄](PF₆)₂ is 1D coordination polymeric linked cycle whereas those of the other five compounds are 2-fold interpenetrated adamantanoid skeletons. The calcination of the present compounds at 500 °C produces micro-sized materials consisting of silver(0) without silicon(IV) oxide. The crystal structures and their physicochemical properties were fully characterized by IR, TGA/DSC, UV/vis, PL, SEM, and single crystal X-ray diffractometer.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-134

발표분야: 무기화학

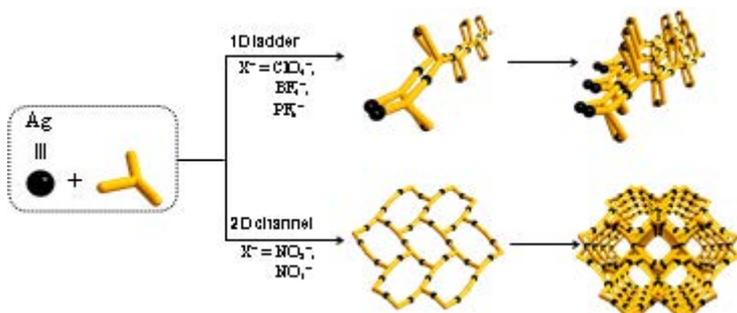
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dimension Control *via* Anion Bulkiness. Synthesis, Structures, and Physicochemical Properties of AgX Bearing *N,N',N''*-Tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide

김은이 정옥상*

부산대학교 화학과

Studies of the anion effects on the molecular construction of a series of AgX complexes with *N,N',N''*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L) ($X^- = \text{NO}_2^-, \text{NO}_3^-, \text{ClO}_4^-, \text{BF}_4^-, \text{and PF}_6^-$) have been carried out. Formation of the skeletal bonds appears to be primarily associated with a suitable combination of tridentate N-donors of L and a variety of coordination geometries of Ag(I) ions. The L/Ag(I) ratios of the products are independent on the nature of the polyatomic anions, but their dimensions are dependent on the bulkiness of counteranions. The structure of $[\text{Ag}_6(\text{L})_4](\text{X})^-$ ($X^- = \text{NO}_2^-, \text{NO}_3^-$) is a kagome 2D grid structure while the structure of $[\text{Ag}_6(\text{L})_4](\text{X})^-$ ($\text{ClO}_4^-, \text{BF}_4^-, \text{and PF}_6^-$) is a 1D structure. Their thermal behavior and photoluminescent properties have been investigated.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: INOR.P-135

발표분야: 무기화학

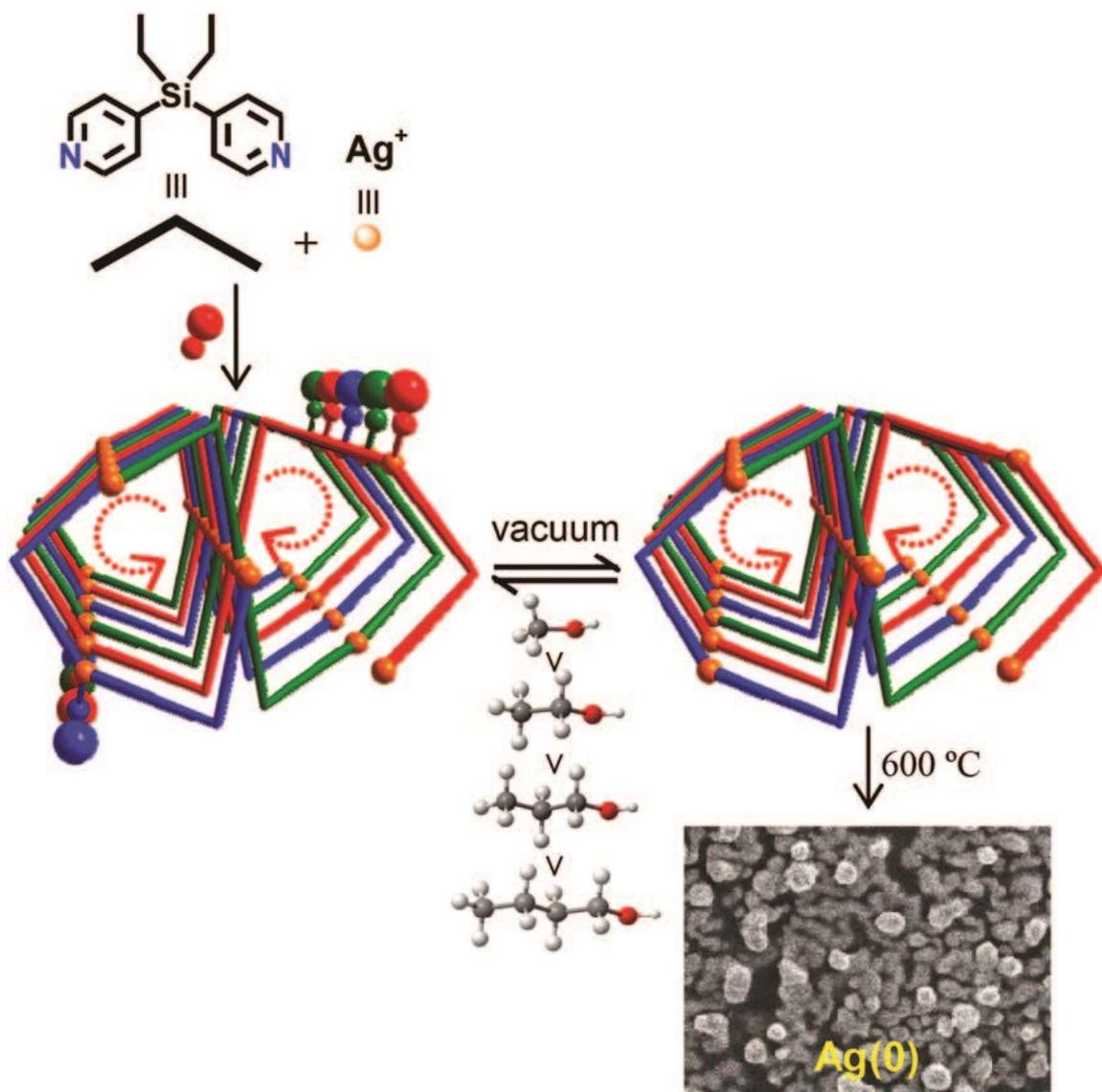
발표종류: 포스터, 발표일시: 수 16:00~19:00

Triple-*meso* Helices as Alcohol Storages and Discriminators: Structural Properties and Thermal Behaviors of Silver(I) Complexes Containing Diethylbis(4-pyridyl)silane

문소연 정옥상*

부산대학교 화학과

Self-assembly of silver triflate with L in alcohol solvent produces characteristic triple-*meso* helices $[Ag_3(L)_3(ROH)](CF_3SO_3)_3$ (L = diethylbis(4-pyridyl)silane; R = Me, Et, *n*-Pr, and *n*-Bu) with six units in each turn. Their unit cell volumes are sensitive to the size of the coordinated alcohol molecules. An unusual “alcohol molecules at triple-*meso* helices” system is a characteristic reversible alcohol container and discriminator *via* appropriate association/dissociation. The *meso* helical solids are favored in the order MeOH > EtOH > *n*-PrOH > *n*-BuOH *via* an interaction between the silver(I) ion and the alcohol molecule. The crystals evaporate the coordinated alcohol molecules at low temperatures, and finally calcination at 600 °C produces micro-sized chaotic surface materials consisting of silver(0) without silicon(IV) oxide.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-136

발표분야: 무기화학

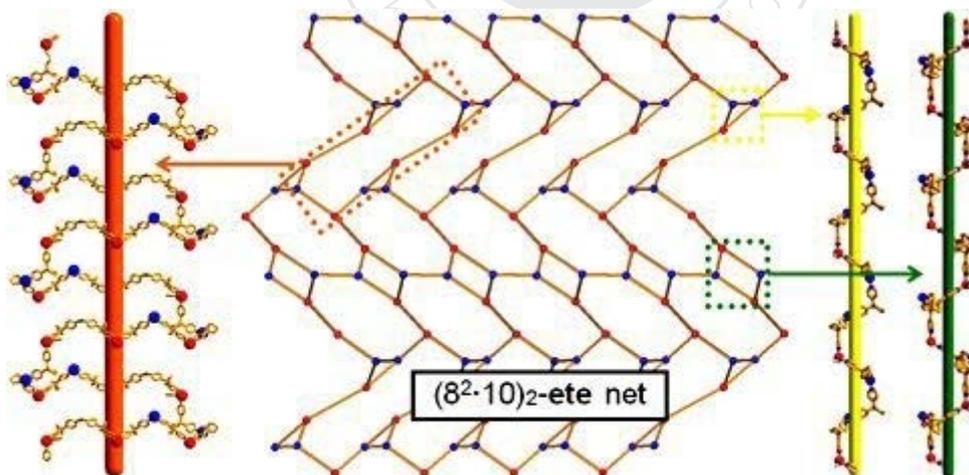
발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction and Characterizations of 4-fold Interpenetrating 3D Silver(I) Coordination Polymer with Bis(4-pyridyl)cyclotetramethylsilane

장재성 정옥상*

부산대학교 화학과

Self-assembly of AgClO_4 with bis(4-pyridyl)cyclotetramethylsilane (L) produces a 4-fold interpenetrating 3D coordination polymeric framework consisting of $[\text{Ag}_5(\text{L})_7(\text{CH}_3\text{CN})_2](\text{ClO}_4)_5 \cdot 2\text{CH}_3\text{CN}$. The topological analysis indicates that the compound is the first example of a binodal 3,3-connected $(8^2 \cdot 10)_2$ -ete net topology. Its thermal behavior and photoluminescent properties have been investigated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-137

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of heterometalic coordination polymers containing chiral nickel(II) macrocyclic complexes with silver(I) cyanide

정아립 신종원 안승현¹ 민길식^{1,*}

경북대학교 화학과 ¹경북대학교 사범대학 화학교육과

We have reported the structures and various characteristic properties of macrocyclic nickel(II) complexes containing chiral pendant groups, i.e. $[\text{Ni}(\text{L}^{S,S})](\text{ClO}_4)_2$ (1) and $[\text{Ni}(\text{L}^{R,R})](\text{ClO}_4)_2$ (2) (L=1,8-di((R/S)-*a*-methylbenzyl)-1,3,6,8,10,13-hexaazacyclotetradecane). To explore magnetic properties in chiral compounds, we have prepared two heterometalic polymers, $[\text{Ni}(\text{L}^{S,S})\text{Ag}(\text{CN})_2](\text{ClO}_4)$ (3) and $[\text{Ni}(\text{L}^{R,R})\text{Ag}(\text{CN})_2](\text{ClO}_4)$ (4), using compounds 1 and 2 with $\text{K}[\text{Ag}(\text{CN})_2]$, respectively. In complexes 3 and 4, nickel(II) ions are coordinated with two N atoms from different $\text{K}[\text{Ag}(\text{CN})_2]$ and four N atoms of amines from macrocycle and displayed distorted octahedral geometry. The crystal structure of 3 and 4 indicate that each nickel(II) macrocyclic complexes coordinated with silver(I) cyanide make 1-D linear polymer complexes. In this poster, the detailed preparation, crystal structure, circular dichromism, magnetic properties will be described.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-138

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and crystal structure, magnetic properties of trinuclear heterobimetallic chiral complexes

안승현 신종원¹ 정아림¹ 민길식*

경북대학교 사범대학 화학교육과 ¹경북대학교 화학과

Chiral compounds have attracted much attention in chemistry, material science and the chemical industry because of their potential and/or practical applications for molecular recognition, catalysis, and separation. Recently transition metal complexes with chiral ligands have been studied in asymmetric catalysis and self-assembly for luminescent materials. Recently, we synthesized the chiral trinuclear heterobimetallic complexes, $[\text{Ni}(\text{L}^{R,R})][\text{HBFe}(\text{pz})_3(\text{CN})_3]_2 \cdot 2\text{CH}_3\text{CN}$ (1), and $[\text{Ni}(\text{L}^{S,S})][\text{HBFe}(\text{pz})_3(\text{CN})_3]_2 \cdot 2\text{CH}_3\text{CN}$ (2), using chiral building blocks $([\text{Ni}(\text{L}^{R,R})](\text{ClO}_4)_2$ and $[\text{Ni}(\text{L}^{S,S})](\text{ClO}_4)_2$ and anionic precursor($[\text{HB}(\text{pz})_3\text{Fe}(\text{CN})_3]^-$), and characterized by various methods. Compound 1 and 2 has same crystal structure except chiral center of chiral building blocks. Interestingly, compound 1 and 2 displayed a ferromagnetic coupling between the Ni(II) ion and Fe(III) ions in the temperature range from 2 to 300 K. In this poster, we will present the detailed preparation of the ligand and metal complexes, crystal structure, magnetic properties.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-139

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single crystal to single crystal transformation of a tetrameric Iron(II) complex to tetrameric Iron(III) complex by the O₂ gas in air as a solid state

신종원 정아림 안승현¹ 민길식^{1,*}

경북대학교 화학과 ¹경북대학교 사범대학 화학교육과

The reaction of stoichiometric amount of iron(II) sulfate heptahydrate, potassium selenocyanate and *N*-(2-Pyridylmethyl)iminodiethanol (H₂pmide) in deoxygenated solvents affords the linear tetranuclear complex, [Fe₄(Hpmide)₄(NCSe)₄]₂·2CH₃OH (1) in good yield under an inert atmosphere of N₂ by using glove box techniques. Complex 1 was very sensitive in air and easily changed to brown color complex, [Fe₄(pmide)₄(NCSe)₂](NCSe)₂·2H₂O (2), which was characterized by single crystal XRD. The asymmetric unit of 1 contains two different iron(II) ions, one (Fe1) is coordinated with a monodeprotonated Hpmide⁻ ligand, two selenocyanate ion, and an ethoxy group of Hpmide⁻ ligand, and the other (Fe2) is bonded with one monodeprotonated Hpmide⁻ ligand and two ethoxy group of Hpmide⁻ ligand. Compared to the complex 1, the asymmetric unit of 2 contains two different iron(III) ions, one (Fe1) is coordinated with a deprotonated pmide²⁻ ligand, one selenocyanate ion, and an ethoxy group of pmide²⁻ ligand, and the other (Fe2) is bonded with one deprotonated pmide²⁻ ligand and two ethoxy group of pmide²⁻ ligand. In order to verify the oxidation states, compound 1 and 2 were also characterized by Mössbauer spectroscopy. The compound 1 and 2 displays antiferromagnetic couplings between the iron ions in the temperature range from 2 to 300 K. In this poster, we will explain the detailed preparation, crystal structure, Mössbauer data, and magnetic properties.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-140**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Controllable Chemical Vapor Deposition Growth of Graphene Films

강철 이진석*

숙명여자대학교 화학과

Graphene is a two-dimensional carbon material whose structure is one-atom-thick planar sheet of sp²-bonded carbon atoms densely packed in a honeycomb crystal lattice. It has drawn significant attention with its distinguished structural and electrical properties. Extremely high mobility and a tunable band gap make graphene potentially useful for innovative approaches to electronics. Although mechanical exfoliation of graphite and decomposition of SiC surfaces upon thermal treatment have been the main method for graphene, they have some limitations in quality and scalability of as-produced graphene films. Solution-phase and solvothermal syntheses of graphene achieved a major improvement for processing, however for device fabrication, a reproducible method such as chemical vapor deposition (CVD) growth yielding high quality films of controlled thickness is required. In this research, we synthesized hexagonal graphene flakes on Cu foils by CVD method and controlled its coverage, density and the size of graphene domains by changing reaction parameters. It is important to control these parameters of graphene growth during synthesis in order to achieve tunable properties and optimized device performance.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: INOR.P-141

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Single-Crystalline InSb Nanowires using CVD method and Study of Growth Mechanism

강은지 박이슬 이진석*

숙명여자대학교 화학과

Indium antimonide (InSb) material has a unique properties due to outstanding electrical characteristic. For instance, they has a narrow band gap of 0.17 eV, effective mass is 0.0135 m_0 , very high electron mobility of 7.8×10^4 cm²V⁻¹S⁻¹ at room temperature and very large Bohr exciton radius of 54 nm. These unique properties makes InSb a wide range of device applications, including high speed field-effect transistors, infrared detectors, magnetic sensors, thermoelectric power generation, and cooling devices. One-dimensional (1D) nanowires are being actively investigated because of their excellent electronic, optical properties, quantum confinement effect, good vectorial transport properties, and large surface area. In addition, the vapor-liquid solid(VLS) mechanism allows the growth of single-crystal. Here, we report the synthesis of the high quality single crystalline InSb nanowires and characterization of their properties. Single-crystalline InSb nanowire was synthesized on SiO₂ wafer via vapor-liquid-solid(VLS) mechanism using chemical vapor deposition method (CVD). According to the source container system(open or close) which contain InSb powder and SiO₂ wafer, the single-crystalline InSb nanowires have different growth mechanisms. We also controlled diameter and thickness of InSb nanowires by changing experiment parameter which is reaction time.

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발표코드: **INOR.P-142**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cellular Adhesion and Growth on the Vertically Aligned Silicon Nanowire Arrays with different flexibility

윤서영 박이슬 이진석*

숙명여자대학교 화학과

According to advanced nanotechnology, the nanostructured materials with various kinds and shape are synthesized easily or produced by process. Recently, researches about interaction between the nanostructured materials and biological system have been progressed actively. The surface topography may influence cellular responses, for example cell adhesion, cell morphology. In this work, we synthesized vertically aligned silicon nanowires (SiNWs) on the Au-covered Si(111) wafer by chemical vapor deposition (CVD) method. We accomplished to control of the SiNWs diameter by regulating thickness of Au film such as 1 nm and 10 nm. These substrates did not isolate cells and just provided surface topography for cell culture. Human Embryonic Kidney 293T cells (HEK 293T cells) were cultured on these substrates for 2 days. We studied the nanotopographical effects on cell morphology, adhesion, and growth which are evaluated on each SiNWs substrate comparing bare glass as control.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-143

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Patterned Growth of Vertically Aligned Silicon Nanowires based on Vapor-Liquid-Solid Mechanism

박이슬 이진석*

숙명여자대학교 화학과

Si nanowires (SiNWs) have been identified as useful building blocks for nanoscale electronic and thermoelectric devices. In order to maximize their entire potential in many applications, SiNWs must be integrated efficiently and economically into various device systems. It is essential to simplify to fabricate devices by eliminating complex processes. Also, an important requirement for device application is the precise control of the location and the size of the SiNWs. According to the vapor-liquid-solid (VLS) growth mechanism, while the length of the SiNWs is determined mainly by the chemical vapor deposition (CVD) conditions such as gas flow rate and growth time, the location and the diameter of the SiNWs are controlled by the diameter and the location of the AuNPs. For this reason, it is important to develop position of AuNPs on the substrate. In this work, we synthesized vertically aligned SiNWs using Au disk pattern as used catalyst for SiNWs growth to obtain precise location of SiNWs. It is possible to manipulate the pitch, diameter, and length of vertically aligned SiNWs by changing the experimental parameters such as various pitch and thickness of Au disk pattern, and growth time. Furthermore, we investigated the SiNWs growth mechanism through the relation between Au and Si precursors using Au-Si phase diagram. We investigated the growth mechanism based on Au-Si phase diagram by amount of Si precursor and temperature in details through the relation between Au and Si precursors using Au-Si phase diagram. Also, various morphologies of SiNWs are synthesized through study of growth mechanism.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-144

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Functionalized Silver Nanocrystals through Polyol Process Using Poly(vinyl pyrrolidone-ran-vinyl acetate) as a Surface Regulating Copolymer

박미라 정임식^{1,*} 송현준^{*}

한국과학기술원(KAIST) 화학과 ¹한국생명공학연구원 세포기능제어연구센터

Many researchers have used poly(vinyl pyrrolidone) (PVP) for synthesizing metal nanocrystals. Because it is believed that tertiary amide groups in PVP are preferentially bound to specific facets of the noble metals and guide the crystal growth direction. [1,2] Also, it is reported that synthesis of gold nanocrystals using polymer including poly(vinyl acetate) (PVAc) generates multiple hydroxyl groups on the surface, which can readily conjugate with versatile functionalities [3]. In the preceding work, we have synthesized silver nanocrystals through the polyol process in the presence of poly(vinyl pyrrolidone-ran-vinyl acetate) (PVP-PVAc). The copolymer, PVP-PVAc, has two distinct moieties including pyrrolidone for nanoparticle formation and acetate for additional functionalization. We have used PVP-PVAc as a surface regulating copolymer for the synthesis of silver nanocrystals and we observed that the shape of silver nanocrystals changes from cubes to wires as increasing reaction temperature. It is anticipated that the choice of well-designed copolymers would be a general methodology for the functionalized metal nanocrystals and serve as a new platform for various applications. References 1.X. Xia, J. Zeng, Q. Zhang, C. H. Moran, Y. Xia, J. Phys. Chem. C, 116, 21647-21656 (2012). 2.J. Zeng, Y. Zheng, M. Rycenga, J. Tao, Z. Y. Li, Q. Zhang, Y. Zhu, Y. Xia, J. Am. Chem. Soc. 132, 8552- 8553 (2010). 3.C. I. Yoo, D. Seo, B. H. Chung, I. S. Chung, H. Song, Chem. Mater. 21, 939-944(2009).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-145

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of a metal-organic framework, iron-benzenetricarboxylate (MIL-100(Fe)), with dry gel conversion method

정범근 정성화*

경북대학교 화학과

Recently, metal-organic frameworks (MOFs), a type crystalline inorganic-organic porous material has made remarkable progress in the field of functional materials. Their huge porosity, the easy tunability of their pores, and the number of potential applications made them one of the important materials with huge prospects. Usually these types of materials are synthesized by solvothermal process, however recently dry gel conversion (DGC) or steam agitated conversion (SAC) have attracted considerable attention to synthesize porous materials. DGC has potential advantages for the synthesis of porous materials, which includes minimum waste disposal, reduced reactor size, reduced consumption of a template and the possibility of continuous production, etc. However, synthesis of a MOF with DGC is not common and we hereby report a synthesis process for MIL-100(Fe) by DGC for the first time. It was found that, a very little amount of solvent can be used to synthesize a MOF by DGC where usually 7 or 8 times of solvent is required for the solvothermal process and hence it is an environmentally benign process. Additionally, the synthesis could be successful without adding any HF or HNO₃ and compared to the solvothermal method the reaction time was very low for the same composition of the reactants. Therefore, it can be established that, the MOFs can be synthesized successfully with DGC with very little amount of solvent (H₂O) and without any requirement of extra acids and hence the procedure is environment friendly. Reference [1] I. Ahmed, N.A. Khan, S.H. Jung, Cryst. Growth Des. 2012, 12, 5878-5881.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-146

발표분야: 무기화학

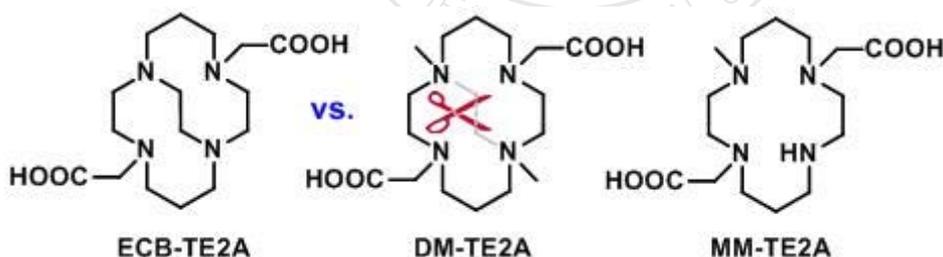
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of non-cross-bridged tetraazamacrocyclic chelator for efficient ^{64}Cu -based radiopharmaceuticals

AJIT V. DALE 김정영¹ 이호춘² 하영수 Nikunj B. Bhatt 이용희 안광일³ 유정수*

경북대학교 의과대학 분자의학교실 ¹한국원자력의학원 방사성의약품연구팀 ²대구경북과학기술원(DGIST) 에너지시스템공학 ³한국원자력의학원 방사성의약품 개발실

N-mono/di-methylated TE2A tetraazamacrocycles (MM-TE2A and DM-TE2A) were synthesized in high yields. Both Cu-MM/DM-TE2A complexes showed increased kinetic stability compared to that of Cu-TE2A, whereas Cu-DM-TE2A showed even higher in vitro stability than that of Cu-ECB-TE2A. MM-TE2A and DM-TE2A were quantitatively radiolabeled with ^{64}Cu ions and showed rapid clearance from the body to emerge as a potential efficient bifunctional chelator.



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장소: 창원CECO

발표코드: INOR.P-147

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

TE2A-Bn-NCS: a new bifunctional chelator for ^{64}Cu -based radiopharmaceuticals

Nikunj B. Bhatt AJIT V. DALE 김정영¹ 이호춘² 하영수 안광일³ 유정수*

경북대학교 의과대학 분자의학교실 ¹한국원자력의학원 방사성의약품연구팀 ²대구경북과학기술
술원(DGIST) 에너지시스템공학 ³한국원자력의학원 방사성의약품 개발실

A new tetraazamacrocyclic bifunctional chelator, TE2A-Bn-NCS was synthesized in high overall yield from cyclam. An extra functional group (NCS) was introduced to N-atom of TE2A for specific conjugation with antibody. The Cu complex of TE2A-Bn-NCS showed high kinetic stability in acidic decomplexation and cyclic voltammetry studies. X-ray structure determination of Cu-TE2A-Bn-NH₂ complex confirmed octahedral geometry, in which copper atom is strongly coordinated by four macrocyclic nitrogens in equatorial positions and two carboxylate oxygen atoms occupy the elongated axial positions. Trastuzumab was conjugated with TE2A-Bn-NCS and then radiolabeled with ^{64}Cu quantitatively at room temperature within 10 min. Biodistribution studies showed that the ^{64}Cu -labeled TE2A-Bn-NCS-trastuzumab conjugates maintain high stability in physiological conditions, and NIH3T6.7 tumors were clearly visualized up to 3 days by ^{64}Cu -immuno-positron emission tomography imaging in animal models.

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장소: 창원CECO

발표코드: **INOR.P-148**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of ZSM-5 from gels containing hexamethylene imine after microwave aging and its application in the dehydration of bioalcohols

전종원 정성화*

경북대학교 화학과

Zeolite ZSM-5 has been synthesized using Hexamethylene imine (HMI) as a template material. For this microwave aging under suitable conditions is essential for the crystallization of ZSM-5 from gels. Moreover, adequate reaction conditions (such as $\text{Al}_2\text{O}_3/\text{SiO}_2$, HMI/SiO_2 and $\text{H}_2\text{O}/\text{SiO}_2$ ratios, pH, reaction time and so on) for ZSM-5 syntheses are also suggested. The obtained ZSM-5, after ion exchange to the proton form, can be applied in acid-catalyzed reactions because the acidity and surface area of the zeolite are very similar to those of commercial ZSM-5 zeolite. For example, the H-ZSM-5 can be applied in the dehydration of bioalcohols such as ethanol and n-butanol into olefins or aromatics, very similar to a commercial H-ZSM-5 zeolite. Reference [1] J.-W. Jun, I. Ahmed, C.-U. Kim, K.-E. Jeong, S.-Y. Jeong, S.H. Jhung, Catal. Today 2013, accepted.

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발표코드: INOR.P-149

발표분야: 무기화학

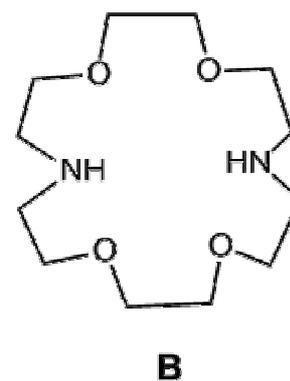
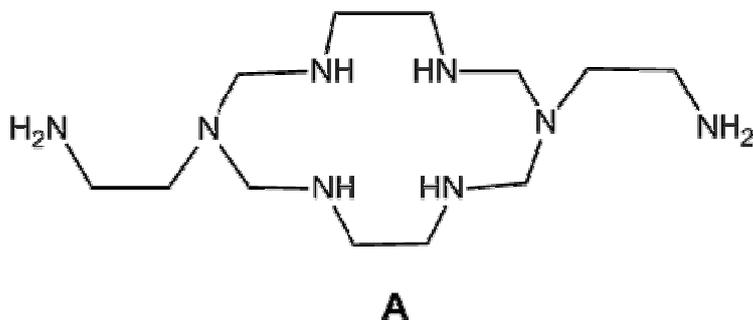
발표종류: 포스터, 발표일시: 수 16:00~19:00

Binding properties of crown ether and azacrown ether against ammonium linked with macrocyclic complexes at various conditions

이재명^{1,*} 곽지훈^{1,*}

순천대학교 화학과¹ 순천대학교 화학교육과

Molecular recognition is an important subject because it is a key concept to develop molecular tectonics, host-guest chemistry, sensor, switch and biological applications. Especially, the study on the selective binding in host-guest chemistry is important to understand the key mechanism of the transport in drug system, to apply in separation, etc. We have worked on the selective binding between ammonium ion attached to copper(II) or nickel(II)-macrocyclic complexes toward 18-crown-6. In this presentation, we will discuss the binding properties of ammonium as a pendant arm of macrocyclic complex (A) toward 1,9-diaza-18-crown-6 (B).



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: INOR.P-150

발표분야: 무기화학

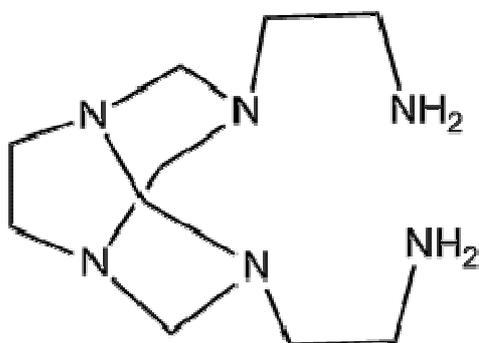
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and properties of some supramolecules obtained from the combination of non-cyclic polyaza complexes and metallocyanides

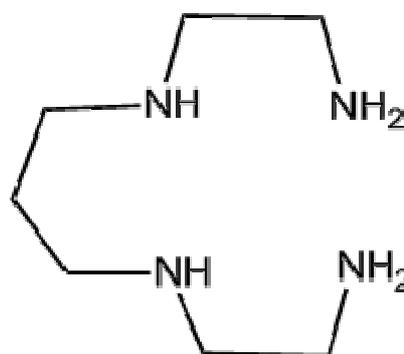
서민지, 곽지훈^{1,*}

순천대학교 화학과 ¹순천대학교 화학교육과

Preparation of supramolecule is important because it gives intrigue and interesting morphology and sometimes, shows interesting physical and chemical properties. Especially, combination of non-cyclic polyaza complex with metallocyanide produces interesting and intrigue multi-dimensional structure such as chain, ladder, rectangular, honeycomb structures. Also, in many cases, they shows unique magnetic properties, photochemical properties and inclusion properties.. We have prepared and structurally characterized some supramolecular complexes by the combination of complexes of non-cyclic polyaza ligands (A and B) and various kind of metallocyanides. In this presentation we will discuss the preparation, X-ray structure and properties of some supramolecules obtained from the combination of non-cyclic polyaza complexes of copper(II) or nickel(II) with metallocyanides.



A



B

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-151**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Supramolecular molecules formed by hexaaza macrocyclic copper(II) complexes

김태영 김주창*

부경대학교 화학과

Hexaaza macrocyclic copper(II) complexes, $[\text{Cu}(\text{L}+2\text{H})](\text{ClO}_4)_4$ and $[\text{Cu}(\text{L})](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$, (L = 3,10-bis(3-(2-methyl-1H-imidazol-1-yl)propyl)-1,3,5,8,10,12-hexaazacyclotetradecane) have been synthesized and structurally characterized by spectroscopic and X-ray diffraction methods. Each structure exhibits a supramolecule by the self-assembly of a monomeric structure. The imidazole pendants on the macrocycle L participate in the formation of supramolecule through hydrogen bonds as well as C-H... π intermolecular interactions. The detailed structures of the complexes as well as the formation of supramolecules will be described in this presentation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-152**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal structures and supramolecular array of macrocyclic nickel(II) complexes

이유정 김주창*

부경대학교 화학과

Hexaaza macrocyclic nickel(II) and copper(II) complexes, $[\text{Ni}(\text{L}+\text{H})](\text{ClO}_4)_3$ and $[\text{Ni}(\text{L})](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$ ($\text{L} = 3,10\text{-bis}(3\text{-(2-methyl-1H-imidazol-1-yl)propyl})\text{-}1,3,5,8,10,12\text{-hexaazacyclotetradecane}$) have been synthesized and structurally characterized by X-ray diffraction method. Both structures form corresponding supramolecules by extending their monomeric unit through various types of intermolecular interactions. Especially, the presence of imidazole pendants on the macrocycle L plays an important role in the formation of supramolecules, respectively. The detailed structures of the complexes as well as the formation of supramolecules by the self-assembly processes will be described in this presentation.

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장소: 창원CECO

발표코드: INOR.P-153

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

**Three Dimensional Frameworks from rare-earth metals and germanium embedding the lithium and indium mixed-site in the void:
 $RE_2Li_xIn_{1-x}Ge_2$ ($RE = La, Nd, Sm$ and Gd ; $0.27 \leq x \leq 0.54$)**

전지은 유태수*

충북대학교 화학과

During our systematic investigation to synthesize the $RE_4LiIn_xGe_{4-x}$ series, which is a derivative of the RE_5Tt_4 ($RE =$ rare-earth metals; $Tt =$ tetrrels) system known for its giant magnetocaloric effect, we serendipitously obtained four members of the $RE_2Li_xIn_{1-x}Ge_2$ system related to the RE_2TtTt_2 ($T = In, Li$) system known for its interesting magnetic property and potential application as electrode in lithium batteries. $RE_4LiIn_xGe_{4-x}$ and $RE_2Li_xIn_{1-x}Ge_2$ systems both contain the identical structural moiety which is a 2-dimensional (2D) layered structure consisting of the AlB_2 -type and $CsCl$ -type units. One particular structural difference is that the $RE_4LiIn_xGe_{4-x}$ series includes In/Ge-In/Ge covalent bonds between pairs of 2D-slabs, while the $RE_2Li_xIn_{1-x}Ge_2$ series does not. Four $RE_2Li_xIn_{1-x}Ge_2$ ($RE = La, Nd, Sm$ and Gd ; $0.27 \leq x \leq 0.54$) compounds were synthesized by high temperature reactions and characterized by both powder and single crystal X-ray diffraction. These quaternary phases crystallize in the tetragonal Mo_2FeB_2 -type structure (an ordered ternary variant of the U_3Si_2 -type structure) and adopt the space group of $P4/mbm$ with $Z=2$ and Pearson's symbol $tP10$. The lattice parameters are $a = 7.6140(3)$, $c = 4.4496(2)$ for $La_2Li_{0.276(2)}In_{0.724}Ge_2$, $a = 7.4368(2)$, $c = 4.3263(10)$ for $Nd_2Li_{0.431(2)}In_{0.569}Ge_2$, $a = 7.3834(3)$, $c = 4.2704$ for $Sm_2Li_{0.432(7)}In_{0.568}Ge_2$, and $a = 7.2885(3)$, $c = 4.2416(2)$ for $Gd_2Li_{0.531(6)}In_{0.469}Ge_2$. A series of theoretical studies using the tight-binding linear muffin-tin orbital (TB - LMTO) method was conducted on the idealized $Gd_2Li_{0.5}In_{0.5}Ge_2$. Density of states (DOS) curves proved its metallic property, and crystal orbital Hamilton population (COHP) analyses showed an antibonding character for Ge_2 dimers around E_F . The slightly unfavorable antibonding character of Ge_2 dimers was compensated by a relatively strong bonding character between Gd and Ge.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-154**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective encapsulation of reactive phosphorus species in a porous coordination network

최완욱 Hiroyoshi Ohtsu Masaki Kawano*

포항공과대학교 첨단재료과학부

White phosphorus (P_4), one of the allotropes of elemental phosphorus, reacts with many chemicals and is used to produce industrially important phosphorus compounds such as phosphoric acids and phosphorus oxides. On the other hand, molecular level reaction investigation of P_4 was rarely conducted due to its instability in ambient condition. Moreover, unique reactions of P_4 are expected in a pore of porous network which works as a molecular crystalline flask.^[1] Therefore, we aimed to trap P_4 and observe unique reaction with I_2 in a powder crystalline porous coordination network. We succeeded in trapping a small phosphorus in a porous coordination network of $[(ZnI_2)_2(TPT)_3]$ (TPT: 2,4,6-tris(4-pyridyl)triazine)^[2] by gas phase diffusion at 380 °C for 8 hrs. After exposure of the network powder to phosphorus vapor generated from red phosphorus, the powder changed from pale yellow to yellow and a XRPD pattern changed. Ab initio XRPD structural analysis and ICP measurement suggest that white phosphorus was encapsulated in the pore of the network. We also investigated the reactions of the encapsulated white phosphorus with iodine in a pore. P_4 -encapsulating network reacted with iodine vapor at 333 K to generate reddish crystalline powder. When the reddish powder was exposed to the air, the color was changed to purple drastically and new phase of crystalline powder was formed. We are analyzing these products by IR, UV-Vis and XRPD. Reference[1]T. Kawamichi, T. Haneda, M. Kawano, M. Fujita, Nature., 2009, 461, 633.[2]K. Ohara, J. Marti-Rujas, T. Haneda, M. Kawano, D. Hashizume, F. Izumi, M. Fujita, J. Am. Chem. Soc., 2009, 131, 3860.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-155**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of Copolymers Containing 1,1-Dihexyl-3,4-diphenylsilole and Disubstitutedsilane along the Main Chain

정영민 장지훈 박영태^{1,*}

계명대학교 화학과 ¹계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-dihexyl-3,4-diphenylsilole as monomer was prepared by the intramolecular reductive cyclization of dihexylbis(phenylethynyl)silane with treatment of 4 mol lithium naphthalenide followed by anhydrous ZnCl₂ and N-bromosuccinimide in situ. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-dihexyl-3,4-diphenyl-2,5-silole and disubstitutedsilane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-dihexyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane using n-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and CHCl₃. 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.

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발표코드: **INOR.P-156**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copolymerizations of 2,5-Dibromo-1,1-diethyl(or 1,1-diisopropyl)-3,4-diphenylsilole with Dichlorodisubstitutedsilanes Using n-Butyllithium

장지훈 정영민 박영태^{1,*}

계명대학교 화학과 ¹계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diethyl(or 1,1-diisopropyl)-3,4-diphenylsilole as monomers were prepared by the intramolecular reductive cyclizations of diethyl(or diisopropyl)bis(phenylethynyl)silane with treatments of 4 mol lithium naphthalenide followed by anhydrous ZnCl₂ and N-bromosuccinimide in situ. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diethyl(or 1,1-diisopropyl)-3,4-diphenyl-2,5-silole and disubstitutedsilane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diethyl(or 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 CHCl₃. 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.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-157**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Diverse reactions of S-K ligand under metal-mediated conditions

임종완 Masahiro Mikuriya^{1,*}

심인고등학교 화학 ¹Kwansei Gakuin University

Variable pyridylpyrimidine-based ligands were used for the study of metal-chelating property in coordination chemistry. The treatment of ligand, potassium 4-(2-pyridyl)pyrimidine-2-thiolate(S-K), with CuCl₂·2H₂O led to the formation of a neutral [Cu(S-S)Cl][CuCl₂], whose X-ray diffraction analysis indicated that S-S bond of the ligand was generated in the course of the reaction. The S-S ligand is bis-(4-(pyridin-2-yl)pyrimidin-2-yl)disulfane. The S-S bond length in S-S ligand equal to 2.0306(10) Å. On the other hand, the main product was metal-free S-S ligand in the reaction with Fe(OAc)₂.

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발표코드: INOR.P-158

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

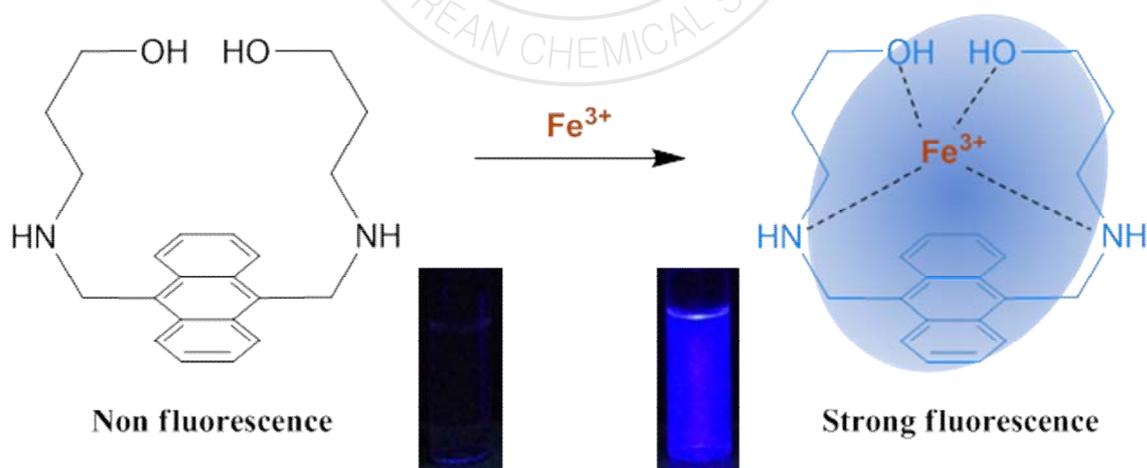
A New Anthracene Based Fluorescent Turn-On Sensor for Fe³⁺

안경룡 신승림¹ 이상오² 고선덕³ 신종일¹ 박수열¹ 박균하* 전근^{1,*}

충남대학교 화학과 ¹한국화학연구원 계면재료공정연구그룹 ²충남대학교 ³성균관대학교 화학

과

A new fluorescent sensor for Fe³⁺ based on anthracene moiety of hydroxyalkylamine was easily synthesized and investigated for photophysical properties. Fluorescent sensor 9, 10-Bis(3-hydroxypropylamino-methyl) anthracene displayed highly selective and sensitive fluorescent “turn-on” toward Fe³⁺ in acetonitrile solution. The 1:1 stoichiometry of sensor complex 1+Fe³⁺ was confirmed by Job’s plots based on fluorescence emission titration. Furthermore, the binding sites of sensor complex 1+Fe³⁺ was properly identified from ¹H NMR study.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-159**

발표분야: 무기화학

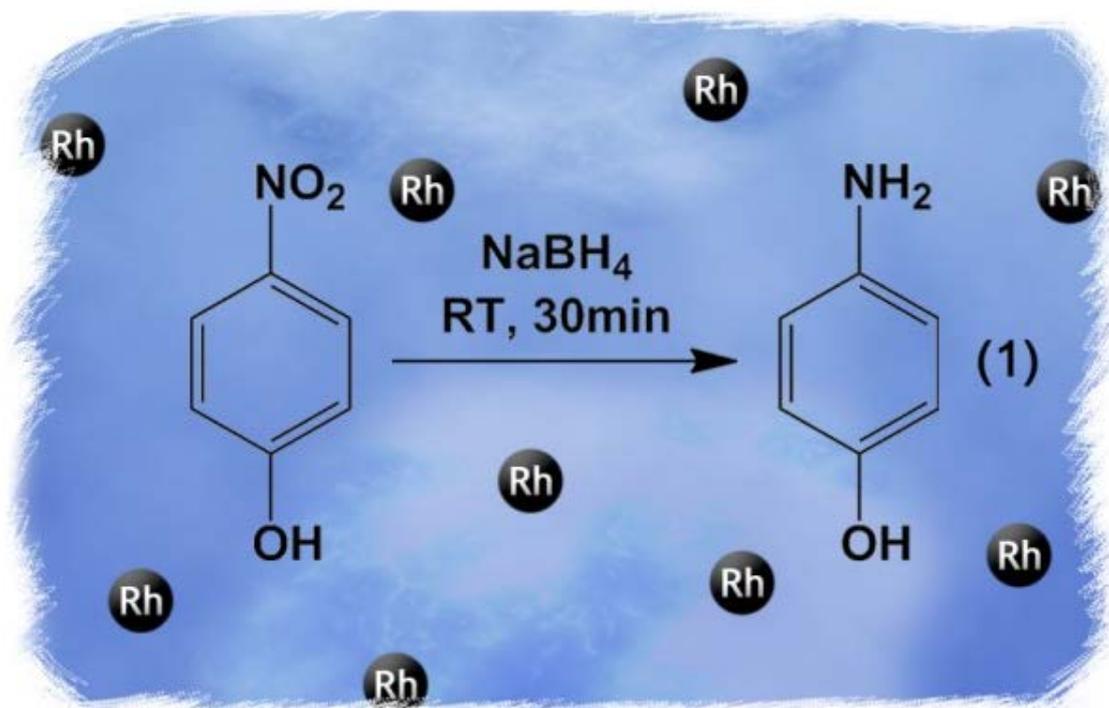
발표종류: 포스터, 발표일시: 수 16:00~19:00

Recyclable Rhodium Nanoparticles as Active and Highly Efficient Catalysts for Reduction of Nitroarenes

황소리 박강현*

부산대학교 화학과

In this work, rhodium nanoparticles were synthesized using hydrothermal method that is simple and easy to use nontoxic supercritical water. The rhodium nanoparticles made preparations formed in uniform size and shape. It also acted as efficient heterogeneous catalyst in reduction of 4-nitrophenol to 4-aminophenol. Moreover, this catalyst has the advantage can be recycled and showed highly efficient catalytic activity for various nitroarenes. This environmentally friendly method with good yields and be suitable for use in the industry.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

TiO₂@GO core - shell nanomaterial decorated with various metal nanoparticles

김미란 박강현*

부산대학교 화학과

Graphene oxide is a versatile solid supporting material to immobilize metal nanoparticles capable of catalyzing a wide array of organic transformations. Similarly, this study describes about the synthesis of hybrid nanomaterial comprised of titanium dioxide core - graphene oxide shell (TiO₂@GO) decorated with various metal nanoparticles including gold, silver, palladium and copper. We examined the effectiveness of supporting material to increase the stability, catalytic activity and recyclability of the nanoparticles. The novel catalytic system open doors for investigating novel reactivity. To investigate furthermore, we made material with various combinations of GO while keeping TiO₂ core shell remains intact. For instance, we synthesized TiO₂ spheres and modified their surface to positive charges in order to wrap negatively charged GO. In addition, we employed TiO₂@GO core shell as templates for the nucleation and growth of metal nanoparticles over their surface exemplified by Au NPs. We expect the metal nanoparticles immobilized on hybrid nanomaterials would be a pioneer catalytic system in a variety of organic reactions. The study on photocatalysis and photovoltaics of these materials are underway.

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발표코드: INOR.P-161

발표분야: 무기화학

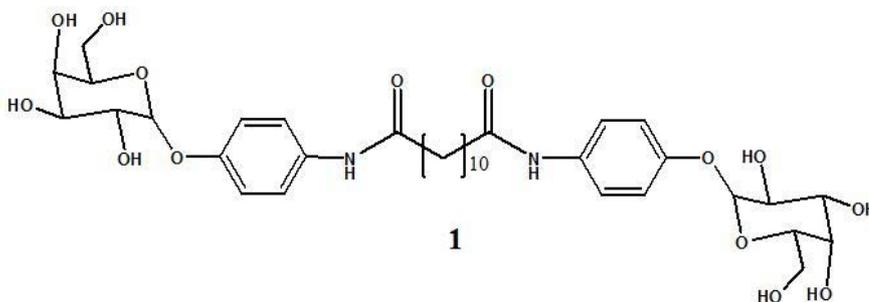
발표종류: 포스터, 발표일시: 수 16:00~19:00

Sugar-Based Composite Hydrogel with Functionalized Graphene Oxide

이지하 정종화*

경상대학교 화학과

We synthesized the β -glucopyranoside-based compound (1) and β -glucopyranoside functionalized graphene oxide (G-GO). A sugar-based bollamphiphile/graphene oxide composite hydrogel has been prepared using simple mixing. The composite gels form at different pH condition. According to SEM observation, the composite gel exhibits a fibrillar structure with a 70-80 nm fiber diameter. As revealed by powder X-ray diffraction (XRD) patterns, the patterns of the composite gel and the native gel were different. The composite gel forms an interdigitated bilayered structure incorporating intermolecular hydrogen-bonding interactions. And then, we observed mechanical and electrochemical properties of gels by rheometer and cyclic voltametry. Interestingly, the mechanical and eletrochemical properties of the composite gel are both dramatically enhanced when compared to the native gel, reflecting that the functionalized graphene oxide layers efficiently act as a intercalator composite gel in the structure.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

다공성 SiO_2 나노입자를 이용한 휴대용 Hg^{2+} 센서의 제조와 형광 특성 연구

이진혁 정종화*

경상대학교 화학과

본 연구는 Hg^{2+} 이온을 검출하기 위해서 리간드 2 를 테더링 방법에 의해서 다공성 입자인 메조포러스 실리카 입자표면에 도입하여 유기-무기 하이브리드 소재(M1)를 제조하였다. 유기-무기 하이브리드 나노소재(M1)은 FT-IR, TGA 및 형광분광기를 이용하여 특성을 연구하였다. 그 결과 리간드 2 는 메조포러스 나노입자 표면에 공유결합에 의해서 20.8% 만큼 도입되었다. 특히 수용액에 분산된 M1 은 397 nm 의 빛을 흡수한 결과 440 nm 에서 강한 방출 스펙트럼을 나타내었다. 따라서 수용액에 분산된 M1 의 형광특성은 다양한 금속이온(Cu^{2+} , Cd^{2+} , Na^{2+} , Zn^{2+} , Ag^{2+} , Pb^{2+} , Mg^{2+})을 첨가하여 연구하였다. 그 결과 M1 의 강한 형광특성은 Hg^{2+} 이온을 첨가 시 소광되었으나, 다른 금속이온 (Cu^{2+} , Cd^{2+} , Na^{2+} , Zn^{2+} , Ag^{2+} , Pb^{2+} , Mg^{2+}) 의 경우에는 큰 변화가 나타나지 않았다. 이는 M1 에 도입된 리간드 2 가 Hg^{2+} 이온과 선택적으로 결합하기 때문으로 예측된다. 나아가 휴대용 센서를 제조하기 위하여 필터페이퍼를 이용하여 형광특성을 연구하여 Hg^{2+} 센서로서의 사용가능함을 연구하였다.



Fig. 1 (A) Structure of **M1** and **M2**, (B) Fluorescence spectra ($\lambda_{ex} = 397\text{nm}$) of **M1** (3×10^{-5} mol) upon addition of metal ions (10 equiv.) in water at pH 7.4



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발표코드: INOR.P-163

발표분야: 무기화학

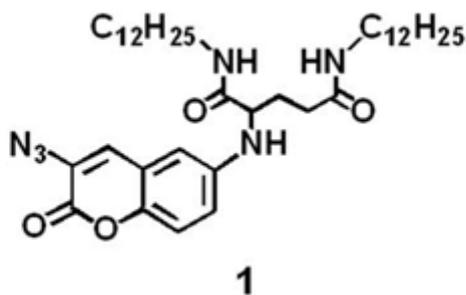
발표종류: 포스터, 발표일시: 수 16:00~19:00

Azidocoumarin-derivative based organogel

박혜경 이지하 정종화*

경상대학교 화학과

본 연구에서는 유기용매에서 초분자 젤을 제조하기 위해서 형광체로 쿠마린기, 그리고 분자간의 수소결합과 소수성 특성을 부여하기 위해서 아미드기를 갖는 알킬 사슬을 도입한 화합물 1은 NMR, IR, MS 및 원소분석을 통하여 구조를 확인하였다. 화합물 1의 초분자 젤 형성은 다양한 용매에서 관찰하였다. 그 결과 화합물 1은 DMSO, Ethanol, Xylene, Toluene, DCM, benzene 에서 자기조립에 의한 초분자 젤을 형성하였다. 그리고 초분자 젤의 분광학적 특성은 UV-Vis, PL, SEM, AFM 등을 이용하여 연구하였다. 형성된 초분자 젤은 파이버 구조를 이루고 있었고, 430 nm 부근에서 강한 형광특성을 나타내었다. 형광의 세기는 용매에 따라 차이가 있었으며 형광의 세기와 젤의 강도는 비례하였다.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Terpyridine-based Metalogel

박소현 정성호 정종화*

경상대학교 화학과

본 연구에서는 리간드와 금속의 당량에 따른 변화를 관찰하였다. 화합물 **1**, **2** 는 거울상 이성질체로서 금속이온과 결합할 수 있는 터피리딘 유도체를 기반으로 하는 물질이다. 긴 알킬사슬은 소수성 상호작용을 위하여 도입하였고, 아민기는 카이랄성을 위하여 부여하였다. 합성된 화합물 **1**, **2** 는 $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, IR, Mass, 원소분석을 이용하여 확인하였다. 화합물 **1**, **2** 는 다양한 용매에서 실험한 결과, THF 에서 Co^{2+} 과 젤을 형성하였다. 형성된 젤의 특성은 UV-vis 분광기, 원편광 이색성 분광기, DSC, 레오미터를 이용하여 수행하였다. 그 결과, 금속 이온의 당량이 변화함에 따라 CD 신호의 방향이 변화하였다. 이러한 현상은 금속 이온과 화합물 **1**, **2** 사이의 배위수의 차이로 인한 것이다.

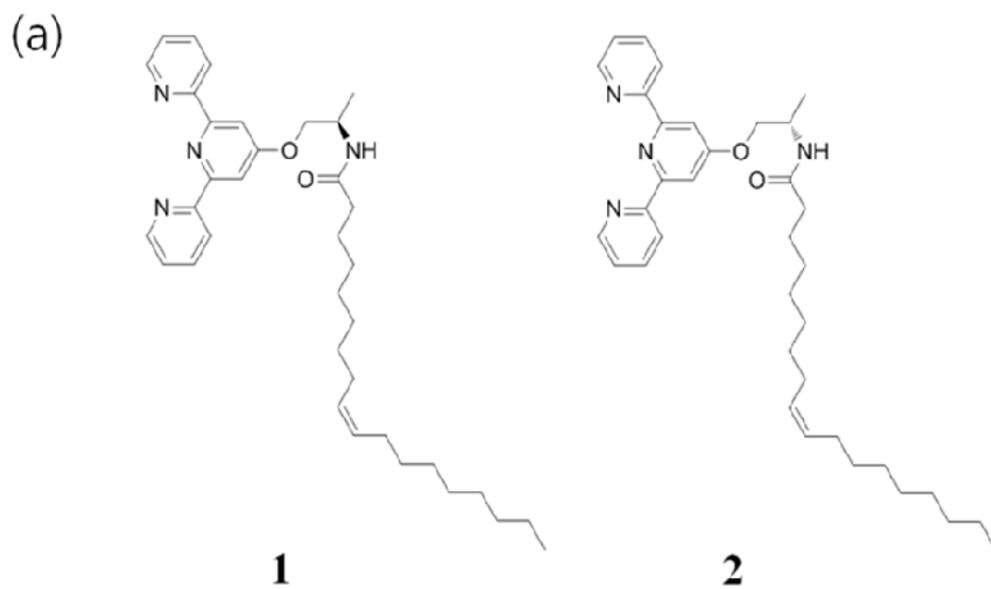


Fig. 1 (a) 터피리딘 유도체를 기반으로 한 화합물 **1, 2**.



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발표코드: INOR.P-165

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

크라운에테르와 칼릭스아렌이 도입된 CdSe와 Au 나노입자를 이용한 도파민 센싱

백영은 안준호 정종화*

경상대학교 화학과

호스트로 칼릭스아렌과 크라운에테르를 도입한 금과 반도체 나노입자가 게스트인 도파민 분자와 파이-파이 스택킹과 수소결합을 하여 입자간 엉김을 유발한다. 그로 인해 반도체 나노입자의 형광 특성의 변화가 나타나게 되는데, 이 변화를 형광광도계, 동적광산란, 투과전자현미경을 통해 분석하였다. 벤젠 유도체를 포함하는 분자를 대조군으로 삼아 형광광도계를 측정하여 센서로써의 활용 가능성을 확인 하였다. 이번 연구를 통해 본 연구진은 호스트-게스트 화학에 금과 반도체 나노입자를 도입하여 보다 간단하고, 미세농도의 도파민을 센싱하는 체계를 구축할 수 있었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-166

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

아조벤젠이 도입된 하이드로 젤의 특성 연구

이정연 정성호 정종화*

경상대학교 화학과

아조벤젠 및 카르복실기를 갖는 트리포달 형태의 젤레이터 1 을 합성하였으며, 젤레이터 1 은 수소결합, 파이-파이 상호작용, 반데발스 상호작용 및 쌍극자-쌍극자 상호작용에 의해 하이드로 젤을 형성하였다. 카르복실기와 이온쌍을 형성 할 수 있는 아민 유도체를 첨가하여 네트워트형 젤을 제조 하였다. 그리고 UV 중합에 따른 아조벤젠의 cis-, trans- 형태의 특성 연구 및 이온쌍 형성에 따른 pH, 농도에 의한 하이드로 젤의 특성을 SEM, NMR, FT-IR 및 CD 분광기를 이용하여 연구하였다.

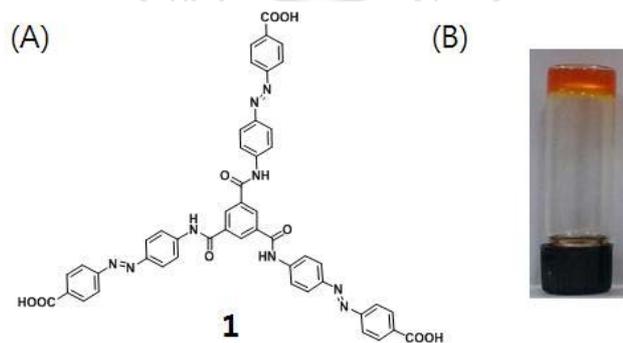


Fig.1 (A) 젤 레이터 1의 구조 (B) 하이드로 젤 1

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-167

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thiacalix[4]arene을 기반으로 한 삼차원 배위 고분자 젤의 알라닌

검출

김가영 정종화*

경상대학교 화학과

자가조립은 분자에 대한 규명과 기능적인 소재로서 개발할 수 있는 기반을 보여준다. 이러한 자가 조립을 바탕으로 형성되는 배위 고분자 젤은 조직 공학, DDS(drug delivery system) 그리고 화학센서로서 광범위한 범위에서 응용되고 있다. 본 연구에서는 MOF (metal-organic framework) 화학에서 널리 바탕으로 사용되는 Calix[4]arene 을 기반으로 화합물 p-tert-butyl-thiacalix[4]arene tetraacetic acid (H_4TCTA , **1**)를 제조하여 Tb^{3+} 과 함께 화학적 센서로서의 배위 고분자 젤의 기능을 연구 하였다. **1** 에 Tb^{3+} 를 첨가하여 DMF/H₂O 조건에서 젤을 제조하였다. 제조된 고분자 젤은 다양한 아미노산 첨가를 통해 관찰된 결과 알라닌에서만 강한 형광을 나타내는 것을 볼 수 있었다. 이러한 결과는 Tb 의 배위 수가 알라닌이 첨가됨으로써 바뀌기 때문이라고 추측된다. 이로 인해 본 발표에서는 Tb^{3+} 배위 고분자 젤의 알라닌 검출 센서의 응용성을 보여주고자 한다.

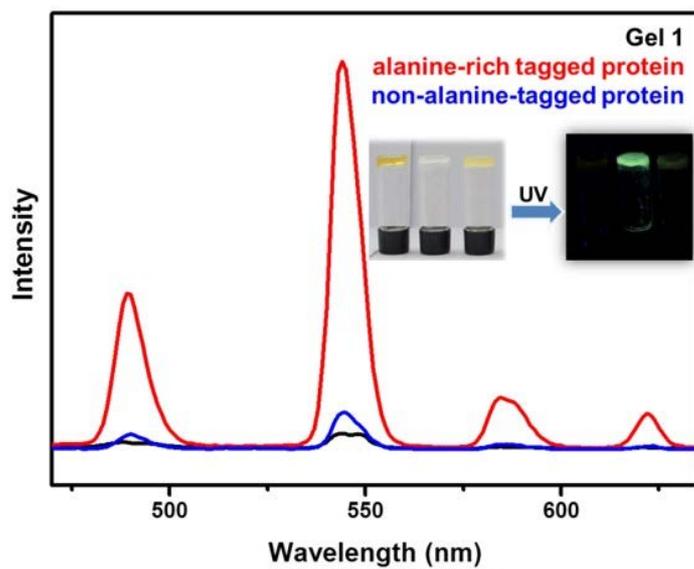


Figure. 알라닌이 풍부한 단백질과 알라닌이 없는 단백질 첨가에 따른 gel 1의 형광 스펙트럼.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-168

발표분야: 무기화학

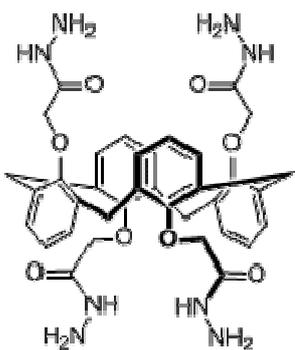
발표종류: 포스터, 발표일시: 수 16:00~19:00

산촉매를 이용한 초분자젤의 고분자화 및 물성연구

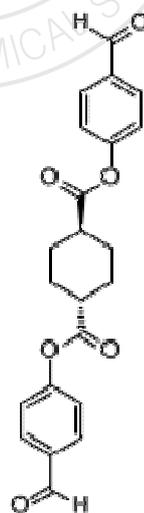
박재현 이지하 정종화*

경상대학교 화학과

알데히드와 하이드라진은 산촉매하에서 하이드라존을 형성한다. 본 연구에서는 하이드라진이 도입된 칼릭스아렌 유도체 1 과 다이알데히드가 도입된 트랜스-사이클로헥세인 유도체 2 를 산촉매를 첨가 하여 상온에서 젤을 제조하였다. 이렇게 제조된 젤은 핵자기공명 분광기, 자외선-가시광선 분광기, 유동계를 통해 젤의 물성을 관찰하였다. 제조된 젤은 시간에 따라 가시광선 영역의 빛을 흡수 하였으며 형광특성을 나타내었다. 젤의 분광학적 특성과 젤의 형성 매커니즘을 연구 하였다.



1



2

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-169**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Two oxidation states of Chromium Complexes derived from the same chromium salt and ligand

김유정 홍수경 이홍인*

경북대학교 화학과

Chromium is the most controversial in terms of the biochemical function. For these reasons, there is considerable interest in developing syntheses for Chromium complexes. Despite several decades of investigation, the biochemistry of chromium has been poorly understood. It is known that Cr interacts with proteins, but the details of the interactions and the safety or the toxicity of Cr are yet to be explored. In this study, we have synthesized Chromium complexes using a tetradentate ligand, called H₂EBPP (=N,N'-(ethylenedi-p-phenylene)bis(pyridine-2-carboxamide)) having carboxamide groups, as a model for investigating chromium-protein binding mechanism. Interestingly, two different oxidation states of Chromium complexes have been identified even though the complexes were derived from the same chromium salt and the ligand. In this poster, we present the syntheses, structures, and physical properties of the complexes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-170

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA가 도입된 금과 산화철@실리카 나노입자 간의 상보적 수소결합을 통한 두 입자의 응집 및 분산 제어와 약물 전달체로의 응용

안준호 정성호 이지하 정종화*

경상대학교 화학과

본 연구는 말단에 황 원자와 아민기를 갖는 DNA를 금(Au-1)과 산화철@실리카($\text{Fe}_3\text{O}_4@\text{SiO}_2$ -1) 나노입자 표면에 고정시켜, 용액 환경의 변화에 따른 두 나노입자의 결합 특성을 관찰하였다. DNA가 도입된 Au-1과 $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -1 나노입자는 적외선 분광기, 라만 분광기, 자외선-가시광선 분광기를 이용하여 DNA의 결합 특성을 관찰하였다. pH 7의 용액에서 Au-1은 $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -1와 상보적인 수소결합을 통해 회합되는 것을 TEM으로 아래의 그림 1과 같이 확인할 수 있었다. 이는 Au-1 나노입자 표면에 도입된 DNA의 아데노신과 $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -1 나노입자의 표면에 도입된 DNA의 티미딘이 상보적인 수소결합을 형성하기 때문이다. 또한 DNA의 상보적인 수소결합에 의해서 회합된 나노입자들은 pH를 산성 쪽으로 변화시키기에 따라 점차적 해리 되는 것을 확인할 수 있었다. 따라서 두 입자의 해리 및 결합은 나노입자 표면의 DNA 간의 수소결합을 조정함으로써 통제가 가능함을 확인할 수 있었다.

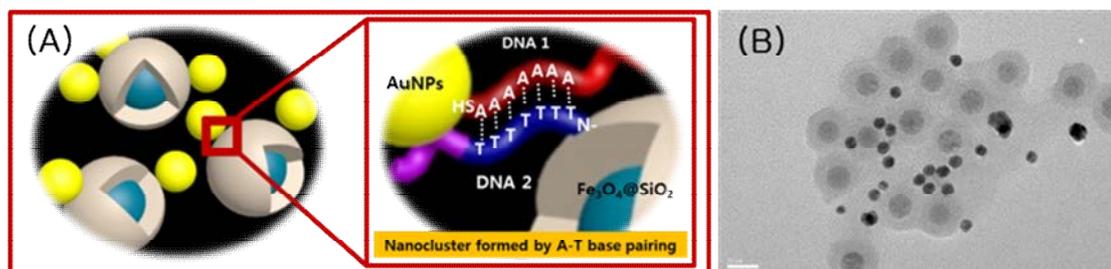


Fig. 1 (A) The mimetic representation and (B) TEM image of aggregated Au-1 and $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -1 nanoparticles

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-171

발표분야: 무기화학

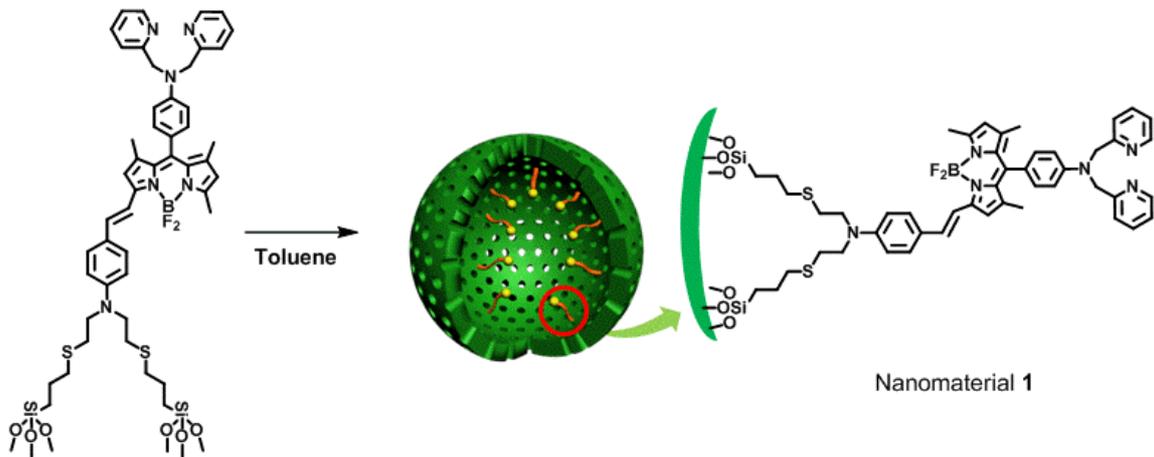
발표종류: 포스터, 발표일시: 수 16:00~19:00

BODIPY 유도체를 기반으로 한 고체 분자 로직 게이트

최희경 이지하 정종화*

경상대학교 화학과

본 연구에서는 특정 금속이온에 의해서 형광특성이 변화하는 유기-무기 하이브리드 소재를 개발하고자 하였다. 먼저 형광특성이 잘 알려져 있는 형광체로 BODIPY 를 이용하였다. 그리고 BODIPY 유도체의 형광특성은 Hg^{2+} 와 Zn^{2+} 이온을 이용하여 제어하였다. 예를 들면 리간드 1 은 Zn^{2+} 이온과 결합하여 강한 발광성을 나타내지만, Hg^{2+} 이 존재할 경우는 형광특성이 나타나지 않는다. 따라서 리간드 1 을 무기 나노소재 표면에 공유결합에 의해서 고정화시켜 유기-무기 하이브리드 나노소재 1 을 형성하였다. 그 결과 유기-무기 하이브리드 나노소재 1 은 푸른색을 나타내었으며 약한 형광 특성을 나타내었다. 따라서 나노소재 1 의 Hg^{2+} 및 Zn^{2+} 에 대한 형광특성을 연구하였다. 본 심포지움에서는 나노소재 1 에 대한 형광특성과 분자 로직 게이트에 대한 연구결과를 소개한다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-172**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrothermal Synthesis of a Nano-sized Co-Prussian Blue Analogue by a Single Source Method

강수민 전영진*

건국대학교 응용화학과

$\text{Co}_3[\text{Co}(\text{CN})_6]_2 \cdot x\text{H}_2\text{O}$, a mixed-valence cobalt(II) hexacyanocobaltate(III) compound, have attracted considerable interest to their many unique properties, such as electrochromic, ion sensing, electrocatalytic photomagnetic phenomena. We report rather than the conventional methods, a simple hydrothermal route to the formation $\text{Co}_3[\text{Co}(\text{CN})_6]$ nanostructure using the only one source. This experimental method offers many merits such as short reaction time, uniform shape, environment-friendly reaction condition. Detailed characterization by using various spectroscopic technics will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-173**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Air-stable Cu(II) Metal-Organic Frameworks with CO₂ Sorption

김동욱 나명수*

울산과학기술대학교(UNIST) 친환경에너지공학부

Even though lots of papers were published about the potential applications of metal-organic frameworks (MOFs) based on their porosities, the reports of their real applications are limited probably because of the hydrothermal instability of the MOFs. Here, we report the preparation and characterization of the structural features of a stable porous MOF, [Cu₃(tetrazole)₄Cl₂], with one-dimensional (1D) channels at even under the water soaking condition for several days. The MOF with the cage-like-pores with small neck-like portals aligned to form 1D channel showed the selective CO₂ adsorption over other gas molecules such as N₂ and CH₄ at 298 K.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-174**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

암모니아 보란 합성 시스템 개발 및 MOF를 이용한 수소발생 특성

향상 연구

박성진

원익머트리얼즈 개발팀

암모니아 보란 합성 Scale-up 시스템 (1 회 100g 이상) 개발 및 합성된 암모니아 보란의 수소 발생 특성평가를 실시하였으며 암모니아 보란을 MOF 에 함침 시켜 기존의 암모니아 보란 보다 뛰어난 수소 발생 특성을 띄는 AB-MOF를 합성하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-175

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Luminescent Solvatochromism of Cu(I) Coordination Polymers and Structural Transformation Between Cubane Cu_4I_4 and Stair-step Cu_4I_4

조성화 전영은 이상진 강기행 김태호 김진은*

경상대학교 화학과

Five copper(I) coordination polymers $[\text{Cu}_2\text{I}_2\text{L}_2]_n$ (1), $[\text{Cu}_4\text{I}_4\text{L}_2]_n$ (polymorphs 2 and 3), $[\text{Cu}_4\text{I}_4\text{L}_2(\text{CH}_3\text{CN})_2]_n$ (4), and $\{[\text{Cu}_4\text{I}_4\text{L}_2]\cdot\text{CH}_3\text{OH}\}_n$ (5), of 2-(*tert*-butylthio)-N-(pyridin-3-yl)acetamide (L), have been successfully synthesized and structurally characterized by single-crystal X-ray diffraction. Coordination polymer 1 shows a 1D loop chain structure, based on rhomboid Cu_2I_2 units. Coordination polymers 2, 3, and 5 have cubane Cu_4I_4 cluster nodes. Coordination polymer 4 has stair-step Cu_4I_4 cluster nodes. Very interestingly, transformation between 3 and 4 was controlled by heat and solvent. Coordination polymer 5 was transformed to coordination polymer 4 by addition of CH_3CN . Coordination polymer 1, 2, 3, 4 and 5 emit blue, red, yellow, blue, and yellow color light, under UV-irradiation respectively. Luminescence color of 4 and 5 depend on solvent molecules in the crystal.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-176

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal Structures and Photophysical Properties of Cu(I) Coordination Polymers

이상진 조성화 전영은 강기행 김태호 김진은*

경상대학교 화학과

Three copper(I) coordination polymers $[\text{Cu}_2\text{I}_2\text{L}^1]_n$ (1), $[\text{Cu}_2\text{I}_2\text{L}^1_2]_n$ (2), $[\text{Cu}_2\text{I}_2\text{L}^2]_n$ (3) with ligands L^1 and L^2 and a complex $[\text{Cu}_2\text{I}_2\text{L}^3]_n$ (4) with L^3 have been successfully synthesized and structurally characterized by single-crystal X-ray Diffraction. Complexes 1-3 show 2D network structures. 1 is composed of cubane Cu_4I_4 Cluster nodes, while 2 and 3 are based on rhomboid Cu_2I_2 cluster nodes. Discrete complex 4 has tetrahedral Cu_4 clusters, which shows cuprophilic interactions. Complexes 1-4 show emission peaks at 571, 480, 502, 595 nm, respectively. possibly, preparation of $[\text{Cu}_2\text{I}_2\text{L}^2]_n$ and $[\text{Cu}_2\text{I}_2\text{L}^3]_n$ will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-177

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper(I) Coordination Polymers Based on Dithioether Ligands with Pyromellitic Diimide

강기행 전영은 이상진 조성화 김태호 김진은*

경상대학교 화학과

Recently, we have explored coordination polymers based on dithioether ligands and $(\text{CuI})_x$. As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we synthesized three dithioether ligands, N,N'-bis[2-(tert-butylthio)ethyl]pyromellitic diimide, (L^1), N,N'-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide, (L^2), and N,N'-bis[2-(benzylthio)ethyl]pyromellitic diimide (L^3). And three Cu(I) coordination polymers 1-3 based on the ligands were prepared by self-assembly reaction between CuI and L^1 , L^2 , L^3 , respectively. Coordination polymers 1-3 are composed of cubane Cu_4I_4 cluster nodes, emitting red-orange light under UV-irradiation. The results of our investigation including syntheses, structural characterization, thermal and photoluminescent properties of three new Cu(I) coordination polymers are presented.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: INOR.P-178

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Structures, and Crystal Transformation Properties of Copper(I) Coordination Polymers Based on 2-(2- benzylthio)ethyl)pyrazine

전영은 조성화 이상진 강기행 김태호 김진은*

경상대학교 화학과

Four copper(I) coordination polymers $[\text{Cu}_2\text{I}_2\text{L}_2]_n$ (1), $\{[\text{Cu}_4\text{I}_4\text{L}_2]2\text{CH}_3\text{CN}\}_n$ (2), and $[\text{Cu}_4\text{I}_4\text{L}_2]_n$ (polymorphs 3 and 4) with 2-(2-benzylthio)ethyl)pyrazine (L), has been prepared by self-assembly reaction between CuI and L. Three coordination polymers 2-4 are supramolecular isomerism by solvent molecules. Compound 1 interconnected by rhomboid Cu-I₂-Cu units is a 2D network structure. Compounds 2 and 3 interconnected by stair-step tetramer Cu₄I₄ units are 1D looped chain structures. Remarkably, crystal structure of 4 composed of zigzag chain (CuI)_n polymer and stair-step (Cu₂I₂)_n polymer units is 1D ribbon-type. Also, transformation between 2 and 3 occurred reversibly by removal of solvent molecular and addition of solvents.

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발표코드: INOR.P-179

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Performance and Synthesis small molecule (TIPS) triisopropylsilylethynyl substituted benzodithiophene (TIPSBDT) and Alkyl-substituted oligothiophene-based in (BHJ)bulkheterojunction Photovoltaics

임남우 백상현 조나라 임기민 고재중*

고려대학교 소재화학과

Organic solar cells are subject to a considerable current interests motivated by the perspective of achieving large area, low-cost, lightweight, and flexible power sources. We believe that Solution-processed SM-OPVs is essential for taking full advantage of OPV technologies. Our work was designed and synthesized with oligothiophenes derivative as a spacer and (TIPS) triisopropylsilylethynyl substituted benzodithiophene (TIPSBDT) based on the donor unit and the several acceptors (3-ethylrhodanine or hexyl cyanoacetate and so on) as electron acceptor bridged by a thiophene unit. Such the TIPS moiety substituent has been used previously to modify acene molecules in organic field effect transistors(OFETs). TIPS substituents are better effective in lowering the lowest unoccupied molecular orbital (LUMO) and HOMO energy level than conventional alkoxy substituents. Furthermore, Alkyl-substituted oligothiophene-based π -conjugated spacers to guarantee good solubility and also to form an effectively long conjugated acceptor?donor?acceptor (A?D?A) backbone structure with strong intramolecular charge transfer and broad absorption. As the photovoltaic devices were fabricated, and the polymers:PC61BM active layer morphology was optimized by adding additive in a single layer device. In this poster, we studied substituent effect on terminal moiety of molecular engineering and controlling of device performance.

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발표코드: **INOR.P-180**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New concept of organic sensitizers with fluorine substituted phenylene spacer for efficient dye-sensitized solar cells

도광석 임남우 고재중*

고려대학교 소재화학과

Exhaustion of fossil fuel reserves and increased global warming are recognized as the most critical problems encountered in this century. In this regard, research targeted at solar energy harvesting is currently under extensive investigation. One useful technology should be ascribed to the dye-sensitized solar cell (DSSC), which is expected to dominate the low-cost niche market of consumer photovoltaics in the future. Due to the relatively high cost of ruthenium element, numerous research groups have expended endeavors to develop metal free organic dyes as the alternative sensitizers. As a result, impressive photovoltaic performances have been reported on various tailor-made organic dyes, which include coumarin, indoline, oligoene, merocyanine, hemicyanine, perylene, spirobifluorene, and even chlorophyll derivatives, showing promising η values in the range of 5~9.8%. Recently, we synthesized a simple organic DSSC dye with fluorine substituted phenylene spacer. A new series of organic sensitizers Ref, Flu-BT-PhF and Flu-IT-PhF with fluorene, 4,4-dimethyl-4H-indeno[1,2-b]thiophene derivatives plus functionalized phenylenes, and cyanoacrylic acid as the donor, π -spacer, and anchoring group, respectively.

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발표코드: **INOR.P-181**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Dye-Sensitized Solar Cells Based on an Alkylation with a Benzothiadiazole and its Properties

박소진 임남우 임기민 도광석 최혜주 조나라 백상현 고재중*

고려대학교 소재화학과

Dye-sensitized solar cells (DSSCs) have been widely investigated their special features, such as controlling absorption range and transparent. DSSCs are composed of donor, acceptor and π -bridge unit. Charge separation is important to achieve high conversion efficiency in the DSSCs. We set up to alkoxy at terminal of donor for application of Cobalt electrolyte. Moreover, our molecular engineering dyes are synthesized as bridging alkoxy at the Benzothiadiazole (BTD) to inhibit aggregation and recombination. In this study, we try to determine the properties and characters of the dyes through a various measurement.

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발표코드: **INOR.P-182**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of redox-active porous coordination network

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포항공과대학교 첨단재료과학부

Proper ligand design is important to realize specific coordination networks which can be applied to bio-mimic materials. Especially, the ligands having multi-interactivity and/or redox activity are particularly attractive in terms of trapping metastable state in the self-assembling process and construction of redox active pores in coordination networks. Here, we will show our recent work using 2,5,8-tripyridyl-1,3-diazaphenylene (TPDAP) including network formation. Considering the result of cyclic voltammetry and the structural properties of TPDAP, we expected that TPDAP can give various kinds of redox-active porous coordination networks. Indeed, the complexation of TPDAP with cadmium nitrate produced redox-active network crystals which have large pore spaces with the size of ca. $20 \text{ \AA} \times 7.1 \text{ \AA}$.

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발표코드: **INOR.P-183**

발표분야: 무기화학

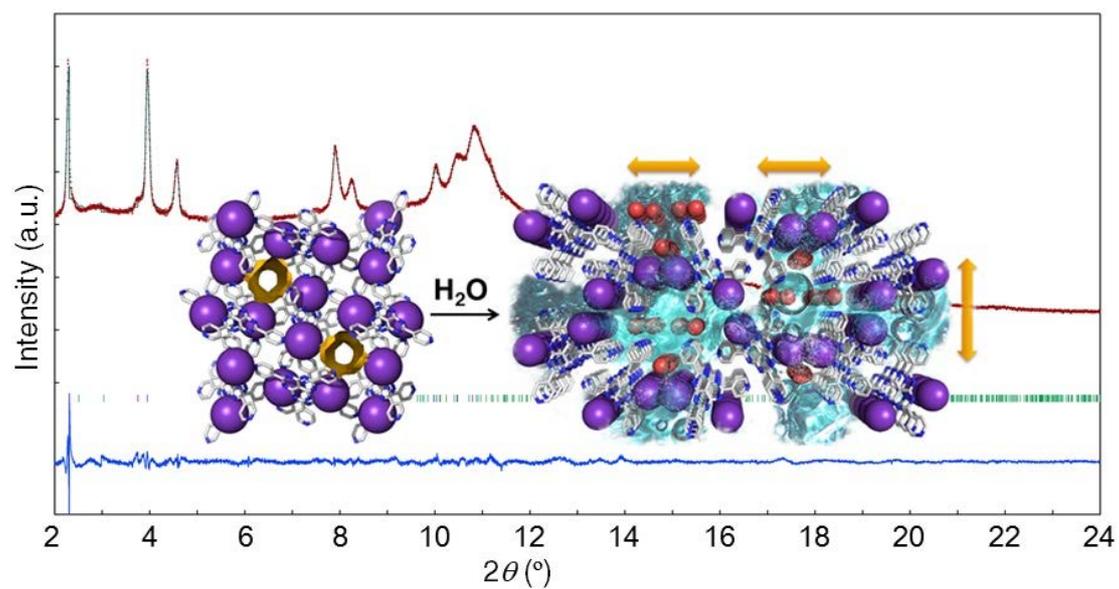
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fast Ionic Conductor based on Multi-interactive Molecule

이길령 Yakiyama Yumi Masaki Kawano*

포항공과대학교 첨단재료과학부

Preparation of efficient ion conducting system is one of the most attractive fields in the material chemistry. To date, introduction of acidic/basic moiety into the system is widely applied to achieve highly effective ionic conductor. However, such a strategy causes problems about cost and stability. In addition, it is not easy to interpret the ionic conduction event by the acidity or basicity of the system. In this context, to clarify the structural information is critical issue. However, it is still difficult to obtain structural information of ion conductive materials in molecular level because most of the reported systems are based on polymer materials. Recently, we have newly designed and synthesized a highly symmetrical multi-interactive ligand, tris(4-pyridyl)hexaazaphenylene (TPHAP). Due to the multi-interactive nature of TPHAP, its alkali metal salts showed enormously high ion conductivity by hydration despite absence of any acidic/basic groups. Here, we discuss the unique ion conducting property of TPHAP based on crystallographic approach, especially ab initio X-ray powder diffraction analysis.



Large water channel formation revealed by XRPD analysis



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

루테늄이온이 배워된 유기 젤의 제조 및 물성연구

이효희 정성호 정종화*

경상대학교 화학과

본 연구는 터피리딘기를 갖는 리간드 1 을 합성하였으며, 루테늄이온과 리간드 1 에 의한 젤을 제조하였다. 제조한 루테늄이온이 배워된 젤의 다양한 물성을 UV-vis, IR, SEM 및 Rheometer 을 이용하여 연구하였다. 그 결과 루테늄이온이 배워된 젤은 π - π stacking 을 형성하지 않았으며, IR 연구에 의하면 리간드 1 은 젤을 형성하기 위하여 분자간 수소결합을 형성하고 있었다. 또한 CV 측정 결과에 의하면 루테늄이온이 배워된 젤의 산화/환원 거동을 확인할 수 있었다. 따라서 본 학회에서는 리간드 1 을 이용하여 제조한 유기 젤의 다양한 물성 및 전기화학적 특성을 소개한다.

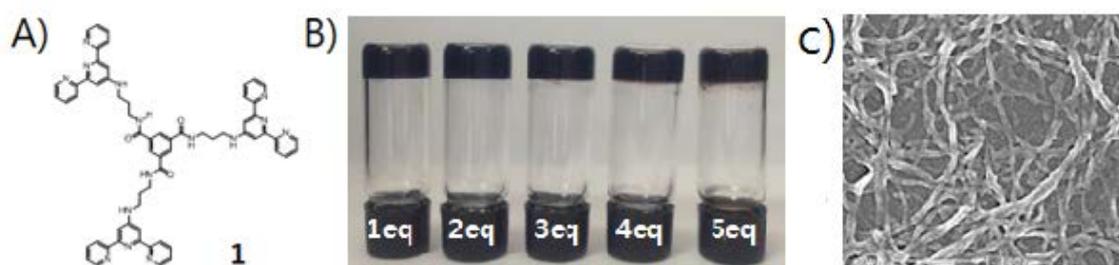


Fig.1 A) 리간드 1의 구조, B) 리간드 1에 대하여 1~5eq의 루테늄을 첨가하여 제조한 루테늄이온이 배워된 유기 젤 사진 C) 루테늄이온이 배워된 유기 젤의 SEM 사진

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장소: 창원CECO

발표코드: INOR.P-185

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses of Various Redox-Active Ligands for the Formation of Network Having Unique Physical Properties

하주연 구진영 Yakiyama Yumi Masaki Kawano*

포항공과대학교 첨단재료과학부

In the field of porous coordination networks, how to design ligands is crucial for realizing the unique functions such as redox-activity and selective guest encapsulation. Recently, we have newly designed and synthesized redox-active as well as multi-interactive 4-[4',7'-bis(4''-pyridyl)-diazaphenalenyl]benzoic acid which contains pyridyl and carboxylic groups as coordination sites in the network structures. This unique nature will enable various network formations by controlling their coordination ability. In addition, we also approached the preparation of 1,4-bis[4',7'-di(4''-pyridyl)2',9'-diazaphenalenyl]benzene which contains two redox active sites in the molecule. This molecule can show the novel mixed-valence state which enables electron transfer from one redox-active part to the other in a molecule. To the best of our knowledge, no such a ligand has been reported in this field and its network will show fascinating and innovative physical properties. In this presentation, we will report the preparation and the properties of diazaphenylene-based new ligands.

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발표코드: **INOR.P-186**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution processable small molecule through molecular engineering based on organic solar cells

백상현 조나라 도광석 최혜주 임남우 박소진 고재중*

고려대학교 소재화학과

Organic solar cells (OPV) have been widely investigated recently due to their potential for light-weight, low-cost, and large-scale roll-to-roll processing. Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. Solution processable small molecule-based donor material has been also attempted as attractive alternative of donor in organic solar cell due to its facile synthesis, purification, and low batch-to-batch variation compared to polymeric materials. Here, we designed and synthesized compound using different acceptor moiety in small molecule organic solar cells. These semiconductors have an unsymmetrical donor A-acceptor-donor B (DA-A-DB) framework composed of stabilized triphenylamine unit. This motif was introduced as donor B in the unsymmetrical DA-A-DB structure to increase solubility in organic solvents and they will have good interaction with PCBM. We suggest direction of research thereby knowing the result of different properties introducing various acceptors with PC71BM BHJ films

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발표코드: **INOR.P-187**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Organic dyes for High Performance Dye-Sensitized Solar Cells

최혜주 백상현 조나라 전무진¹ 고재중*

고려대학교 소재화학과 ¹연세대학교 화학과

Increasing energy demands and environmental issues such as fossil fuel shortage and global warming have leads to the need for clean renewable energy. Dye-sensitized solar cells are attracting widespread interest for a renewable energy source as a cost-effective alternative to conventional solid-state solar cells. Triphenylamine derivatives have been widely investigated for the use in organic electronics, because they are characterized by good optical properties and p-type charge transport mobilities, allowing their use as hole-transport layers in organic field-effect transistors (OFET) or organic light emitting diodes (OLED). In this study, we expect to the introduction of cyclic thiourea/urea groups induces an extension of electron-donating ability.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Co(II) Complexes with N,N',-bispyazole Ligands Based on N-alkyl or N-cycloalkyl amine Derivatives

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We have synthesised and characterised a series of new cobalt(II) complexes, CoLnCl_2 with ligands Ln ($L_1 \sim L_4$), where ($L_1 = \text{N,N-bis}((1\text{H-pyrazol-1-yl)methyl)benzenamine}$, $L_2 = \text{N,N-bis}((1\text{H-pyrazol-1-yl)methyl)cyclohexanamine}$, $L_3 = \text{N,N-bis}((1\text{H-pyrazol-1-yl)methyl)-3-methoxypropyl-1-amine}$) $L_4 = \text{N,N-bis}((1\text{H-pyrazol-1-yl)methyl)-1-(furan-2-yl)-methanamine}$). All new Co(II) complexes are characterized by spectroscopic methods and X-ray single crystal diffraction. Depending on the substituents of amine group in Ln ligands, Co(II) complexes have shown a 5-coordinated geometry or a 4-coordinated geometry.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Crystal Structure and MMA Polymerization of Binuclear Zinc(II) Complexes with Tetradentate Pyrazolyl Ligand

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경북대학교 화학과 ¹경북대학교 자연과학대학 화학과

The reaction of ZnCl_2 with ancillary ligands, including 1,4-bis-(N,N-di-(1H-pyrazolyl-1-methyl)amine)benzene (L_1) and 4,4'-bis-(N,N-di(1H-pyrazolyl-1-methyl)phenyl)methane (L_2), in ethanol yields Zn(II) chloride complexes, i.e., 1,4-bis-(N,N-di-(1H-pyrazolyl-1-methyl)amine)benzene(dichloro)Zn(II) [L_1ZnCl_2] and 4,4'-bis-(N,N-di-(1H-pyrazolyl-1-methyl)phenyl)methane(dichloro)Zn(II) [L_2ZnCl_2]. The molecular structures of Zn(II) complexes were determined by X-ray diffraction method. In addition, the catalytic activity of [L_1ZnCl_2] and [L_2ZnCl_2] for MMA polymerization was investigated and compared to the corresponding monomeric Zn(II) complex.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis , Structural characterization and Reactivity of Cobalt(II) complex with N,N-bispyridine amine Derivative

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경북대학교 화학과 ¹경북대학교 자연과학대학 화학과

The mononuclear cobalt(II) complex $[\text{Co}(\text{L}_1)\text{Cl}_2]$ with ligand L_1 ($\text{L}_1 = \text{N,N-bis(pyridine-2-ylmethyl)3-methoxypropylamine}$) has been synthesized and structurally characterized. Molecular structure of $[\text{Co}(\text{L}_1)\text{Cl}_2]$ revealed that the nitrogen of 3-methoxypropylamine group (Co1-N2 bond length: 2.2476(8) Å) are coordinated to the cobalt metal to achieve 5-coordinated complex around cobalt metal. However, oxygen atom of 3-methoxypropylamine group was not coordinated (Co1-O1 bond length: 5.823 Å) to the metal centre. In addition, the catalytic activity of $[\text{Co}(\text{L}_1)\text{Cl}_2]$ for MMA polymerization was investigated.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cu(II) Complexes with Multidentate Pyridyl Ligand with Tri- and Tetradentate Pyridyl Ligand

이수연 정현진 임세리¹ 박경세² 이동현*

전북대학교 화학과 ¹전북대학교 자연대/화학과 ²군산대학교 화학과

Transition metal complexes with two or three chelate pyridyl ligands have been studied in detail, largely because of their catalytic abilities, biological significance and sensor application. Copper complexes have been particularly fruitful since pyridine ligands support a range of coordination numbers, geometries, and nuclearities for copper(II). We have synthesized different multidentate pyridyl ligands and their Cu(II) complexes. These compounds were characterized by a single crystal X-ray crystallography and EPR (Electron Paramagnetic Resonance) spectroscopic methods. The *N,N'*-dimethyl-*N,N'*-bis(pyridin-2-yl)methanediamine (DMPA, 1) ligand reacts with one equivalent at Cu(ClO₄)₂ salts to give [(DMPA)₂Cu](ClO₄)₂, 2. Slow decomposition of 2 under aerobic condition in methanol, unexpectedly led to the formation of an alkoxo-bridged tetranuclear copper(II) cubane 3, which is considered to be a product of an oxidative N-dealkylation reaction. We also synthesized *N,N'*-(Pyridine-2,6-diylbis(methylene))bis(*N*-methyl(Pyridin-2-yl)methanamine) (L^{N5}, 4) and its Cu^{II}(L^{N5}) complex 5, which was characterized by X-ray crystallography. To investigate of O₂ reactivity, We plan to investigate Cu(I)/O₂ reactivity using there new ligands and their Cu(I) complexes.

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Synthesis of Pentacene Crystal Wires via Solvent Vapor Annealing Process and their Photoluminescence Properties

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포항공과대학교 첨단재료과학부 ¹포항공과대학교 화학과

Photoluminescence (PL) is an important optical property that has been widely studied for the development of light-based applications, such as displays, lasers, sensors, and biotags. In contrast with the PL from individual molecules in ensemble states, PL commencing from solid state crystals needs careful studies for its origin because interaction between incoming excitation light and the fixed orientation of molecules in specific crystal planes determine the absorption cross-section and eventually overall quantum yield. Although very little is known about the influence of the crystal plane for organic crystals, we have recently reported the crystal plane-dependent PL activity of pentacene 1D wires and 2D disks synthesized by physical vapor process: high PL from pentacene 1D wires but low PL from 2D wires owing to the presence of (010) plane only in the 1D wires. In this presentation, we present new pentacene 1D wires that are synthesized by solvent vapor annealing (SVA) process and exhibit homogeneous PL from all surfaces of wires. The morphology and crystal structure information were obtained by scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), energy-filtering transmission electron microscopy (EF-TEM), and selected area electron diffraction pattern (SAED). The PL spectra and images of the wires are different from those of the previously reported pentacene crystals. This unique PL property is attributed to the solvent inserted in the wires.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Deprotonated-Pyridyldicarboxamide Copper Complex as a Catechol Oxidase Model System: Kinetics and Mechanism

shuranjan sarkar 이홍인*

경북대학교 화학과

Catechol Oxidase, a type 3 copper enzyme, is isolated from phytogetic materials. The dinuclear copper active site of the enzyme mediates a two-electron transfer reaction during the oxidation of a wide range of catechols to the corresponding o-quinones by molecular oxygen. In this study, we have synthesized a dinuclear Cu(II) complex Cu_2L_2 ($Cu_2L_2 = di(N,N'-(ethane-1,2-diyldi-o-phenylene)-bis(pyridine-2-carboxamide)dicopper(II))$) as a model for the enzyme to investigate the catalytic reaction mechanism. Single crystal X-ray crystallography of Cu_2L_2 revealed that the two copper centers are apart at 6.992 Å, allowing this non-bridged dicopper(II) complex to be a model for the active sites of catechol oxidase. The oxidation reaction was spectrophotometrically studied by following the appearance of the o-quinone, at basic pH and room temperature. In this poster, we present the possible reaction pathway of the catalytic action of the complex.

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발표코드: **INOR.P-194**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Phenothiazine Exfoliatable Crystal *via* VCR process and Its Field-effect transistor Device Application

이민경 박지은 박치범 최희철*

포항공과대학교 화학과

Discovery of graphene has attracted scientist in various fields spanning from fundamental researches to applications based on the unique chemical, electrical, optical and mechanical properties of 2D quantum structures and also developing diverse carbon-based crystal. Recently, organic single crystal has collected much interest as a mimic or alternate of graphene. The successful synthesis of disk-typed organic crystals are expected to provide a new strategic direction for the realization of graphene-like organic layered structures. In this presentation, we present that phenothiazine molecules are grown into exfoliatable layered structure. The phenothiazine layered crystals have been successfully synthesized by vaporization-condensation-recrystallization (VCR) process. The synthesized PTZ crystal shows p-type behavior with the average hole charge carrier mobility of $1.15 \times 10^{-4} \text{ cm}^2/\text{V}\cdot\text{s}$ and photoresponses under UV light. Furthermore, the assembled phenothiazine crystal can be mechanically exfoliated into stacked individual layers to exhibit various colors depending on the thickness, has revealed that single layer of phenothiazine crystal can be also obtainable.

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발표코드: INOR.P-195

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ni(II) Complex with a Pyridine Substituted N-Heterocyclic Carbene Ligand and It's Catalytic Property

정현진 문건우¹ 박경세² 이동현*

전북대학교 화학과 ¹전북대학교 자연과학대학 화학과 ²군산대학교 화학과

N-heterocyclic carbenes(NHCs) have been accepted as a mightily important class of ligands in organometallic chemistry or catalysis reaction. A nickel(II) complex of a NHC ligand containing two pyridyl substituents has been synthesized and characterized by x-ray crystallography. The crystal structure indicated that the nickel ion forms a square planar geometry around it with two sets of a pyridyl nitrogen and a carbene carbon. Those two sets of N and C are from two NHC ligands. Here we report on the synthesis and characterization of nickel(II) complex of pyridine substituted N-heterocyclic carbene ligand. Especially, focus on electrocatalytic reduction of CO₂. We investigated the activation/reduction of CO₂ by a $(((\text{MepyCH}_2)_2\text{-Im})_2\text{Ni})(\text{PF}_6)_2$ by using cyclic voltammetry. In the N₂ atmosphere, we observed first reduction peak at -1.214V vs Ag/AgCl and second reduction peak at -1.630V vs Ag/AgCl of $(((\text{MepyCH}_2)_2\text{-Im})_2\text{Ni})(\text{PF}_6)_2$. And when it was in the CO₂ atmosphere, we observed the current enhancement at first & second reduction peak and strong reduction peak at -2.486V vs Ag/AgCl. For this reason, we tentatively suggest that CO₂ binds to the center the nickel(II) and is activated. A thorough investigation is in under way to find what the reduced products of CO₂ might be and the possible reduction mechanism.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-196

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct Synthesis of High Quality Single Layer Graphene on Amorphous SiO₂ Substrate via Copper Vapor-Assisted Chemical Vapor Deposition

김형기 송인택 박치범 최희철*

포항공과대학교 화학과

We demonstrated that high quality single layer graphene (SLG) on SiO₂/Si substrate can be grown by copper vapor-assisted growth method where copper foil is located right above the SiO₂/Si substrate at a few micrometer distance. At 1000 °C of growth temperature, the vaporized copper from copper foil catalyzes the dehydrogenation of methane and the nucleation on SiO₂/Si substrate. It results in the growth of high quality SLG on amorphous SiO₂/Si substrate. Raman spectroscopy clearly shows that the SLG is grown on the SiO₂/Si substrate and has very low defect level which is comparable to the quality of graphene grown on copper foil. Also, intensity profile of electron diffraction pattern using transmission electron microscopy (TEM) supports that the graphene grown on substrate is single layer. The FET device fabricated with graphene grown on SiO₂/Si substrate clearly the ambipolar behavior and Dirac point in the resistance versus gate voltage curve which is typical electronic properties of graphene. The carrier mobilities of electron and hole are about 800 cm²V⁻¹s⁻¹ and 700 cm²V⁻¹s⁻¹ which are comparable to the graphene grown on Cu foil. Copper-vapor-assisted growth method can be applied to other substrate such as h-BN and quartz substrate.

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장소: 창원CECO

발표코드: INOR.P-197

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Unprecedentedly High conductive quenched DPPH crystal by ascorbic acid treatment

박지은 최희철*

포항공과대학교 화학과

An important goal for organic materials is to enhance electrical conductance for application such as flexible OLED, organic solar cell. Likewise, the impurity atoms participate in electronic conduction in inorganic semiconductor, such as silicon and germanium, with n type or p type impurity, respectively, free electron by metal doping or polarity by inserting organic molecules as a donor in organic crystal could be induced higher current level than original organic crystal. But, due to the migration of metal and difficulty of dopant stoichiometric analysis in organic crystals, radical molecule with unpaired electron as a dopant or defect can be possible candidate for conducting organic materials. However, the handling of radical molecules is very difficult due to instability in the air at room temperature. So we synthesized DPPH (2,2-diphenyl-1-picrylhydrazyl) single crystal from DPPH molecules, which is well known as one of the stable radical molecules, by SVA (Solvent-Vapor-Annealing) system. Electrical measurement shows that as-grown DPPH single crystal exhibits lower electrical conductivity than what was expected, but intentionally quenched DPPH crystal by ascorbic acid, we confirmed that electrical conductivity can be dramatically increased and mobility is $1.21 \text{ cm}^2\text{V}^{-1}\text{S}^{-1}$. the DPPH crystal changed to core-shell structure. The unexpected phenomenon will be attributed to electron movement of quenched DPPH molecules like doping by ascorbic acid treatment. The phenomenon can be explained by reduced band gap in ultraviolet photoelectron spectra.

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장소: 창원CECO

발표코드: INOR.P-198

발표분야: 무기화학

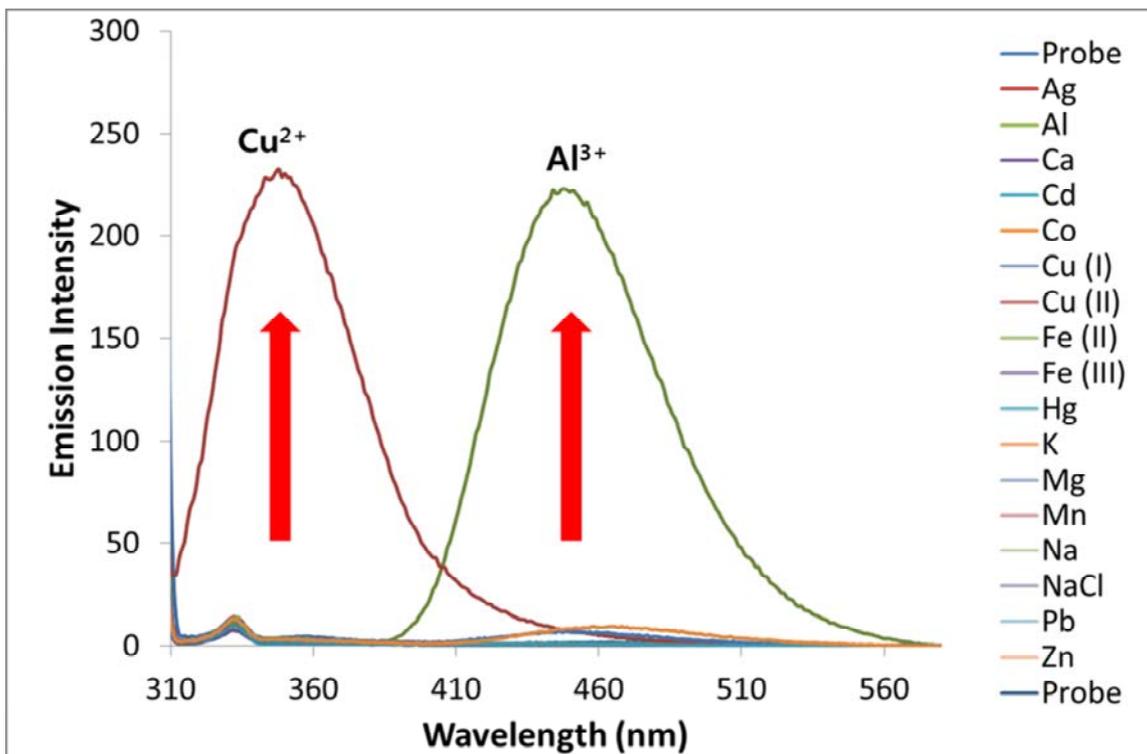
발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbamoyl phenol group protection promotes novel and surprising chemosensing versatility: strong fluorescence turn-on dual Cu(II) sensing reversible with biothiols, Al(III) sensing, and Al(III)-triggered Cu(I) 1:2 DEMULTIPLEXING

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한국과학기술원(KAIST) 화학과

A novel Schiff base probe (N,N'-bis(N-dimethylcarbamoyl)salicyl-imine)carbohydrazone) was prepared and explored for chemosensing potential which showed surprising strong exclusive fluorescence 'turn ON' for Cu²⁺ at 345 nm (85-fold) and Al³⁺ (771-fold) at 445 nm which is the first of its kind for this general motif. Ligand: metal binding stoichiometries and binding constants for Cu²⁺ and Al³⁺ were 1: 2 (2.93 x 10⁹ M⁻²) and 1: 1(2.36 x 10⁴ M⁻¹), respectively. Detection limit of Cu²⁺ and Al³⁺ were 0.0467 μM, and 0.769 μM in acetonitrile, respectively. In the presence of Al³⁺, Cu⁺ showed fluorescence 'turn-ON' signal (32-fold) at 360 nm. Density functional theory (DFT) calculations revealed approximately C_{2v} symmetrical structure of probe₂Cu²⁺. The most stable form was 2₂Cu²⁺, triplet ground state, which was from the two unpaired electrons of Cu²⁺ ions through calculations of optimization energy. When the 2₂Cu²⁺ complex was treated with a variety of biothiols (L-cysteine, homocysteine, glutathione, N-acetyl cysteine), fluorescence were found to decreased to probe levels, which shows the reversibility. Through the biological application, sensing potential for copper ions was shown in human blood plasma. From Al³⁺, Cu⁺, Cu²⁺ and L-cysteine input fluorescence data, 'INHIBIT' and '1:2 DEMULTIPLEXERS' molecular logic gating behavior can be represented.



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장소: 창원CECO

발표코드: INOR.P-199

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Blue Phosphorescent Organic Light-Emitting Diodes with excellent external quantum efficiency

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강원대학교 과학교육과 ¹강원대학교 화학과 ²강원대학교 일반대학원 화학과

Heteroleptic Ir(III) complexes, $(C^{\wedge}N)_2Ir(L^{\wedge}X)$, are considered to be promising phosphorescent metal compounds for application in OLEDs because they have both high thermal stability and phosphorescent efficiency. Recently, we have developed a series of deep-blue phosphorescent Ir(III) complexes. These molecules have the general formula of $Ir(C^{\wedge}N)_2(L^{\wedge}X)$ where $C^{\wedge}N = 2',6'$ -difluoro-2,3'-bipyridine (dfppy), and $L^{\wedge}X =$ ancillary ligand such as acetylacetonate, acac (1, 3) or dipivaloylmethanoate, dpm (2) as shown in Figure 1. Recently, we have reported double-layer electroluminescent devices using compounds 1 and 2 as the dopant. These EL devices showed pure blue color with high efficiency (EQE: 10% ~ 15%). However, the optimization of device condition is still needed because the lack of energy transfer between host and dopant and exciton confinement in emitting layer was observed in this structure. Therefore, a optimized condition using mCP as host and TSPO1 as a hole blocking and electron transporting material was developed for efficient blue PhOLEDs of the following structure: ITO/PEDOT:PSS/TAPC/mCP/ mCP:x%-1, 2 and 3/TSPO1/LiF/ Al, as show in Figure 2. The device of compound 2 doped into mCP host at the doping level of 3 wt% has the best performance with EQE of 20% at the brightness of 100 cd/m² and the maximum current efficiency of 25.3 cd/A(CIE, x = 0.14, y = 0.18).

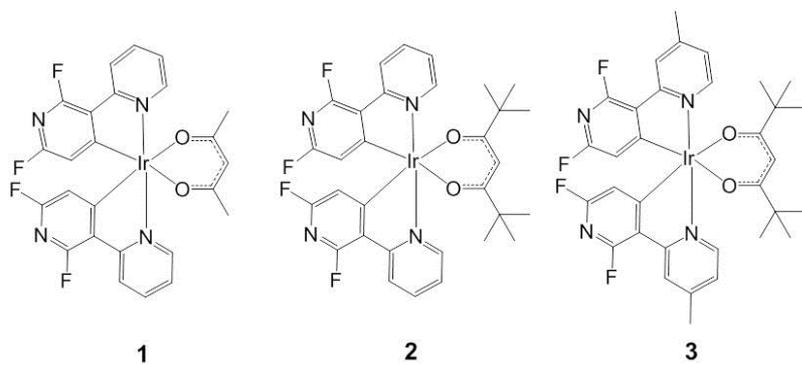


Figure 1. Molecular structure of deep blue Iridium complexes **1** – **3**.



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장소: 창원CECO

발표코드: INOR.P-200

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Isorecticular and Polymorphic Metal-Organic Frameworks via Combination of Solvothermal Reactions and Subsequent Postsynthetic Ligand Exchanges and Insertions

정석 신선영 박정인¹ 나명수*

울산과학기술대학교(UNIST) 친환경에너지공학부 ¹울산과학기술대학교(UNIST) 나노생명화학
공학부

The metal-organic frameworks (MOFs), [Ni(HBTC)(pz)] (3) (hms net topology) (where, H₃BTC = 1,3,4-benzenetricarboxylic acid; pz = pyrazine) and [Ni(HBTC)(bipy)] (4) (gra net topology) (where, bipy = 4,4'-bipyridine) that were unattainable via conventional synthetic approach, were prepared via the postsynthetic ligand exchanges of 3-D MOFs, [Ni(HBTC)(bipy)] (1) (hms net topology) and [Ni(HBTC)(pz)] (2) (gra net topology), respectively. The MOFs, [Ni(HBTC)(pz)] (5) (gra net topology) and [Ni(HBTC)(bipy)] (6) (gra net topology) that are the same as 2 and 4, respectively, were prepared via the postsynthetic ligand insertions into 2-D MOF [Ni(HBTC)(DMF)] (hcb net topology). 1 and 4 (or 6) are the polymorphic MOFs of the same 3,5-connected but of different net topologies, hms and gra net topologies, respectively, with the same [Ni(HBTC)(bipy)] formula. 2 (or 5) and 3 are also the polymorphic MOFs of the same formula unit, [Ni(HBTC)(pz)]. 1 and 3 are the isorecticular structures of the same hms net topology and 2 and 5 also are the isorecticular structures of the same gra net topology.

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장소: 창원CECO

발표코드: **INOR.P-201**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

***In-situ* monitoring of conductance change during alkali doping into polycrystalline C₆₀ thin film**

박지범 이진호 최희철*

포항공과대학교 화학과

Since the discovery of superconductivity in alkali doped C₆₀, people have studied the optical and electrical properties of alkali metal - C₆₀. During the exposure of alkali metal vapor to polycrystalline C₆₀ film, the conductance is first increased and decreased again according to sequential filling of electrons into the lowest unoccupied molecular orbitals (LUMO). In previous reports, the conductance change of polycrystalline C₆₀ film occurs smoothly without any significant signal change. Here, we show discrete conductance change of C₆₀ thin film during vapor form potassium doping process, implying that the polycrystalline C₆₀ thin film also follows a granular metal system. The clear peaks or plateaus are observed in conductance - time plot which is believed to correspond to the number of doped alkali metal atoms. This hypothesis is confirmed by Raman spectroscopy, X-ray photoelectron spectroscopy and temperature dependent conductance change.

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장소: 창원CECO

발표코드: **INOR.P-202**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Shape controlled synthesis of water soluble NaGdF₄:Yb,Er upconversion nanoparticles

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Upconversion (UC) is a unique type of photoluminescence in which lower-energy excitation (near-infrared light) is converted into higher-energy emission (visible light) via multi-photon absorption processes. Currently, great effort has been devoted to the synthesis of rare-earth ion doped upconversion nanoparticles (UCNPs) due to their emerging application in many fields such as bioimaging, photodynamic therapy, UC lasers, photovoltaics, and optical memory. Great efforts have been devoted to synthesize monodisperse NPs with a small size, uniform morphology, through thermolysis method, and hydro-/ solvothermal reactions. However, the as-synthesized NPs are normally capped by hydrophobic ligands such as oleic acid or oleylamine on the surface, making them insoluble in aqueous solutions, which greatly restricts their potential biomedical applications. So it is highly desirable to synthesis water soluble upconversion nanoparticles. Herein, we present the synthesis of water soluble upconversion nanoparticles with different shapes using polyethyleneimine (PEI) as surfactant through solvothermal approach. The effect of the solvent on the shape of the nanoparticles has been studied.

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발표코드: **INOR.P-203**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis of p-type semiconducting Picene Single Crystal

이진호 최희철*

포항공과대학교 화학과

Since superconductivity is discovered in alkali-doped C_{60} , organic hydrocarbons, especially highly conjugated molecules have been gathering great interest for the possibility of new superconducting material that shows high T_C . One important issue in organic superconductor is the influence of specimen structure on the superconducting properties. However, the difference of T_C from superconducting materials in powder form to either in thin film or single crystal form has been rarely studied. For the successful study of the correlation between structure and superconductivity, we need to synthesize organic superconductor molecules into geometry- controlled single crystals. Recently, picene molecules in polycrystalline bulk powder form has been reported to show the superconductivity at low temperature when doped with alkali metal. However, the synthesis of picene single crystals is still challenging due to its low solubility in organic solvents. In this presentation we report the synthesis of one-dimensional (1D) picene single crystals by drop-drying method. We analyzed the structure of picene crystal by synchrotron X-ray diffraction. The surface morphology of picene 1D crystal has been studied with scanning electron microscopy (SEM) and atomic force microscopy (AFM). The electrical property of picene 1D crystal has been examined using picene 1D crystal-field effect transistor (FET) devices.

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발표코드: INOR.P-204

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stepwise Synthesis of Metal-Organic Frameworks Using Metal-Organic Polyhedra as an intermediate

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While the Zn-MOF $[Zn_{24}(\text{mip})_{24}(\text{dabco})_6(\text{H}_2\text{O})_{12}]$ (where H_2mip = 5-methylisophthalic acid; dabco = 1,4-diazabicyclo[2.2.2.]octane) based on the cuboctahedral MOP $[Zn_{24}(\text{mip})_{24}(\text{H}_2\text{O})_{12}]$, as a 12-connected node could only be prepared via one-pot solvothermal reaction, similar attempts to prepare isorecticular Cu-MOFs via conventional one-pot synthetic approach in presence of 5-hydroxyisophthalic acid (H_2hip) and various linkers between the potential MOP intermediate, $[\text{Cu}_{24}(\text{hip})_{24}(\text{H}_2\text{O})_{12}]$, only produced metal-organic polyhedron (MOP), $[\text{Cu}_{24}(\text{hip})_{24}(\text{DMF})_{12}(\text{H}_2\text{O})_{12}]$. A series of isostructural and isorecticular Cu-MOFs, $[\text{Cu}_{24}(\text{hip})_{24}(\text{L})_6(\text{H}_2\text{O})_{12}]$ (where L = dabco; pz = pyrazine; bipy = 4,4'-bipyridine), could only be obtained via stepwise reactions using the cuboctahedral MOP, $[\text{Cu}_{24}(\text{hip})_{24}(\text{DMF})_{12}(\text{H}_2\text{O})_{12}]$, as an intermediate.

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장소: 창원CECO

발표코드: INOR.P-205

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stability of Hybrid Bimetallic Metal-Organic Frameworks and Its Large CO₂ Uptake Capacity

오민학 한승완 나명수*

울산과학기술대학교(UNIST) 친환경에너지공학부

A series of isostructural hybrid bimetallic metal-organic frameworks (MOFs), Ni_xM_{1-x}-ITHDs (M = Zn(II), Co(II)), have been prepared via a solvothermal syntheses using H₃BTB(4,4',4''-Benzene-1,3,5-triyl-tris(benzoic acid)) and bipy(4,4'-bipyridine) ligands with the mixed metal salts. While a critical amount of the doped Ni(II) ion (more than 0.2 mole fraction) is needed to have any enhancement of the framework stability of the hybrid bimetallic Ni_xZn_{1-x}-ITHDs, even a very small amount of the doped Ni(II) ion (0.1 mole fraction) produced a full enhancement of the framework stability of the hybrid bimetallic Ni_xCo_{1-x}-ITHDs. The highly porous and rigid Ni_xCo_{1-x}-ITHDs activated via a conventional vacuum drying process shows a BET specific surface area of 5,370 m² g⁻¹, which is comparable to that of pure Ni-ITHD. The CO₂ uptake capacities of Ni-ITHD and Ni_{0.11}Co_{0.89}-ITHD (2.79 g g⁻¹ and 2.71 g g⁻¹, respectively) at 1 bar and 195 K are larger than those of any other reported MOFs at similar conditions and the excess CO₂ uptake capacity at 40 bar and 295 K (1.50 g g⁻¹) is comparable to those of other MOFs, which are activated via the supercritical carbon dioxide drying process, with similar pore volumes.

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장소: 창원CECO

발표코드: INOR.P-206

발표분야: 무기화학

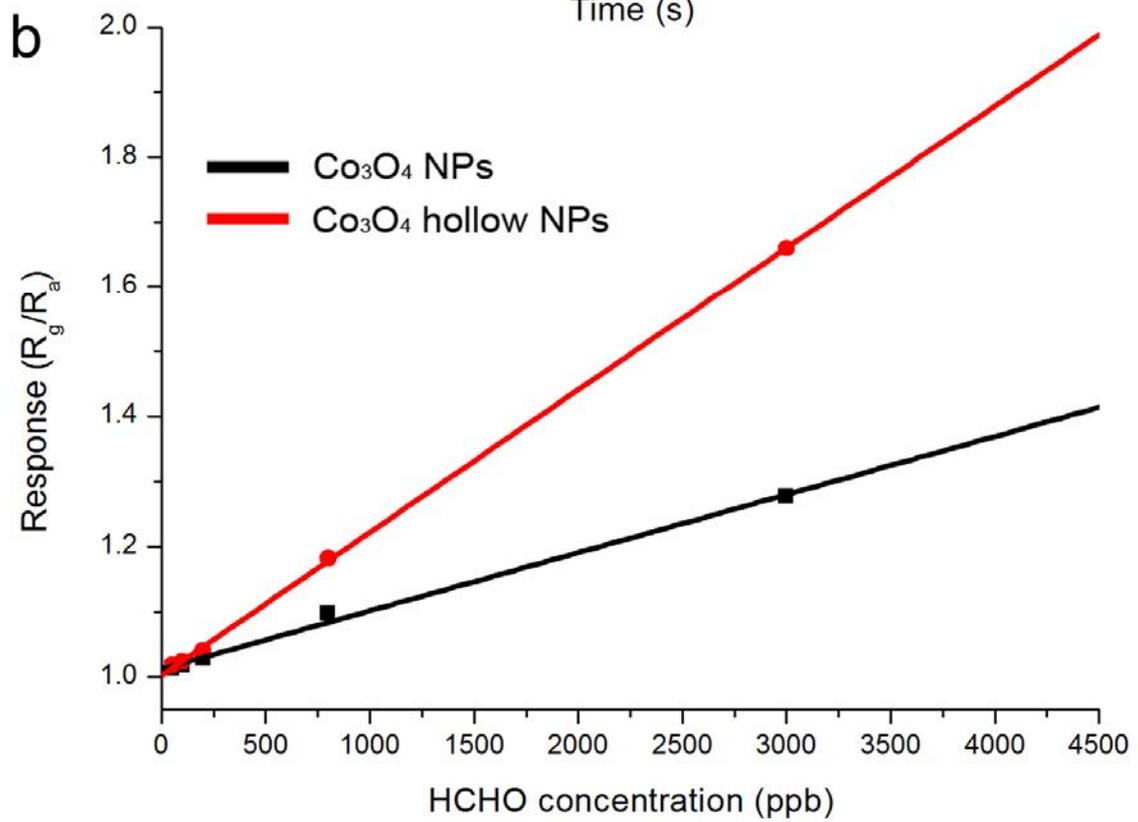
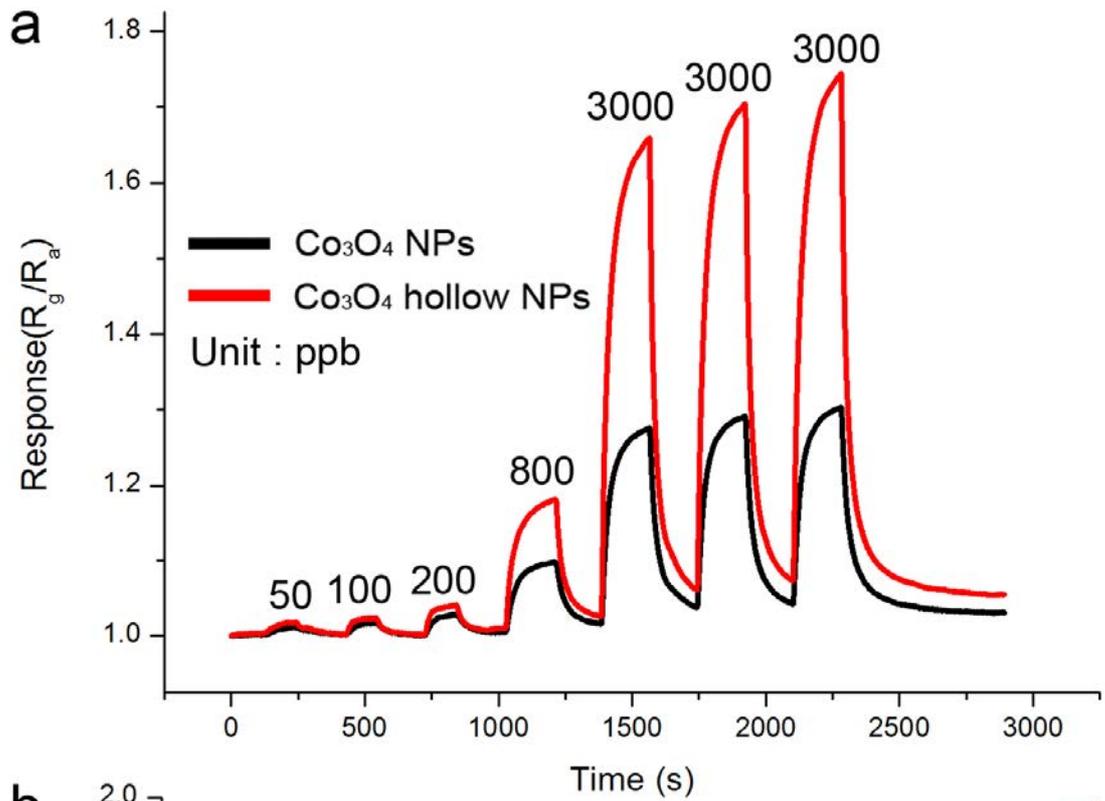
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Co_3O_4 nanocrystal-aggregated hollow nanostructure for high sensitive aldehyde gas sensor

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한국과학기술원(KAIST) 화학과 ¹한국전자통신연구원 바이오메드연구실 ²한국전자통신연구원 (ETRI) 바이오메드팀

Formaldehyde is an industrial chemical that is widely used to manufacture building materials and numerous household products. Formaldehyde has a great impact on human health, because of its potentially carcinogenic and mutagenic properties and its capability of forming intermediate and stable species of toxic and phototoxic radicals. The World Health Organization has set a standard for safe exposure of 0.1 mg/m^3 averaged over 30 min. However, the traditional techniques to detect HCHO (such as based on gas chromatographs, mass spectroscopy, FTIR analysis, etc.) are often costly, time-consuming and cannot realize real-time measurements. In this study, we fabricate Co_3O_4 hollow nanostructure by removing ZnO part from ZnO@Co(OH)_2 core-shell nanostructure. The synthesized Co_3O_4 hollow nanoparticles were used for semiconductor type gas sensor for HCHO detection. The sensor showed responses to formaldehyde gas at sub ppm, as a function of operating temperatures and gas concentrations. The lowest detection limit is HCHO 50 ppb. Also, we used benzene, nitrogen dioxide, and carbonmonoxide for test the gas sensor's selectivity.



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장소: 창원CECO

발표코드: INOR.P-207

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Germanium and Antimony Chalcogenides Nanomaterials by Thermal Decomposition of Metal Precursors for Phase Change Random Access Memory Device

김효숙 박보근^{1,*} 손성욱* 김창균^{1,*} 정택모^{2,*}

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“Phase-change” applications utilize differences in optical or electrical properties between the crystalline and amorphous phases of the same materials. Two metal chalcogenide materials like germanium antimony telluride (GST) are predominantly one of the most potential candidates for phase change random access memory (PRAM) device. Moreover, some electronic devices as PRAM using them have been already produced using atomic layer deposition by electronic companies in some countries. An alternative route to germanium antimony chalcogenide materials was investigated by thermal decomposition of the molecular precursors combination of germanium telluride and antimony telluride. The studies include the facile preparation, structural characterization, and spectroscopic analysis of the new precursors of germanium as well as antimony. In this presentation, we will discuss synthesis and characterization of new metal chalcogenide precursors such as germanium and antimony on the basis of molecular design. Also the application of the precursors for the preparation of chalcogenide materials containing germanium and antimony by thermal decomposition method at comparatively low temperature will be disclosed.

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발표코드: **INOR.P-208**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Alloy Formation for the Growth of Atomic Layers of MoS₂

송인택 최희철*

포항공과대학교 화학과

Semiconducting transition metal dichalcogenides (TMDCs) have become one of the most significant materials in nanoelectronics as an alternative to graphene. The lack of growth method to accomplish all of scalability, uniformity, and patternability, however, hinders further development and study of this nanomaterial. Herein in this presentation, we present a novel way to prepare atomic layers of MoS₂ by chemical vapor deposition using surface alloy. In addition, we demonstrate that atomic layers of MoS₂ can be grown in specific patterns by simply defining the pattern of underneath metal catalyst film. We used Raman spectroscopy and atomic force microscopy (AFM) to confirm that our sample is composed of continuous few layers of MoS₂. HRTEM and X-Ray photoelectron spectroscopy (XPS), and device fabrication measurement were used for the characterization. Combined study of XPS and AFM as well as literature study on STM characterization of alloy-analogues have confirmed the successful formation of highly confined surface alloy.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Ruthenium Precursors for Electronic Device using Chemical Vapor Deposition

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한국화학연구원 화학소재연구본부 ¹한국화학연구원 화학소재연구단

Ruthenium (Ru) has attractive material properties for semiconductor microelectronic devices applications, such as a low resistivity ($7.1 \mu\Omega\text{cm}$ in the bulk), a high work function of 4.7 eV, and feasibility for the dry etch process. Ru is also chemically stable toward oxygen, forming a stable and conductive oxide, RuO₂ (Resistivity: $20 \mu\Omega\text{cm}$ in the bulk). Thus, it has been widely investigated, as an electrode for the capacitor in dynamic random access memory (DRAM), as a gate for metal-oxide semiconductor transistors, and as a seed layer for Cu metallization. Due to the continuous shrinkage of devices, better deposition processes for Ru thin films are critically required with excellent step coverages in high aspect ratio (AR) structures. In these respects, atomic layer deposition (ALD) is a viable solution for preparing Ru thin films because it enables atomic-scale control of the film thickness with excellent conformality. A recent investigation reported that the nucleation of ALD-Ru film was enhanced considerably by using a zero-valent metallorganic precursor, isopropyl-methylbenzene-cyclohexadiene Ru(0) (IMBCHRu, C₁₆H₂₂Ru) and O₂ molecules, compared to the utilization of precursors with higher metal valences. In this study, we investigated new zero-valent Ru metallorganic precursor, and characterized by NMR, elemental analysis and TGA/DTA.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Template-Free Vertical Crystallization of Fullerene Molecules (C_{60}) by Solvent Vapor Annealing

김정아 박치범 박지은 최희철*

포항공과대학교 화학과

Vertical alignment of organic structures attracts much attention for photonic sensing device, flexible light emitting device, high surface area solar cell, superhydrophobic surface and so forth. Despite its importance, it has rarely been reported about obtaining vertically grown structures of organic materials compared with inorganic materials which have totally different characteristics of organic materials. For this reason, a new kind of method for vertical growth of organic structure is required, and it has high scientific importance, either. We used fullerene (C_{60}) which continuously attracts attention due to not only its unique structure, but also its electrical and optical properties. Especially, it is already reported that various morphologies of C_{60} nanocrystals could be synthesized by facile synthetic methods such as LLIP or drop-drying. However, these methods have limit to control the growth direction which should be random or lateral to the substrate. To overcome this limitation, we applied SVA process as a method for minimizing lateral force and maximizing vertical force generated by solvent movement. As a result, we successfully crystallized C_{60} molecules into vertical nanowires on the substrate without any templates. Vertically grown C_{60} structures have been confirmed by scanning electron microscopy (SEM) and structural analysis has been done by X-ray diffraction (XRD) data and selected area electron diffraction (SAED) patterns. Proposed mechanism of vertically crystallized C_{60} nanowires will also be discussed.

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발표코드: **INOR.P-211**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In situ observation of H-D exchange in LiBD₄-MgH₂-MWCNT composite by neutron diffraction measurement

조인화 강승기 이희주 최용남*

한국원자력연구원 중성자과학연구부

LiBH₄-MgH₂ composite is a promising candidate for overcoming obstacles of LiBH₄ (high dehydrogenation temperature and extreme conditions for hydrogen uptake etc.) to be exploited as on-board hydrogen storage material. The composite has been known that the total enthalpy change of the reaction is reduced by forming MgB₂ and LiH as final products. However, overall reaction rate remains slow which is partly attributed by raising the decomposition temperature of MgH₂. To elucidate controversial dehydrogenation mechanism of the system clearly, we measured in situ neutron diffraction patterns of isotope-labeled ⁷Li₁₁BD₄-MgH₂(-MWCNT) composite varying temperatures. Based on the report of hydrogen exchange effect between LiBH₄ and MgH₂ on decomposition of MgH₂ [1], we are trying to show how much hydrogen exchange occurs from results of neutron diffraction, TG-MS, and x-ray diffraction.[1] L. Zeng et al., J. Phys. Chem. C, 114 (2010), 13132

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발표코드: **INOR.P-212**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Temperature Evolution of the Spin Structure in $\text{Cu}_3(\text{BTC})_2$ (HKUST-1)

이희주 최용남* 최상범¹ 김자현¹

한국원자력연구원 중성자과학연구부 ¹승실대학교 화학과

Two adjacent copper ions (distance is ~ 2.68 Å) are coupled with each other via direct exchange interaction (energy splitting, $J \sim 300$ cm^{-1}). The eigen states of this exchange coupled spin system are composed of a singlet state (ground) and a triplet state (excited). At room temperature, all the dimers lie in the triplet states ($S=1$). At low temperature, the spin systems transformed into the ground state ($S=0$). The nearest spin dimers are connected by a 1,3,5-benzenedicarboxyl ligand and their distance is ~ 9.3 Å. Four nearest spin dimers lie on the middle edges of a tetrahedron and a superexchange interactions between them are expected. Electron Spin Resonance with a temperature variation (4~300K) and magnetic susceptibility data, $\chi(T)$, will be presented and discussed in terms of its spin structures.

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발표코드: **INOR.P-213**

발표분야: 무기화학

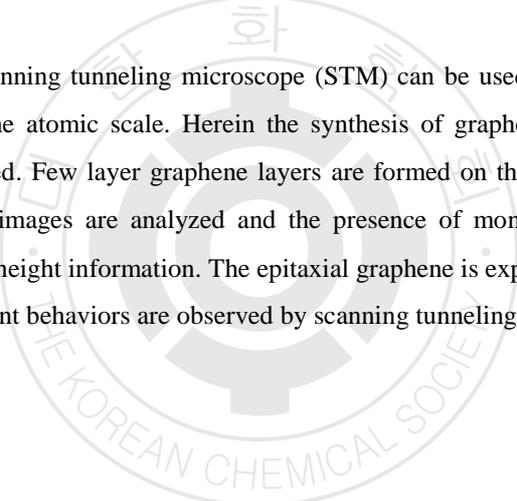
발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidized epitaxial graphene on SiC(0001) analyzed by STM

김태수 최희철*

포항공과대학교 화학과

it is recently shown that scanning tunneling microscope (STM) can be used to study various electronic properties of graphene at the atomic scale. Herein the synthesis of graphene under ultrahigh vacuum (UHV) condition is presented. Few layer graphene layers are formed on the SiC substrate heated up to 1200°C. STM topographic images are analyzed and the presence of monolayer and bilayer epitaxial graphene is confirmed from height information. The epitaxial graphene is exposed to oxygen molecules to induce oxidation, and different behaviors are observed by scanning tunneling spectroscopy (STS).



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장소: 창원CECO

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Nickel Sulfide Precursor

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Nickel sulfide (NiS) have attracted much attention owing to their potential applications as transformation-toughening agent for materials used in semiconductor applications, catalysts, and cathodic materials in rechargeable lithium batteries. Recently, single source precursor chemistry has attracted considerable interest for the growth of semiconductor thin films and nanoparticles. Herein we report on the synthesis and characterization of new nickel sulfide complex with designed aminothiolate ligand, and show up thermal decomposition of novel complex. The novel complex has been characterized by means of ¹H-NMR, elemental analysis, thermo gravimetric analysis (TGA), and thermal decomposition of novel complex X-ray Diffraction (XRD) and scanning electron microscope (SEM).

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장소: 창원CECO

발표코드: INOR.P-215

발표분야: 무기화학

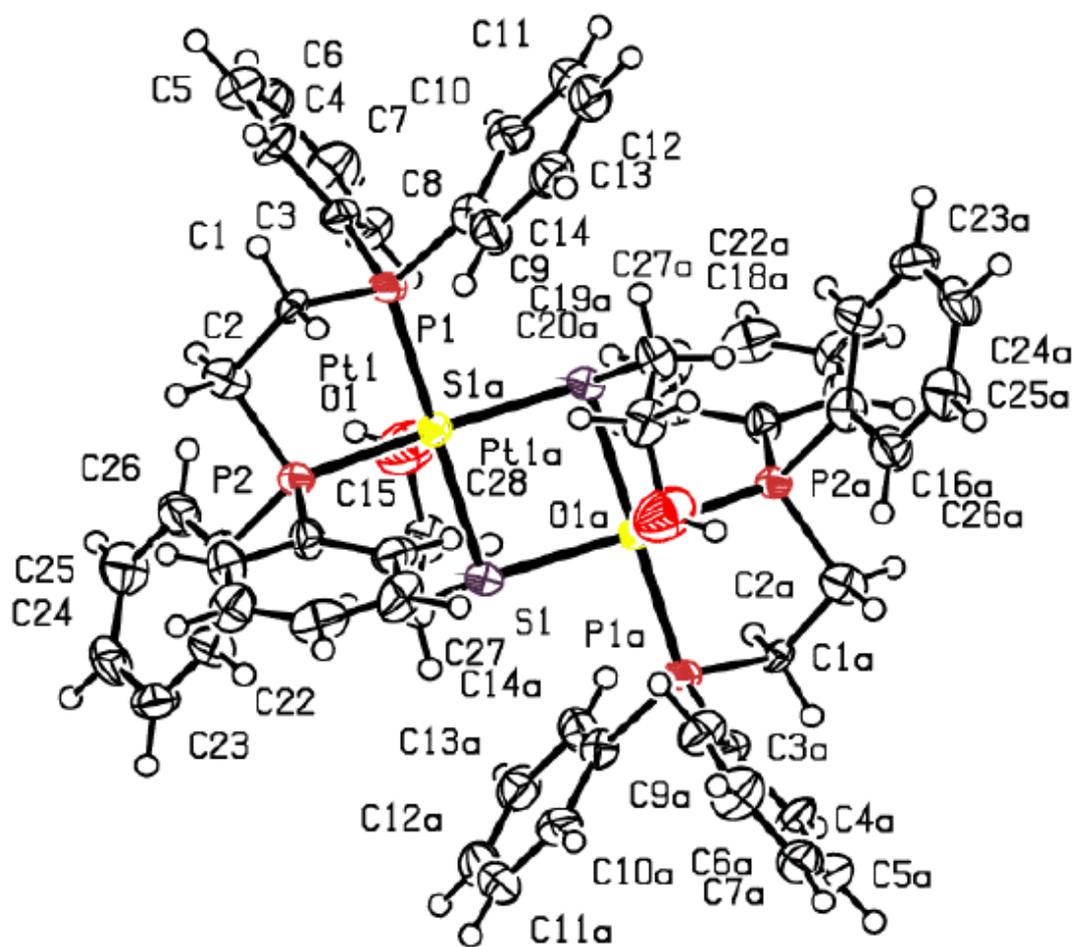
발표종류: 포스터, 발표일시: 수 16:00~19:00

**Diphosphine-dependent Oxidative Dimerization of
(diphosphine)Pt(SEtOH)₂ where diphosphine = dppe (1,2-
bis(diphenylphosphino)ethane) and dppf (1,1'-
bis(diphenylphosphino)ferrocene)**

전효경 노동윤*

서울여자대학교 화학과

The oxidative dimerization process of (dppe)Pt(SEtOH)₂ (dppe = 1,2-bis(diphenylphosphino)ethane) afforded dicationic bimetallic Pt(II) complex formulated as [(dppe)Pt(μ-SEtOH)₂Pt(dppe)]²⁺ (Fig.1). On the other hand, the reaction of (dppf)Pt(SEtOH)₂ (dppf = 1,1'-bis(diphenylphosphino)ferrocene) with the oxidizing reagent (TCNQ) led to an unsymmetrical cationic Pt(II) complex, formulated as [(dppf)Pt(μ-S)(μ-SEtOH)Pt(dppf)]⁺ based on the elemental analysis. The differences of crystal morphology, color, and physical properties between two complexes will be presented. (NRF 2013-0011478)



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발표코드: INOR.P-216

발표분야: 무기화학

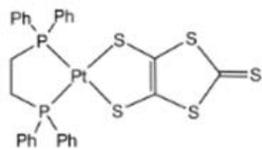
발표종류: 포스터, 발표일시: 수 16:00~19:00

**>C=S...Hg(II) Interactions in (dppe)Pt(dmit) / Hg(II)X₂ System
(dppe:bis(diphenylphosphino)ethane, dmit: 1,3-dithiolo-2 thione-4,5
dithiolate)**

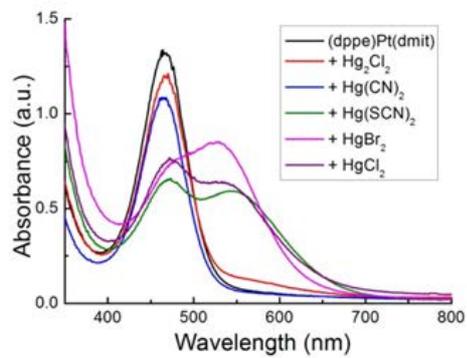
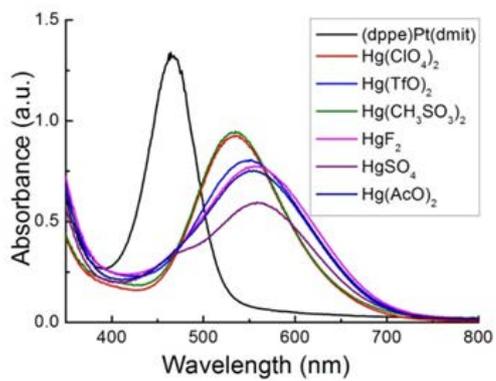
전소희 노동윤*

서울여자대학교 화학과

The terminal >C=S group in dmit (1,3-dithiolo-2thione-4,5dithiolate) ligand of (dppe)Pt(dmit) (dppe: bis(diphenylphosphino)ethane) is obviously known to be coordinated by Hg(II) ion. This is clearly shown by the bathochromic shift of the band for $\pi \rightarrow \pi^*$ transition in H₂O/CH₃CN solution. The band shifts are strongly anion (X⁻)-dependent: when an equimolar of Hg(II)X₂ (X = AcO⁻, ClO₄⁻, TfO⁻, CH₃SO₃⁻, 1/2SO₄²⁻, F⁻) is added, an obvious bathochromic shift is observed due to a strong >C=S...Hg(II) interaction. In contrast, no band shift (X = CN) or a mixed state (X = SCN, Br, Cl) is observed (Fig.1), possibly due to the stronger interaction between Hg(II) and four anions (X = CN, SCN, Br, Cl). These results are likely related to the binding constant of Hg(II) ions with (dppe)Pt(dmit). The binding constant was determined by UV/vis spectroscopic method. The results on the binding constant for each HgX₂, together with the absorption results, are to be presented. (NRF2013-0011478)



(dppe)Pt(dmit)



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장소: 창원CECO

발표코드: INOR.P-217

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Morphological Diversity of Mn(III) Metalloporphyrin-Based Nano- and Microsize CPAs Assembled via Kinetic and Thermodynamic Controls and Their Application in Heterogeneous Catalysis

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고려대학교 화학과

Porous coordination polymers (PCPs), also called metal-organic frameworks (MOFs) for three-dimensional (3D) PCPs, have received much attention due to their potential applications. Currently, nano- and micro-sized PCPs (nPCPs or mPCPs) have often been reported with promising applications. Their novel and/or enhanced performances are frequently reported with potential applications in catalysis, separation, gas storage, drug delivery, biosensing, and imaging. Particularly, metalloporphyrins would be good building blocks for the construction of such functional materials because of their unique structure evidenced by a wide range of molecular architectures, such as molecular boxes, self-assembled arrays, and PCPs with various applications in catalysis, gas storage, and separation. In particular for the catalysis application, the utilization of PCPs would be the best strategy in order to avoid catalyst degradation via μ -oxo dimer formation of metalloporphyrin-based homogeneous catalysts. So we describe herein the preparation and use as heterogeneous catalysts of Mn(III) metalloporphyrin that contain size-controlled amorphous and crystalline nano- and micro-sized coordination polymer aggregates (CPAs). Particularly, we focused on the conversion of kinetically controlled amorphous assemblies into thermodynamically controlled crystalline structures based on the self-assembly of a (porphyrin)Mn(III) biscarboxylic acid and $\text{Co}(\text{OAc})_2$.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A metastable zeolitic imidazolate framework and its structural transformation

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승실대학교 화학과 ¹승실대학교 의생명시스템학부

Zeolitic imidazolate frameworks (ZIFs) are composed of tetrahedral metal centers, mainly zinc ions, and imidazolate linkers. As their connection mimics the Si-O-Si bent bonds of zeolites, the resulting ZIF networks resemble zeolite structural types. Until now, about 40 ZIF network types are known to exist. Most ZIFs have large structural and chemical stability while some of them undergo structural transformation at elevated temperature and pressure. Herein we report a new ZIF which adopts ilc net. Although this ZIF-ilc is obtained as single crystals, it easily converts into ZIF-61 (zni net) in common solvents. The crystal structure of ZIF-ilc is presented in comparison with that of ZIF-61.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A microporous metal-organic framework containing zinc and calcium mixed-metal centers

노경규 오유진 홍지수 김자현 박상연^{1,*}

승실대학교 화학과 ¹승실대학교 의생명시스템학부

A new metal-organic framework, ZnCaBTB was built from mixed-metal (Zn(II)/Ca(II)) trinuclear clusters and benzene-1,3,5-tribenzoate (BTB). A cluster consists of two tetrahedral zinc ions and one octahedral calcium ion. The crystal structure shows that BTBs connect in pairs both Zn(II) and Ca(II) ions to form honeycomb-like two-dimensional layers. These layers are stacked alternatively through efficient π -stacking of the BTBs. The evacuated ZnCaBTB was stable under vacuum, and could adsorb nitrogen gas.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cu^{II} complex with Tetrathiafulvalene bis (4 (5) Carboxy-1, 3-dithiolidene)

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경북대학교 화학과

Tetrathiafulvalene (TTF) and its derivatives are well-established organic π donors which have been extensively studied for various applications, in particular, in the field of conducting organic materials involving intermolecular charge-transfer interactions with various π -accepting molecules. A variety of mono- or polydentate coordinating functional groups have been attached to the TTF moiety, and the corresponding metal complexes have been reported. In this study, we have done the synthesis of the transition metal coordination polymer containing a tetrathiafulvalene (TTF) moiety substituted with a dicarboxylic group of the formula [CuL] BCDT-TTF (L = 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hezaazacyclotetradecane) (BCDT = Bis(4,5-carboxy-1,3-dithiolidene). It has been characterized by various analytical methods.

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발표코드: **INOR.P-221**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Water vapor adsorption in amine-functionalized UiO-67

고낙은 유래경 최판규 양진국*

승실대학교 화학과

Absorbents for heat transformation applications demand large water adsorption-desorption at a pressure range of $P/P_0 = 0.1 \sim 0.3$, and naturally high stability in water vapor. The UiO series of MOFs, which consist of Zr ions and linear aromatic carboxylates, can meet these requirements. We have synthesized a new Zr-MOF (UiO-67-NH₂) which has a same structure as the well-known UiO-67 formulated as Zr₆O₄(OH)₄(BPDC)₆ (BPDC = biphenyl-4,4'-dicarboxylate). Water adsorption isotherms for these MOFs indicate that the amine-functionalization can make the water uptake of UiO-67-NH₂ happen in the desired pressure range with capacity of 0.15 g H₂O/gMOF.

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발표코드: **INOR.P-222**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluoro-functionalized HKUST-1 metal-organic framework and its gas adsorption behavior

교낙은 김태민¹ 여미소 김자현 박상연^{2,*}

숭실대학교 화학과 ¹숭실대학교 ²숭실대학교 의생명시스템학부

HKUST-1 formulated as Cu_3BTC_2 (BTC = benzene-1,3,5-tricarboxylate) is one of the most studied MOFs. We prepared a fluoro-functionalized form (CuBTC-F) of HKUST-1 by a solvothermal reaction between $\text{H}_3\text{BTC-F}$ and copper nitrate. Activated CuBTC-F showed a BET surface area of $1404 \text{ m}^2/\text{g}$, and resulted in an increased amount of carbon dioxide adsorption at 298K by ca. 10 % compared with that of more porous HKUST-1. CuBTC-F could uptake hydrogen up to ca. 2 wt% at 77K and 1 bar.

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발표코드: INOR.P-223

발표분야: 무기화학

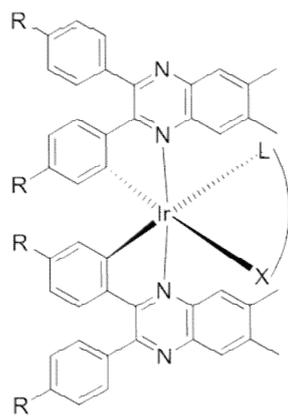
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Red Phosphorescent Heteroleptic Ir(III) Complexes Based on 2,3-Diphenylquinoxaline Derivatives

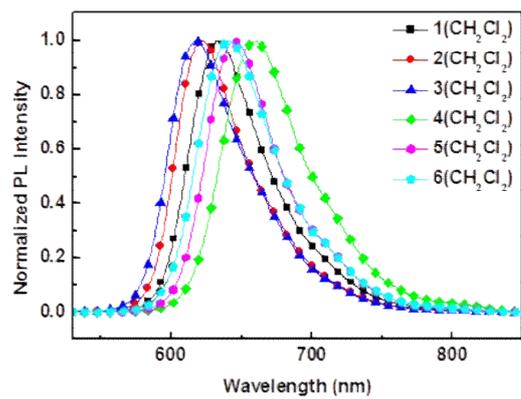
윤성재 송영광¹ 강성권² 김영인^{3,*}

부산대학교 첨단정보및디스플레이소재협동 ¹부산대학교 첨단정보 및 디스플레이소재협동과
정 ²충남대학교 화학과 ³부산대학교 화학교육과

Recently, the iridium(III) complexes chelated with a 2,3-diphenylquinoxaline ligand (dpq) were reported to exhibit deep red phosphorescence at 677 nm. Herein, we have designed and synthesized new red phosphorescent iridium(III) complexes using diphenylquinoxaline derivatives. Variation of the substituents in the 2,3-diphenylquinoxaline ligand backbone led to tune the emission color. The 2,3-bis(4-fluorophenyl)-6,7-dimethylquinoxaline (dfpdmq) and 2,3-bis(4-methylphenyl)-6,7-dimethylquinoxaline (dmpdmq) were synthesized as main ligands and acetylacetonate (acac), 1,1,1-trifluoro-2,4-pentanedione (tfacac) and picolinic acid (pic) were used as ancillary ligands in phosphorescent heteroleptic Ir(III) complexes; (dfpdmq)₂Ir(acac) (1), (dfpdmq)₂Ir(tfacac) (2), (dfpdmq)₂Ir(pic) (3), (dmpdmq)₂Ir(acac) (4), (dmpdmq)₂Ir(tfacac) (5) and (dmpdmq)₂Ir(pic) (6). The complexes exhibited the photoluminescence peaks at 618 ~ 659 nm and quantum yields of 16 ~ 57% in CH₂Cl₂ solution.



- (1) R=F, L[^]X= acac
- (2) R=F, L[^]X= tfacac
- (3) R=F, L[^]X= pic
- (4) R=H, L[^]X= acac
- (5) R=H, L[^]X= tfacac
- (6) R=H, L[^]X= pic



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-224

발표분야: 무기화학

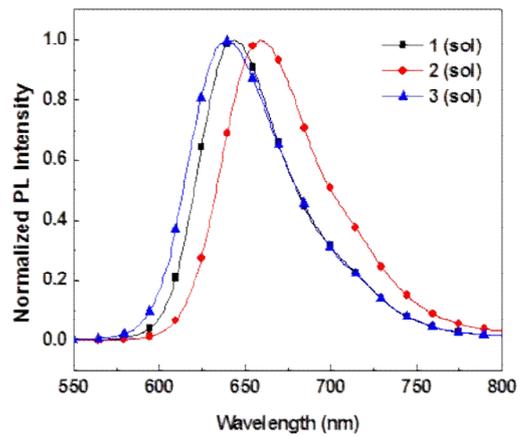
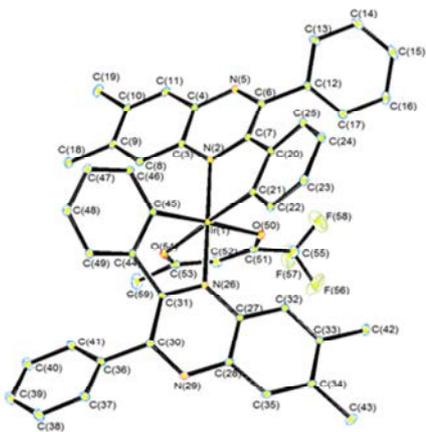
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Red Phosphorescent Iridium(III) Complexes Based on 6,7-Dimethyl-2,3-diphenylquinoxaline for Organic Light-Emitting Diodes (OLEDs) : The Effects of the Ancillary Ligand

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부산대학교 첨단소재화학협동과정 ¹부산대학교 화학교육과 ²부산대학교 화학교육학과 ³충남대학교 화학과

The phosphorescent OLEDs exhibit highly efficient electroluminescence, which significantly exceeds the accepted theoretical limitation of the external quantum efficiency (η_{ex}), 5%, for conventional fluorescence-based OLEDs. The cyclometalating ligands for efficient red phosphorescent iridium(III) complexes were synthesized and characterized ; (dmdpq)₂Ir(L^X), where dmdpq = 6,7-dimethyl-2,3-diphenylquinoxaline and L^X = ancillary ligand such as 1,1,1-trifluoro-2,4-pentanedione, tfacac (1), acetylacetonone, acac (2) and picolinic acid, pic (3). The structures were determined using single crystal X-ray method and revealed that complex 1, 2 and 3 adopted distorted octahedral geometries around iridium metal ion with cis-C, C and trans-N, N positions. The phosphorescence properties of complexes 1~3 showed red emission at 600~639 nm in PL spectra and exhibited quantum yield of 28~41 % in dichloromethane solution. Compounds 1~3 showed a red-shift in the order of 3<1<2.



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발표코드: INOR.P-225

발표분야: 무기화학

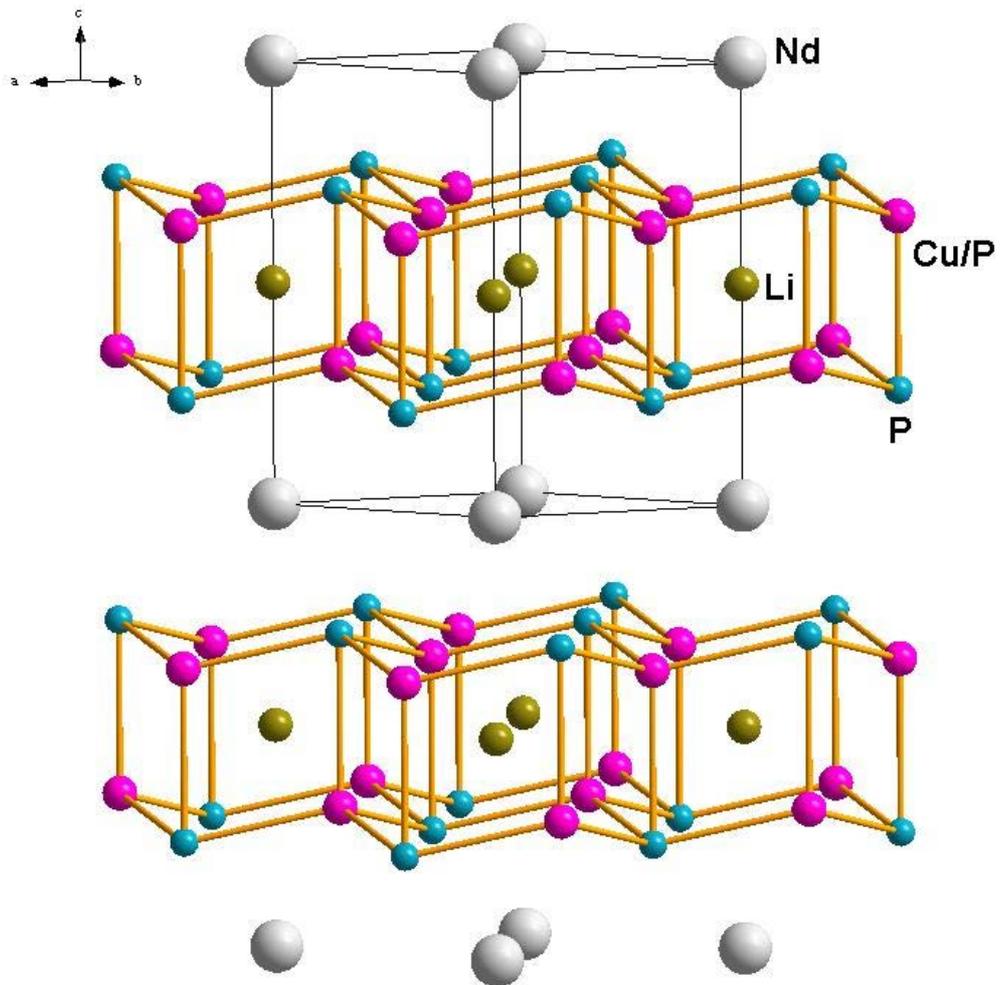
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Series of Novel Rare-Earth Metal Containing Phosphides: $RELi_{1+x}Cu_{2-y}P_{2-x+y}$ ($RE = La, Nd$ and Gd)

장은영 유태수*

충북대학교 화학과

Three quaternary rare-earth metal phosphides $RELi_{1+x}Cu_{2-y}P_{2-x+y}$ ($RE = La, Nd, Gd$) have been successfully synthesized with a potential thermoelectric application in mind. The high temperature synthetic method using Nb-ampoules was exploited, and the crystal structures were characterized by powder and single crystal X-ray diffractions. They adopt the trigonal $LaLi_3Sb_2$ -type structure (space group $P3-m1$, Pearson symbol $hP6$) with the mixed-occupation of Cu and P at the $2d$ site. The lattice parameters are as follows: $a = 4.0967(15) \text{ \AA}$, $c = 6.7961(32) \text{ \AA}$ for $LaLiCu_{1.53}P_{2.47}$, $a = 4.0614(1) \text{ \AA}$, $c = 6.7023(3) \text{ \AA}$ for $NdLiCu_{1.23}P_{2.77}$, and $a = 4.0240(2) \text{ \AA}$, $c = 6.5966(4) \text{ \AA}$ for $GdLi_{1.16}Cu_{1.07}P_{2.78}$. The crystal structure of $RELi_{1+x}Cu_{2-y}P_{2-x+y}$ can be described as a combination of the 2-dimensional (2D) layers of $[Li_{1+x}Cu_{2-y}P_{2-x+y}]$ and the space-filling cations located between 2D layers. In particular, the layered structure can further be considered as an assembly of two puckered hexagonal layers including Cu/P and P connected along the c -axis direction. The voids located in between double corrugated hexagonal layers are occupied by Li atom, and the cationic site is surrounded by three Cu/P mixed-sites and three P atoms forming a distorted-octahedral environment. Theoretical investigations have been conducted based on a structural model with an ideal composition of $NdLiCuP_3$ using TB-LMTO-ASA method. Electronic structure was further studied based on the analyses of DOS and COHP curves.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-226

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Sonochemical Synthesis of High Performance Core-Shell Fluorescent Nanocrystals Containing Non-toxic Silver, Indium, Zinc, Sulfur Components

정종진 이승재¹ 박자영 장혜미 박정규^{2,*}

한국화학연구원 나노기술융합연구단 ¹연세대학교 화학과 ²한국화학연구원 형광물질연구팀

ZAIS - (Zn_xAg_yIn_z)S₂ - fluorescent nanoparticle has been developed to replace II-VI quantum dots (QDs) due to its cadmium free non-toxic nature, and facile synthesis of the nanocrystal library by ultrasonic and combinatorial chemistry. Although ZAIS shows better fluorescence intensity than QD without photoblinking, it is necessary to enhance its brightness and quantum efficiency for the expansion of its uses, from a cell imaging probe to LED and cosmetic dyes. Here, we developed a rapid and facile synthesis method of ZnS shell surrounding ZAIS nanoparticle core through ultrasonic chemistry. After adding zinc and sulfur sources to as-prepared ZAIS core in TOP (trioctylphosphine) and ODE (octadecene) solution mixture, ZnS shell was successfully formed around two different types of ZAIS cores ? ZAIS 57: (Zn_{0.0}Ag_{0.3}In_{0.7})S₂: red and ZAIS 59: (Zn_{0.2}Ag_{0.1}In_{0.7})S₂: green, respectively, following the sonication for 10 minutes with an appropriate power. ZnS shells raise their fluorescence intensity up to five or ten times because the sonochemical shell synthesis prevents a lattice mismatch between core and shell, and interface strain due to increasing thickness of shells. Moreover, the quantum efficiency of ZAIS-ZnS core-shell nanoparticle increases dramatically from 0.13 to 0.81 in chloroform. For the further application as a bioimaging probe and cosmetic dyes, we prepared MPA (mercaptopropionic acid) coated ZAIS-ZnS core-shell nanoparticle to make it dispersed in physiological solution. The population of breast cancer cell didn't change due to the less-toxic nature of ZAIS-ZnS nanoparticles although high concentration of nanoparticles were added (200 µg/ml).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-227**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel rare-earth oxides Precursor

이의진

한국화학연구원 화학소재연구본부

The rare-earth oxides M_2O_3 ($M=La, Pr, Gd$) are good insulators due to their large band gap (3.9eV for Pr_2O_3 , 5.6eV for Gd_2O_3), they have high dielectric constants (Gd_2O_3 $K=16$, La_2O_3 $K=27$, Pr_2O_3 $K=26-30$) and, compared to ZrO_2 and HfO_2 , they have higher thermodynamic stability on silicon making them very attractive materials for high-K dielectric applications. Another attractive feature of some rare-earth oxides is their relatively close lattice match to that of silicon, offering the possibility of epitaxial growth and eliminating problems related to grain boundaries in polycrystalline films. Metal-organic chemical vapor deposition (MOCVD) has been preferred to PVD methods because of the possibility of large area deposition, good composition control and excellent conformal step coverage. Herein we report on the synthesis of rare-earth oxide complexes with designed alkoxide and aminoalkoxide ligand. These novel complexes have been characterized by means of FT-IR, elemental analysis, and thermogravimetric analysis (TGA).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **INOR.P-228**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemical Probes for Selective Fluorescence Assay of Aluminum Ions

김진홍* 김수진 이가예 강희경

이화여자대학교 화학·나노과학과

The frequent use of aluminum foil, vessels, and trays for convenience might moderately increase the Al^{3+} concentration in food. After absorption, aluminum will become distributed to all tissues in humans and animals, and accumulates in the bone. The iron binding protein is the main carrier of Al^{3+} in plasma and Al^{3+} can enter the brain and reach the placenta and fetus. Al^{3+} may persist for a very long time in various organs and tissues before it is excreted in the urine. Al^{3+} has been implicated as a causative factor in Alzheimer's Disease and has been associated with damage to the central nervous system in humans. In this study, A phenol-pyridylimine probe was utilized as an optical sensor to quantify the presence of aluminum ions using a turn-on fluorescence enhancement approach. The high sensitivity was the result of FRET amplification of the receptor subunit fluorescence emission. The complex stability constant (K_s) for the stoichiometric 1:1 complex of the sensor with aluminum ions was obtained by fluorimetric titration. Remarkably, fluorescence output was not significantly affected by other trivalent cations, particularly Ga^{3+} and In^{3+} .

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-229

발표분야: 무기화학

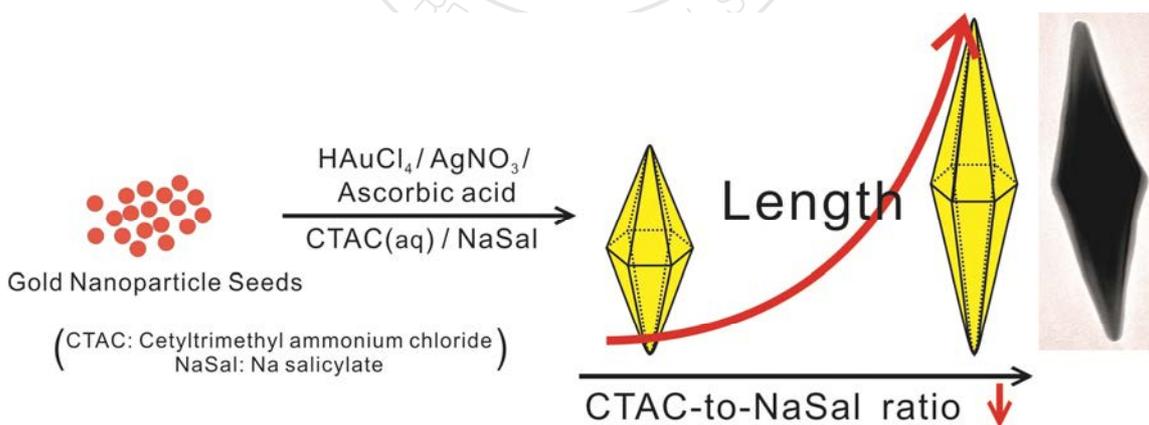
발표종류: 포스터, 발표일시: 수 16:00~19:00

Size-controlled synthesis of gold bipyramids using an aqueous mixture of CTAC and salicylate anions as the soft template

유효종

한림대학교 자연과학대학 화학과

One-dimensional (1D) gold (Au) bipyramids are successfully synthesized through a facile seed-mediated method using cetyltrimethylammonium chloride (CTAC), Au seed nanoparticles, Ag^+ ions, and ascorbic acid. The length and optical properties of the synthesized Au bipyramids are controlled with precision by varying the amount of salicylate anions (Sal⁻) added during the synthesis. The micelles formed from CTA^+ -Sal⁻ mixtures in aqueous solutions act as effective templates for the size-controlled synthesis of 1D nanocrystals.



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발표코드: **INOR.P-230**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nonionic Surfactant-Assisted, Seed-Mediated Synthesis of Gold Nanotoroids

유효종

한림대학교 자연과학대학 화학과

Recently, syntheses of unique Au microcrystals using nonionic Brij surfactants, which are used as reducing, capping, and structure directing agents, have been reported by our research group. Triangular or hexagonal crystalline Au microrings were synthesized using a $\text{Au}^{\text{n}+}$ precursor and nonionic Brij35 $((\text{C}_2\text{H}_4\text{O})_{23}\text{C}_{12}\text{H}_{25}\text{OH})$ surfactant in aqueous solution. Hexagonal multilayered Au spirangles were also synthesized in a controllable fashion and in high yields, through a simple process in Brij 700 $((\text{C}_2\text{H}_4\text{O})_{100}\text{C}_{18}\text{H}_{37}\text{OH})$ aqueous solution. Herein, we report a novel and simple solution-based seed-mediated method using the nonionic Brij35 surfactant to synthesize Au nanotoroids with ring-like structures and vacancies at their center. The relative amount of 2 nm Au seed nanoparticles significantly affected the formation yield of Au nanotoroids and the morphologies of the resulting Au nanostructures. Using the Au seed nanoparticles solution in the optimal range of 50 ~ 200 μL led to the formation of Au nanotoroids in high yield. Mechanistically, the Au nanotoroids may have originated from the Brij35-assisted etching of the initially grown platelike intermediate Au nanoparticles, which in turn could have been generated from the inner holes as defects and the edges of the Au plates. Our investigation of the formation mechanism and optimization of the synthesis methods for Au nanotoroids can help in preparing other hollow noble metal nanomaterials with potential applications in a variety of fields.

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장소: 창원CECO

발표코드: **INOR.P-231**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Oxidation of Bio-based Compounds over Raspberry-Like Gold Nanoparticles (Au RLNPs)

서기욱 유효종^{1,*}

한림대학교 화학과 ¹한림대학교 자연과학대학 화학과

We successfully synthesized raspberry-like gold nanoparticles (Au RLNPs) in high yield through the reduction of HAuCl_4 by Brij 35 surfactant in basic conditions. The synthesized Au RLNPs possess high surface area, which is possibly useful structural factor for the catalytic applications. The unique, highly-red shifted surface plasmon resonances (SPRs) of Au RLNPs originate from the rough, raspberry-like surface of Au RLNPs. The generated Au RLNPs were stable in basic or neutral conditions, however show the structural changes in acidic conditions. In particular, the Au RLNPs showed high catalytic activities in the aerobic oxidations of a variety of biomass sources such as the conversion of 5-hydroxymethylfurfural (HMF). The improved catalytic activities compared with other Au nanoparticles are mainly due to the high surface area and stability in a basic condition. In addition, we also deposited Au RLNPs on the silica substrate for the easier recoveries and reusabilities in the repeated catalytic cycles. The effects of pressure, temperature, substrate to catalyst ratio, and pH were studied to find the most suitable reaction conditions for the highest catalytic results.

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발표코드: **INOR.P-232**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of Copper-based One-Dimensional Inorganic Polymer, $[\text{Cu}(\text{PDA})(\text{DMF})]_n$

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One-dimensional (1D) inorganic polymer, $[\text{Cu}(\text{II})(\text{PDA})(\text{DMF})]_n$ was successfully synthesized through the reaction of $\text{Cu}(\text{NO}_3)_2$ and 2,6-dicarboxylic pyridine (PDA) in dimethylformamide (DMF). X-ray crystal structure of this polymer shows that each building unit around a copper center has a 5-coordinate square pyramidal geometry. A tri-dentate chelating PDA and a DMF molecule are coordinate to a copper center. An oxygen atom in the carboxylate from the next building unit coordinates to the copper center, and this coordination repeats to generate the resultant 1D polymeric structure. As excess pyridine was added in the formation reaction, coordination of pyridine molecules instead of DMFs occurred to generate a different 1D inorganic polymer, $[\text{Cu}(\text{II})(\text{PDA})(\text{pyridine})]_n$. Interesting physical properties were observed from these 1D polymer crystals using spectroscopic techniques. The structure, reactivity and physical properties of the synthesized 1D inorganic polymers will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: INOR.P-233

발표분야: 무기화학

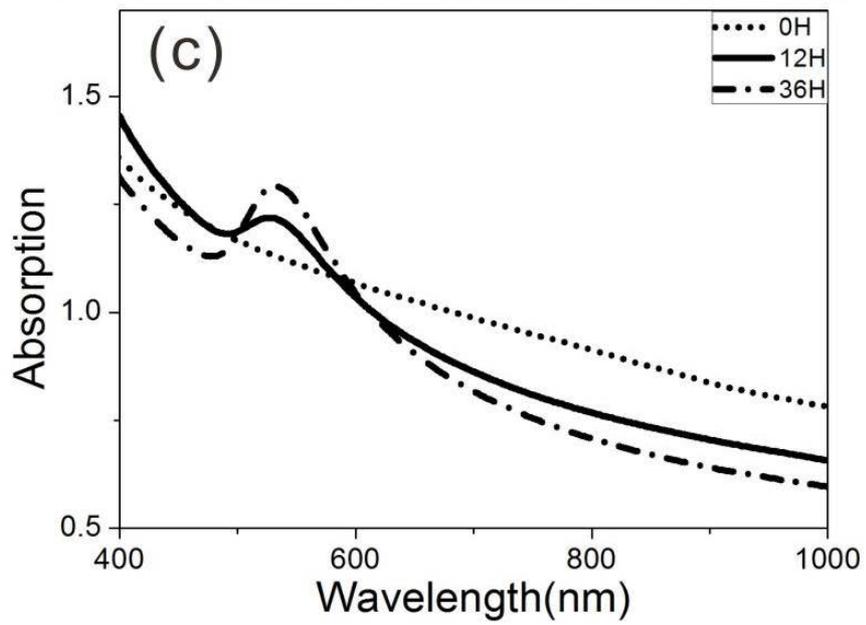
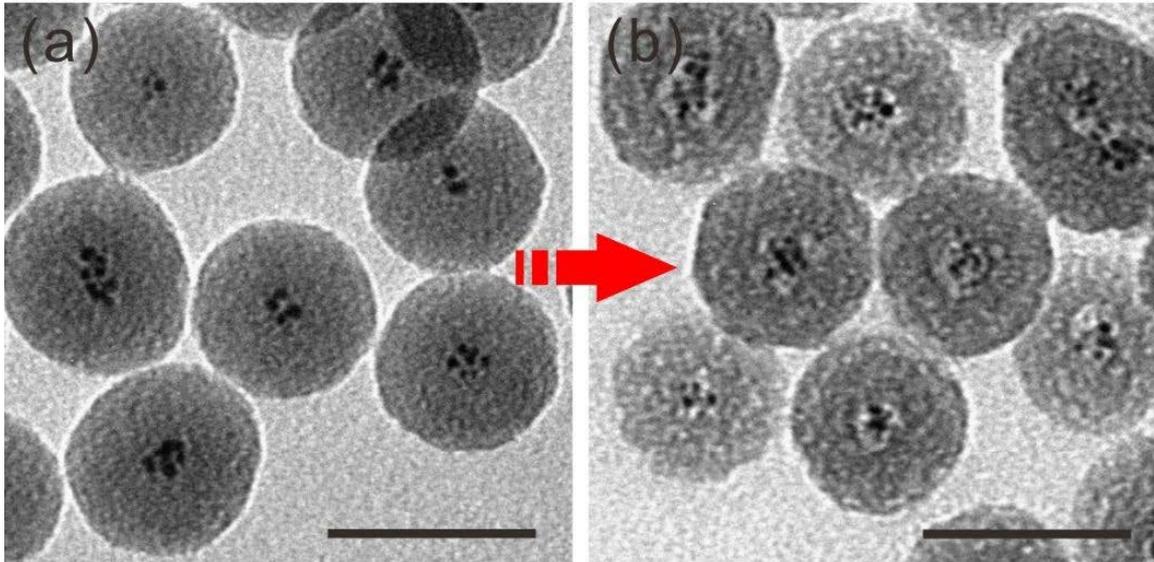
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis and catalytic application of spherical nanoparticles with a porous silica shell and multiple Au nanodots as the core

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Highly spherical nanoparticles with a core comprising multiple gold (Au) nanodots and a silica shell (multi-Au@SiO₂ NPs) 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 solution. Multiple Au nanodots with a maximum diameter of ~5 nm could be encapsulated within a silica matrix during the growth process. The size of the multi-Au@SiO₂ NPs and the number of Au nanodots doped could be controlled by varying the water-to-Brij35 ratio and the amount of the precursor of cationic gold ions. Further, the multi-Au@SiO₂ NPs could be softly etched by thermal treatments to give multiple Au nanodots core-mesoporous silica shell nanoparticles (multi-Au@mesoporous-SiO₂ NPs). By heating multi-Au@SiO₂ NPs in aqueous media, the mesopores were successfully generated over the silica shell without change of the size and number of multiple Au nanodots. The multi-Au@mesoporous-SiO₂ NPs showed much higher catalytic activity in the reduction of 4-aminophenol compared to other Au core-silica shell nanoparticles. The enhanced catalytic activity is mainly due to the efficient diffusion of reactants onto the multiple Au nanodots through mesopores within the silica shell as well as the possible interparticle couplings of Au nanodots within mesoporous silica matrix. This is a novel and simple synthetic approach for generating hybrid Au-silica nanomaterials by encapsulating multiple Au nanoparticles within a silica matrix.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and structural properties of multi-Pt@SiO₂ and multi-Au/Pt@SiO₂ nanoparticles

박준성 유효종^{1,*}

한림대학교 화학과 ¹한림대학교 자연과학대학 화학과

Multiple platinum (Pt) nanodots core- and hybrid multiple Au/Pt nanodots core- silica shell nanoparticles (multi-Pt@SiO₂ NPs and multi-Au/Pt@SiO₂ NPs) were successfully fabricated through a reverse microemulsion (water-in-oil) based method. The morphologies and structural properties of the synthesized core-shell nanoparticles were completely characterized through the transmission electron microscopy (TEM) and X-ray energy dispersive spectroscopy (EDS). The sequential reduction of HAuCl₄ and K₂PtCl₄ by Brij35 surfactant within reverse micelles, followed by the condensation of TEOS gave the hybrid multiple metal core-silica shell nanoparticles. By the amount changes of the additional reducing agent (ascorbic acid), the reduction yield as well as the size and property of metallic nanodots were interestingly varied. The size of silica shell was also effectively controlled by changing the water to surfactant ratio. The catalytic activities of multi-Pt@SiO₂ NPs and multi-Au/Pt@SiO₂ NPs in a variety of reactions have been also tested.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: INOR.P-235

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a Small Molecule Targeting Multiple Facets of Brain Disease

임미희* Todd J. Eckroat¹ Keith D. Green² Akiko Kochi³ Sylvie Garneau-Tsodikova²

울산과학기술대학교(UNIST) 나노생명화학공학부 ¹Department of Medicinal Chemistry, University of Michigan, USA ²Department of Pharmaceutical Sciences, University of Kentucky, USA ³Department of Chemistry, University of Michigan, USA

While the etiology of Alzheimer's disease (AD), a fatal form of dementia, still remains elusive, multiple neuropathological factors, such as misfolded proteins (e.g. A β and tau), metal ions, and acetylcholinesterase (AChE) have been proposed to be involved in AD neuropathogenesis. Metal ions and AChE have been observed to be deposited with accumulated A β plaques; however, the correlation between all three factors (A β , metal ions and AChE) have yet to be elucidated. The interaction between two factors (A β and metal ions or AChE), has been studied and reported. Metal binding to A β have seen suggested to facilitate A β aggregation and generate reactive oxygen species.² Inhibition of AChE, a serine protease that hydrolyzes the neurotransmitter acetylcholine (ACh), has been shown to temporarily reduce cognitive decline in addition to A β aggregation, due to inhibition of the peptide binding to the AChE peripheral site. Therefore, in order to target metal-associated A β species and AChE concurrently, a multifunctional small molecule containing bifunctionality (A β interaction and metal chelation) and AChE inhibitory activity was designed.⁴ Herein, the design, synthesis, and characterization of the hybrid will be presented. In addition, we will report the activities of our hybrid toward AChE inhibition with A β and/or metal ions as well as metal-free and metal-induced A β aggregation in the absence and presence of AChE.

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발표코드: **INOR.P-236**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Calculation of Germafluorene Derivatives

엄성용 이성기 조보민 김성웅 손홍래*

조선대학교 화학과

Various functionalized germafluorene derivatives were used to investigate their optical and electronic properties. The germafluorene compounds were synthesized by a stepwise reactions from 1,2,4,5-tetrabromobenzene to 2,2'-dibromobisfluorene with germanium tetrachloride in THF at room temperature. The germafluorene compounds were characterized by ¹H-NMR, UV-Vis absorption, and photoluminescence spectroscopy. The optical absorption spectra showed an absorption edge at 285 nm, while a strong UV-vis photoluminescence at 350 nm is observed. These germafluorene compounds are served as light emissive layers. They possess relatively low LUMO energy levels while maintaining high HOMO-LUMO optical gaps. Differential scanning calorimetry measurements reveal that these germafluorene compounds exhibited very good thermal stability at extremely high temperature ca. above 350 °C. Organic light-emitting diodes have been fabricated by using thermal evaporation technique and shows blue emission with an excellent diode behavior under the forward bias. 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. 2012H1B8A2026282)

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Phenyl-Vinyl-Based Polysiloxane Resins by Using Oligohydrosiloxanes

정성은 이성기 조보민 신동희 손홍래*

조선대학교 화학과

For the synthesis of phenyl-vinyl-based polysiloxane resins, novel cross-linking agents containing silicon-hydride such as linear hydrosiloxane oligomers have been discovered via hydrosilylation reaction. Phenyl-vinyl-based oligosiloxanes were synthesized from the reaction of diphenylsilanediol and vinyltrimethoxysilane through a nonhydrolytic sol-gel condensation. linear hydrosiloxane oligomers containing Si-H moiety were obtained from the reaction of dichlorodimethylsilane and dichlorophenylsilane. Dimethylchlorosilane was used as a ending group for the linear hydrosiloxane oligomers. The reaction of phenyl-vinyl-based oligosiloxanes and linear hydrosiloxane oligomers in the present of Pt catalyst was carried out for the synthesis of polysiloxane resins. The prepared phenyl-vinyl-based polysiloxane resins showed a good refractive index, high hardness, and great transmittance. The comparison to previously known phenyltris(dimethylsiloxy)silane as a cross-linking agent has been reported. This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation . (2012H1B8A2026282)

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발표코드: **INOR.P-238**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Camptothecin-Capped Silicon Quantum Dots for drug Delivery Application

백상수 김성룡 정성은 김강빈 손홍래*

조선대학교 화학과

Camptothecin(CPT)-capped silicon quantum dots (Si QDs) were successfully synthesized. Optical characterizations of Si QDs were achieved by using ultraviolet-visible (UV-Vis) and photoluminescence (PL) spectroscopy. The morphologies of Si QDs were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), nuclear magnetic resonance (NMR) and infra-red (IR) spectroscopy. Bare Si QDs and CPT emitted the light at 450 and 425 nm with an excitation wavelength of 400 and 370 nm, respectively. However, CPT-capped Si QDs emitted the light at 570 nm with an excitation wavelength of 480 nm, which shifted to the longer wavelength. Optical characteristic of drug-capped Si QDs were investigated in PSB buffer solution. The release of CPT was investigated by the measurement of fluorescence intensity of Si QDs using UV-vis spectrometer to obtain a release profile. Quantum yields for Si QDs, CPT, and CPT-capped Si QDs were measured. 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. (2012H1B8A2026282).

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultra-Fast Curing of Epoxy-Based Polysiloxane Resins Showing High Refractive and Transparent Optical Properties for LED Encapsulats

김성웅 엄성용 김종준 안지훈 손홍래*

조선대학교 화학과

The epoxy-based oligosiloxanes were synthesized from the reaction of 3-glycidoxypropyltrimethoxysilane, diphenylsilanediol (DPSD). Previously known cross-linking agent such as a methyl hexa-hydrophthalic anhydride (MHHPA) for the synthesis of epoxy-based polysiloxane resins in the present of amine catalyst showed disadvantage in terms of long curing time. To obtain suitable hardness for polysiloxane resins, the curing time to complete the reaction requires 12 hours. Here, we reported new aromatic anhydrides as a ultra-fast curing agent for the synthesis of epoxy-based polysiloxane resins. The curing process with non-aromatic anhydride requires usually more than 12 hours. However the curing process with aromatic anhydrides requires only about 30 min to obtain a suitable hardness. Prepared epoxy-based polysiloxane resins exhibited an ultra-fast curing time, good refractive index, and high hardness and transmittance. 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. 2012H1B8A2026282)

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Evaluation of LED Encapsulants Based on Phenylvinyl Polysiloxane Resins with Various Phenyl Derivatives

김성룡 안지훈 신기루 김종준 손홍래*

조선대학교 화학과

Evaluation of LED encapsulants based on phenylvinyl polysiloxane (PVPS) resins with various phenyl derivatives has been successfully achieved. The phenyl derivatives used in phenylvinyl polysiloxane resins for OLED encapsulant application are phenyl and mesityl group. Thermally stable transparent PVPS resins with high refractive index was synthesized by the thermal curing reaction of phenylvinyl oligosiloxanes (PVOS). PVOS was obtained by a sol-gel condensation process between vinyltrimethoxysilane (VTMS) and diphenylsilanediol (DPSD). We have investigated the effect of phenyl derivatives on PVOS resins. Instead of using DPSD, dimethylsilanediol (DMSD) was used for the synthesis of mesitylvinyl oligosiloxane (MVOS). DMSD was synthesized from the reaction of 2 equivalents of mesityllithium and silicon tetrachloride. To obtain mesitylvinyl polysiloxane (MVPS) resins, MVOS was thermally cured at 150 oC for 3 hours. The comparison with DPSD was achieved. The physical properties such as an optical transmittance, refractive index, and harness were measured. This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation (No. 2012H1B8A2026282).

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장소: 창원CECO

발표코드: **INOR.P-241**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of Graphene-Silicon Nanowire Composite Materials

신동희 안지훈 김종준 신기루 손홍래*

조선대학교 화학과

Silicon nanowire(SiNW)-graphene hybrimer was synthesized from the reduced GO and Si NW via hydrosilylation in the presence of platinum catalyst. Single-crystalline SiNWs were fabricated by using an electroless metal assisted etching of bulk silicon wafers with silver nanoparticles deposited by a spin-casting. The etching of SiNWs was carried out in an aqueous solutions of hydrofluoric acid and hydrogen peroxide. Free-standing SiNWs were then obtained using ultrasono-method in chloroform. GO was prepared by the modified Hummer's method and reduced by a microwave to give a reduced grapheme which was used for the synthesis of SiNW-graphene hybrimers. The morphology of SiNW-graphene hybrimers were characterized by EDS, TEM, and FE-SEM. Covalent bond between graphene and SiNW was confirmed by using XPS and FTIR spectroscopy. BET measurement showed that SiNW-graphene hybrimer had a mesoporous. 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.(2012H1B8A2026282)

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발표코드: **INOR.P-242**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

FRET Efficiency between Silicon Quantum Dots and Silole Fluorophore

김강빈 엄성용 김성웅 김성룡 손홍래*

조선대학교 화학과

Silicon Quantum Dots (Si QDs) capped with organic fluorophore such as siloles were successfully synthesized. Optical characterizations of Si QDs were achieved by using UV-Vis and photoluminescence spectroscopy. The morphologies of Si QDs were achieved by SEM and TEM. Silole-capped Si QDs were characterized by NMR and IR spectroscopy. The emission wavelengths of hydrogen-terminated Si QDs and silole were 450 and 520 nm with an excitation wavelength of 400 and 360 nm, respectively. The synthesized Si QD/silole (core/shell) nanoparticles exhibited an absence of PL of Si QDs but showed an enhancement of PL of silole by 40 times. This result could be interpreted by the efficient fluorescence resonance energy transfer (FRET) from Si QDs having large band gap to silole moiety having small band gap. This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282).

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발표코드: INOR.P-243

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Bis(triptycene)silafluorene Derivatives for Explosive Sensor

이성기 김성룡 백상수 김강빈 손홍래*

조선대학교 화학과

The synthesis, spectroscopic characterization, and fluorescence quenching efficiencies of metallafluorene were reported. The synthesized compounds were characterized by ^1H and ^{13}C 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 chemosensor to detect various type of explosives such as (1,3,5-trinitroperhydro -1,3,5-triazine, RDX), nitroaromatics (1,3,5-trinitrotoluene, TNT), and nitrate esters (PETN). The results of detection efficiency showed that both compounds were served as an excellent chemosensors and other metallafluorene derivatives were synthesized and their photonic behaviors were investigated. 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 (2012H1B8A2026282).

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Graphene-Silicon Quantum Dot Hybrimer via Hydrosililation

안지훈 조보민 정성은 백상수 손홍래*

조선대학교 화학과

Graphene-silicon quantum dot (Si QD) hybrimers have been successfully synthesized and characterized for the possible application of supercapacitor. Graphene oxide was synthesized by using modified Hummer's method and exfoliated by microwave to give a reduced graphene. Hydride-terminated Si QDs were synthesized from the reaction of ammonium chloride and magnesium silicide. Reduced graphene was reacted with H-terminated Si QDs via hydrosilylation in the presence of platinum catalyst. Graphene-Si QD hybrimers were characterized by XRD, TEM, and FE-SEM. Specific surface area was measured by the Brunauer-Emmett-Teller (BET) method. 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.2012H1B8A2026282).

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장소: 창원CECO

발표코드: INOR.P-245

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Phenyl-Vinyl-Based Polysiloxane /Metal Oxide Nanoparticle Hybrimer for LED Encapsulats

신기루 김강빈 정성은 백상수 손홍래*

조선대학교 화학과

Phenyl-vinyl-based polysiloxane (PVPS)/metal oxide nanoparticles (MONPs) hybrimer was synthesized from the reaction of PVPS and MONPs via hydrosilylation in the presence of platinum catalyst. MONPs were surface-derivatized from the reaction of MONPs with dimethylchlorosilane to give SiH-terminated MONPs. Si-H moiety of the MONPs was used for a covalent attachment with vinyl group of PVPS via hydrosilylation. The physical properties such as an optical transmittance, refractive index, and harness of PVPS/ MONPs hybrimer were investigated with various curing times and precursor compositions. Optical characterizations of MONPs were achieved by using UV-Vis and photoluminescence spectroscopy. To tune the refractive index of PVPS/ MONPs hybrimer, thermal stability was investigated upon baking. This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2012H1B8A2026282).

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발표코드: INOR.P-246

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Diphenyl Polysiloxane Resins Having Methacrylate and Epoxy Group for the Application of LED Encapsulats

김종준 이성기 신동희 신기루 손홍래*

조선대학교 화학과

New oligosiloxanes having both methacrylate- and epoxy-group were synthesized from the reaction of 3-(methacryloyloxy)-propyltrimethoxy-silane (MPTS), 3-(glycidoxy)-propyltrimethoxysilane (GPTS), and diphenylsilanediol (DPSD). Barium hydroxide monohydrate was used as a catalyst and promotes the direct condensation reaction between the methoxy radical of MPTS and GPTS and the diol radical of DPSD to form siloxane bonds. These oligosiloxanes contained bi-functional groups such as methacrylate and epoxy group for the further condensation. New methacrylate- and epoxy-containing polysiloxanes resins were obtained by using both photo-curing and thermal curing methods. The epoxy moiety of oligosiloxane was heat-treated for the photo-curing and the methacrylate moiety of oligosiloxane was photo-treated for the thermal curing, respectively. An optical transmittance, refractive index, harness were investigated according to the curing time and precursor composition. 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. 2012H1B8A2026282).

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발표코드: **INOR.P-247**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optical Characterization and Crystal Growth of Silicon Quantum Dots

조보민 엄성용 김성용 신동희 손홍래*

조선대학교 화학과

Silicon quantum dots (Si QDs) have been successfully synthesized and their photoluminescence (PL) and quantum yields have been investigated. The change of quantum yield and optical characterization of Si QDs are measured at various reaction conditions. Luminescence intensity was increased as the reaction time increased. Investigation for the crystal growth of Si QDs has been studied by using TEM and the TEM topograph of as-prepared Si QDs reveals that Si QDs exhibited the tetrahedral geometry. The SAED pattern has been obtained from the several particles shown in the TEM image and single zone axis patterns are observed. The [111] zone axis pattern for diamond cubic is observed. FTIR measurement indicated that the Si QDs consisted of only silicon and hydrogen atom. Optical characterizations of Si QDs were measured by UV-Vis and PL spectroscopy. The size distribution and orientation of Si QDs were measured by TEM and XRD. TEM image displays the spherical Si QDs with the size of 2-4 nm. 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 (2012H1B8A2026282)

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발표코드: **INOR.P-248**

발표분야: 무기화학

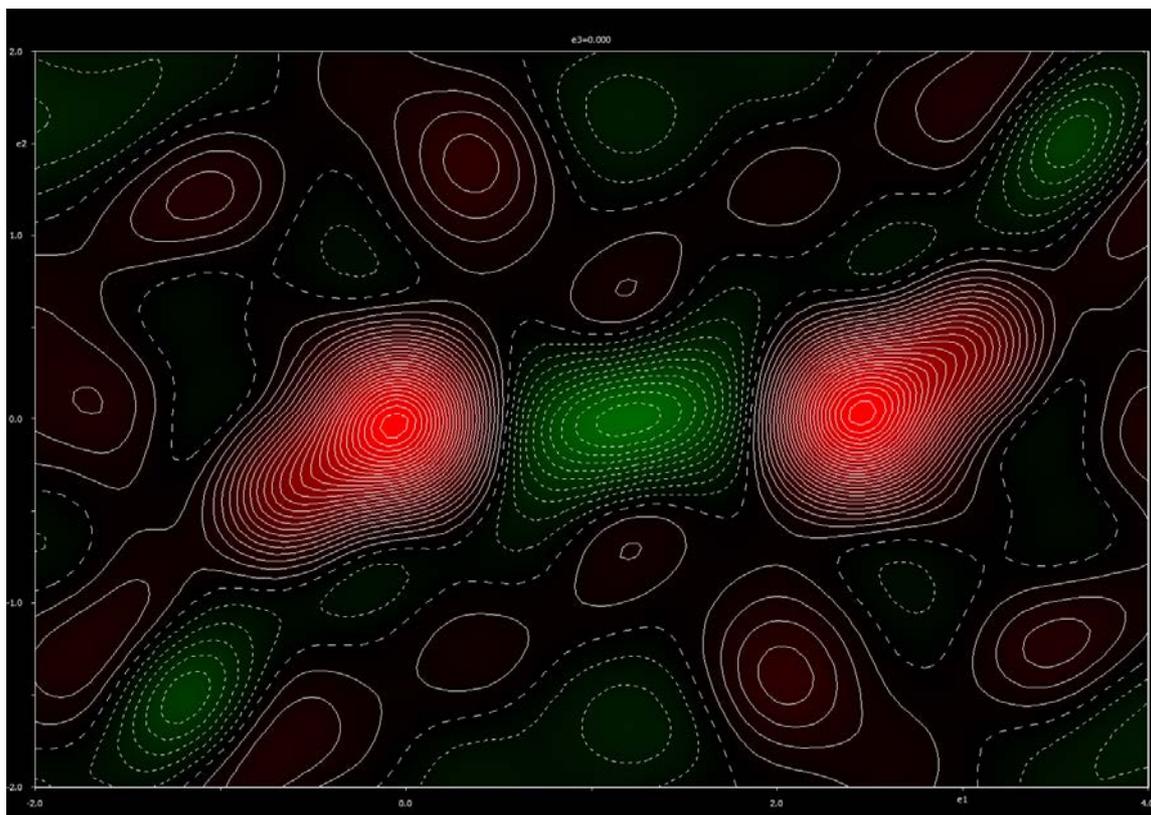
발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of the symmetrical hydrogen bond in the $\text{SO}_4\text{-H-SO}_4$ dimer in $\text{K}_3\text{H}(\text{SO}_4)_2$ by neutron diffraction

오인환* 손유정¹ Martin MEVEN¹ Gernot Heger¹

한국원자력연구소 중성자과학연구부 ¹RWTH Aachen, Germany

The mineral letovicite $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ belongs to the well-known structure family of compounds with the general formula $\text{M}_3\text{H}(\text{XO}_4)_2$ ($\text{M} = \text{NH}_4^+$, K^+ , Rb^+ , Cs^+ , Tl^+ ; $\text{X} = \text{S}^{6+}$, Se^{6+}). The characteristics of these compounds are the strong hydrogen bonds between two XO_4^{2-} ions and the superprotonic conductivity. In the letovicite, two types of the disorder related with the hydrogen atoms, the rotational disorder of the NH_4^+ groups and two maxima along the $\text{SO}_4\text{-H-SO}_4$ dimers, are reported. Although letovicite shows various phase transitions due to the proton ordering at low temperature, $\text{K}_3\text{H}(\text{SO}_4)_2$ without the possibility of an orientational disorder of NH_4^+ undergoes no phase transition at low temperature. At room temperature, the title compound is isostructural to letovicite with a monoclinic space group A2/a and has an inversion center in the middle of the $\text{SO}_4\text{-H-SO}_4$ dimer. Based on the analysis of the anisotropic displacement parameters and the elongation of the hydrogen atom toward the two oxygen atoms by neutron single crystal diffraction at 2.3K, it seems that the hydrogen bond in the title compound can be classified as centered hydrogen bond or intermediate form between the low-barrier hydrogen bond (LBHB) and the ultrashort centered hydrogen bond.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

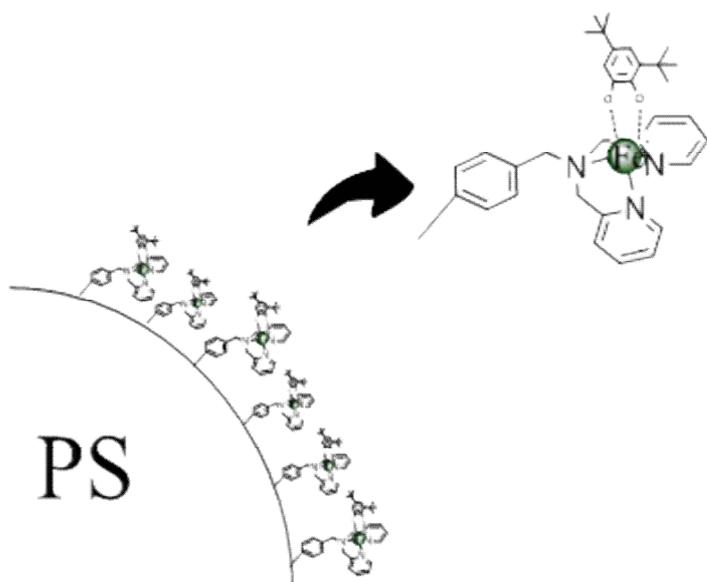
Poly styrene nanoparticle에 카테콜(catechol) 분해 촉매를 연결하여

신개념 나노촉매의 개발

박광호 윤성호*

국민대학교 생명나노화학과

Aromatic ring 을 갖는 phenol, catechol 등 환경오염물질 처리 기술이 현대 사회에서 매우 중요한 연구 목표가 되고 있는 실정임. Catechol 분해는 자연계에서 catechol dioxygenase 를 포함하는 soil bacteria 등이 공기 중 산소와 이용하여 분해하는 것이 잘 알려져 있음. 자연계의 효소는 열에 약하고 고가라는 단점으로 인하여 향후 산업계에서 사용의 제한이 있을 수 있음. 따라서 많은 연구는 효소의 활성화 자리만을 유기/무기화학을 통해 모사하여 mimicking catalyst 를 개발하기 위해 추진되어 왔음. 하지만 Mimicking catalyst 를 구현함에 있어 단순한 리간드를 이용 할 경우 dimerization 에 의해 활성이 존재 하지 않는 배위 화합물이 형성되는 것이 알려짐. 본 실험에서는 Di-(2-picoly)amine 와 같은 간단한 리간드를 이용하여 Poly styrene nanoparticle 에 표면 개질 통해 dimerization 없이 non-heme iron catalyst 를 합성하고, heterogeneous 촉매로서의 가능성을 확인하고자 함



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Cp* -Iridium complex을 통한 이산화탄소의 전기화학적 전환

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국민대학교 화학과 ¹국민대학교 생명나노화학과

이산화탄소는 지구온난화의 주된 원인으로 알려져 있다. 또한 이산화탄소는 무해하고 자원의 양이 무한하므로 이를 전환하여 사용하는 연구를 진행하고 있다. 하지만 이산화탄소는 매우 안정하기 때문에 전환하기에 많은 에너지가 소모된다. 따라서 이산화탄소를 전환하는 촉매의 연구가 활발히 진행되고 있다. 그 중 이산화탄소의 환원을 통해 포름산을 생성하는 연구는 화학반응에 비해 부산물이 적으며 섬유염색, 피혁가공 등 부패방지에 많이 사용되며 수소저장 등 다양한 분야로 이용되어 반응이 관심을 받고 있다. Transition metal complex 를 사용한 촉매의 경우 광화학, 전기화학적으로 이산화탄소의 환원촉매로 사용되었다. Iridium, Rhodium 등 귀금속의 경우 초임계 상태에서 이산화탄소를 포름산으로 빠르게 전환된다고 보고되었다. 본 실험에서는 Cp* -Iridium complex 를 촉매로 사용하여 이산화탄소의 전기화학적 전환에 따른 포름산의 생성에 대해 연구하여 보고한다.

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발표분야: 무기화학

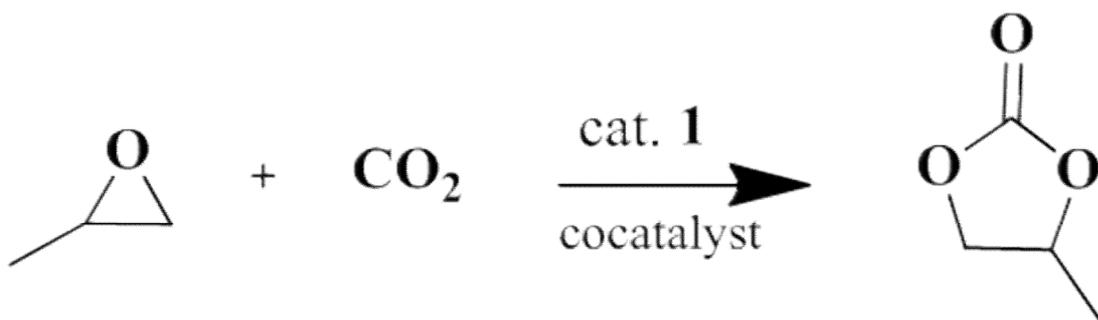
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Cp^{*}-Rh complex catalyzes formation of cyclic carbonate from CO₂ and Propylene oxide under mild condition

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Activation or utilization of carbon dioxide (CO₂) is widely studied, owing to their environmental concerns and high abundant and CO₂ has the most attractive applications as C1 source in organic synthesis due to their non-toxic and non-corrosive nature. However, the inertness of CO₂ makes it very difficult to activate. Several methods have been developed, and among them, one of the very interesting methods is atom-economical synthesis of five membered cyclic carbonates from CO₂ and propylene oxides (Scheme 1). Due to the various applications of the cyclic carbonates such as aprotic polar solvents, electrolyte, starting material of poly carbonates and polyurethane, and raw material for the chemical reactions, conversion of CO₂ to cyclic carbonate has gained much attention. Previously, Co(III), Al(III) and Cr(III) complexes with salen ligand derivatives were studied elaborately with different cocatalysts. Similarly, ionic liquids were used to successfully convert the CO₂ to cyclic carbonate with propylene oxides. However synthesis of cyclic carbonate from CO₂ and propylene oxide using the metal complexes and the ionic liquids was conducted at high CO₂ pressure and temperatures. Additionally some of the catalysts afford the mixture of polycarbonate and cyclic carbonate, and most of the metal catalysts were highly sensitive to water molecule which deactivates the catalyst. Herein, we report the Cp^{*}-Rh(III) complex, where Cp^{*} is pentamethylcyclopentadiene, catalyzed formation of cyclic carbonate from CO₂ and propylene oxide, under mild conditions without the influence of moisture.



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발표코드: **INOR.P-252**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dimensional transformation of metal coordinated polymer by controlling the size of pendant

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한국과학영재학교 화학생물학부 ¹아주대학교 분자과학기술학과 ²아주대학교 공업화학과

Metal coordinated polymer is composed of metal cations and organic linkers and their structures can be controlled on the substituents that are present on the organic linkers. For example, 2,5-disubstituted H2BDC analogues, in which the substituents were long alkoxy chains-like octyloxy chains, first formed a 3D MOF structure that then transferred to a 1D coordinated structure. When more bulky substituents such as 3-(9H-carbazol-9-yl)octyloxy groups were introduced on a H2BDC linker, only 1D coordinated structure was obtained. Here, we investigated a novel metal coordination polymer based on an organic H2BDC analogue to determine the influence of the substituents of the organic linker, 2,5-bis(3-(9H-carbazol-9-yl)propoxy)benzene-1,4-dicarboxylic acid, and the resulting single crystals of [Zn(CZ3)(DMF)] polymer exhibited 2D metal coordinated structure.

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발표코드: **INOR.P-253**

발표분야: 무기화학

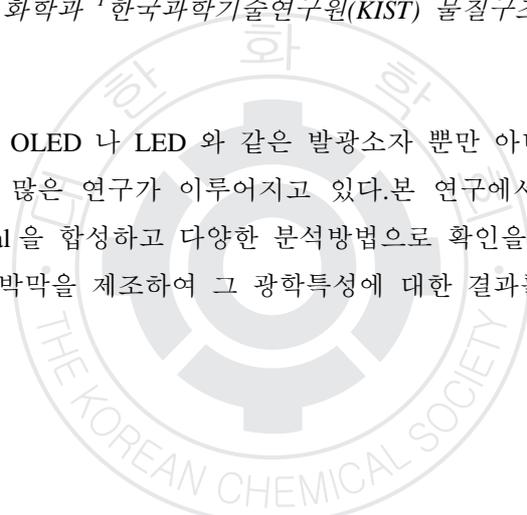
발표종류: 포스터, 발표일시: 수 16:00~19:00

형광체를 포함한 박막의 제조와 특성 연구

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한남대학교 화학과 ¹한국과학기술연구원(KIST) 물질구조 제어 연구단

형광체를 포함한 박막은 OLED 나 LED 와 같은 발광소자 뿐만 아니라 태양전지 관련분야에 적용할 수 있기 때문에 많은 연구가 이루어지고 있다. 본 연구에서는 quantum dot 과 같은 photo luminescence material 을 합성하고 다양한 분석방법으로 확인을 하였다. 또한 발광물질을 포함한 유기 또는 무기 박막을 제조하여 그 광학특성에 대한 결과를 발표할 예정이다.



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발표코드: INOR.P-254

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction and Reactivity of Synthetic Flavonoids with Metal-Free and Metal-Associated Amyloid Species

임미희* Hyuck Jin Lee¹ Alaina S. DeToma¹

울산과학기술대학교(UNIST) 나노생명화학공학부 ¹Department of Chemistry, University of Michigan

Disturbed metal ion homeostasis in conjunction with amyloid- β ($A\beta$) aggregation in the brain has been implicated in Alzheimer's disease (AD) pathogenesis. To uncover the interplay between metal ions and $A\beta$ peptides, multifunctional small molecules have been employed to monitor $A\beta$ aggregation and toxicity in vitro. Naturally occurring flavonoids have emerged as a valuable class of compounds for this purpose due to their ability to modulate both metal-free and metal-induced $A\beta$ aggregation leading to non-toxic amorphous peptide products; however, the structural moieties of flavonoids responsible for such reactivity have not been fully identified. Herein, we designed, synthesized, and characterized a set of synthetic flavonoids that interact with metal ions and $A\beta$ species, modulate metal-free $A\beta$ and metal- $A\beta$ aggregation in vitro, and regulate toxicity induced by metal-free $A\beta$ /metal- $A\beta$. Overall, through our studies we obtained valuable insights on the requirements for parity among metal chelation, intermolecular interactions, and substituent variation using synthetic flavonoids, which offer a basic fundamental understanding of a structure-interaction-reactivity relationship between metal-free $A\beta$ and metal- $A\beta$ species with the flavonoid family.

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장소: 창원CECO

발표코드: INOR.P-255

발표분야: 무기화학

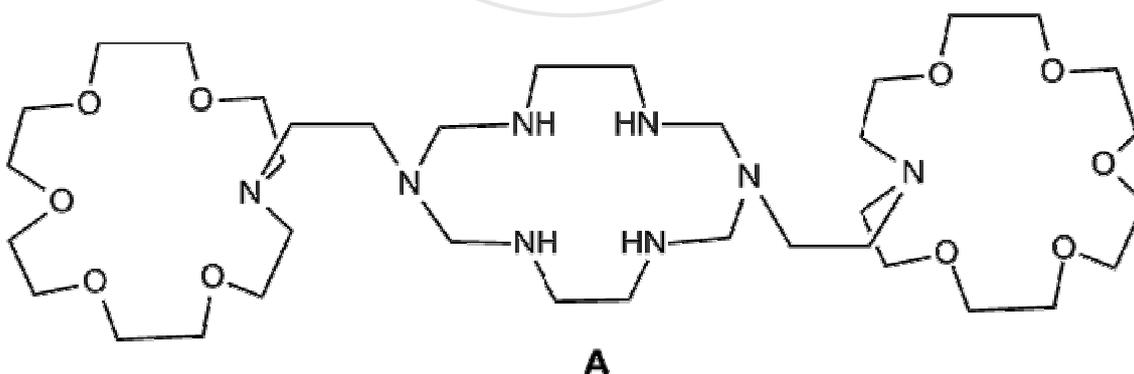
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Binding Properties of Macrocyclic Complex as a Redox Active Center Having Crown Ether Type Receptor

곽지훈* 이재명¹

순천대학교 화학교육과 ¹순천대학교 화학과

Molecular sensing is one of the interesting fields in molecular recognition. Usually, this sensing is derived from the selectivity toward the guest ions or molecules. In a certain sense, the reverse behavior of this sensing is switching. We had studied this sensing and switching with the nickel(II) macrocyclic complexes containing crown ether by measuring binding properties of crown ether. We prepared more developed system of the complex of crown-macrocycle-crown(A) for the study of selective binding properties of it toward metal ions. In this work, the preparation and the binding properties of it toward alkali metal ions will be presented



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Sensitive SERS Detection Based on Raman Reporter-labeled Au@SiO₂ Core-shell for Immunoassay

사영조 Lei Chen¹ Bing Zhao¹ 정영미* Xu Wang¹

강원대학교 화학과 ¹Jilin University, China

A highly sensitive SERS detection based on immunoassay has been developed by using Au@SiO₂ core-shell nanoparticles which are combining Raman reporter-labeled Au aggregates on a SERS-active substrate. The features of those aggregates were characterized by TEM images, UV-vis spectra and SERS spectra. Au aggregation can be induced by simply mixing Raman reporter with gold nanoparticles, which could produce high SERS enhancement. In this study, we will present a rapid and straightforward procedure for the preparation of Au@SiO₂ core-shell. The Au@SiO₂ core-shell nanoparticles are functionalized with anti-immunoglobulin G (anti-IgG) for immunoassay exhibited a potential application in biosensing. Characterization of Au@SiO₂ core-shell nanoparticles and application in SERS-based biosensing will be discussed in details.

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발표코드: **PHYS.P-257**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of Gold-coated Magnetic Nanoparticles for Protein Detection by Using SERS-based Immunoassay

신민화 Lei Chen¹ 이영주 Xu Wang¹ Bing Zhao¹ 정영미*

강원대학교 화학과 ¹State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China

Gold-coated magnetic nanoparticles are an effective means for the separation of proteins via application of an external magnetic field. With the integration of high sensitivity, unique spectroscopic fingerprint, and nondestructive data acquisition, the surface-enhanced Raman scattering (SERS) technique has been developed for the identification and detection of biology system. Easy separation of proteins by using gold-coated nanoparticles magnetic particles and sandwich type immunoassay are applied to obtain ultrasensitive SERS spectra simply. In this presentation, characterization of gold-coated magnetic particles and application in the immunoassay by using SERS will be discussed in details.

Acknowledgements

This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (MEST) (No. 2009-0087013).

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발표코드: **PHYS.P-258**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of Li-ion battery at high voltage: The chemical additive effect on cathode surface

신수현 박연주 최현철¹ 정영미*

강원대학교 화학과 ¹전남대학교 화학과

Li-ion battery has thermal stability problem under high voltage condition due to distortion of cathode structure, formation of insulating film, and generation of gas and heat during charge-discharge process. In our previous study, the formation mechanism of surface-electrolyte interface (SEI) film on the cathode at high voltage has been investigated to understand the safety problem. Based on these results, we used organic additives such as vinylene carbonate (VC) and fluoroethylene carbonate (FEC) in Li-ion battery, to improve the stability of cathode at high voltage. In this study, we investigated the formation mechanism of SEI film in Li-ion battery with various additives by using CV curve, cyclic voltammetry and spectroscopies. Details on the effect of additives in Li-ion battery will be discussed.

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장소: 창원CECO

발표코드: **PHYS.P-259**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal behavior of polyhydroxyalkanoate-based blend films investigated by two-dimensional correlation spectroscopy

박준후 박연주 Isao Noda¹ 정영미*

강원대학교 화학과 ¹Materials Science and Engineering, University of Delaware

Poly(3-hydroxybutyrate-co-3-hydrohexanoate) (P(HB-co-HHx)), which is the polyhydroxyalkanoate (PHA) family, has been extensively studied as environment-friendly polymer. Physical properties of P(HB-co-HHx) can be improved by blending with polyethylene glycol (PEG). To study the thermal dynamics of spin-coated films of P(HB-co-HHx)/PEG blend, temperature-dependent IRRAS spectra were analyzed by two-dimensional correlation spectroscopy and chemometrics. The details of thermal behavior of P(HB-co-HHx)/PEG blend will be discussed.

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발표코드: **PHYS.P-260**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

**Study of highly excited states of a Li₂ molecule by the MRCI method
and comparison of potential energy curves obtained from experiments
by RKR and IPA and from other theoretical methods**

이천우

아주대학교 화학과

Lithium dimer is a molecule for which extensive experimental and theoretical work have been performed. For most of states (~30 states) related asymptotically to Li (2s) + Li [nl (n=2,3,4, l = s, p, d, f)] and Li (2p) + Li (2p), potential energy curves (PECs) are determined by RKR and IPA using conventional and OODR spectroscopic methods. Although many theoretical studies have compared their PECs with those of RKR and IPA, still there are highly excited states for which the comparisons are not made. For the latter states, comparisons are made with our PECs obtained using Kaufmann's Rydberg basis functions.

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발표코드: **PHYS.P-261**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of photoionization of N₂ molecules by various methods

이천우

아주대학교 화학과

We report the progress on the study of photoionization of N₂ molecules by an one-center expansion method. We have tried two methods to study the photoionization of N₂. One is the one-center expansion method and the other is the *R*-matrix method using the UK molecular code. One-center expansion method by Faisal, Sinfailam and Burke is adopted to our work. Their codes seem to contain parts specific to their site. We spent a lot of time to get rid of such parts specific to their computer system and to make a workable code in our system. Since electron and target states in their calculation are treated separately, their method suffers from the orthogonalization problem between scattering states and target states. Thus it may be better to use the method which treat the target and photo-electron together. For this purpose, we tried to adopt the UK molecular *R*-matrix method. We report the progress.

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장소: 창원CECO

발표코드: **PHYS.P-262**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies of Rydberg states by ECP and CPP methods and comparison with the methods using Rydberg basis functions

이천우

아주대학교 화학과

Recently, we made a lot of calculations of potential energy curves (PECs) of valence and Rydberg states of molecular dimers made of second-row atoms and diatomic hydride. For the ground and lower-excited states, the multi-reference configuration interaction (MRCI) calculations using CASSCF wavefunctions reproduce experimental PECs obtained by RKR or IPA methods quite well. But, for the highly excited states, strangely the calculated MRCI PECs at the asymptotic range of R where dissociation takes place are lower than the experimental PECs for all second-row elements, which is contradict to the variation theorem that the calculated energies are always higher than the true experimental ones. [This greatly contrasts to the case of diatomic hydrides or dimers made of hydrogen or helium where excellent agreements between theoretical and experimental PECs.] Interestingly, such discrepancies do not appear if the effective core-potentials (ECP) in conjunction with core-polarization potentials (CPP). Can ECP method with CPP provide us the explanation for the contradiction of the theoretical results with the experimental ones? We report on the progress of studies of Rydberg states by ECP and CPP methods and comparison with the methods using Rydberg basis functions.

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장소: 창원CECO

발표코드: **PHYS.P-263**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Concerning the Reaction Channel for the Solvolyses of Benzoyl Chlorides

고한중

전주교육대학교 화학교육과

The ortho-effect of substituents upon the kinetics of reactions taking place at a reaction center attached to an aromatic ring has long been a topic of interest. For benzoyl chloride solvolyses, it was shown by Bentley and co-workers that the 2,6-dimethyl-derivative followed an ionization pathway with characteristics very similar to those for the solvolyses of p-methoxybenzoyl chloride. We have carried out a Grunwald-Winstein equation treatment of the solvolyses of 2,6-dichlorobenzoyl chloride, with similar size chlorines replacing the methyl groups but now with an overall electron-withdrawing influence of the ortho-substituents. In this way the reactivity is moderated and the study can be extended to the important fluoroalcohol-containing solvents. For the 30 solvents studied, an ionization pathway with a moderate nucleophilic solvation component is indicated. For comparison purposes, the treatment has also been applied to the 2,4-, 3,4-, and 3,5-dichloro-derivatives. For the 2,4-dichloro-derivative, the two reaction channels are clearly visible and the solvents included for each channel are consistent with their solvent properties.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Na⁺, F⁻, Br⁻ and Cl⁻ on ice surface: Theoretical Studies of Dissolution and Ion Segregation Processes

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경북대학교 일반대학원 화학과 ¹경북대학교 화학과

By the Antarctic Ozone Hole discovery and the recognition of dominant role of the atmospheric ice particle in the chemical composition of the atmosphere determination, the interest of the chemical reactions between gases and ice surface has raised extensively. In the troposphere, reactions between sea-salt aerosols and ice particles with ozone and organic species are considered to play a significant role to produce reactive halogen species. Water-solvated Cl⁻ and F⁻ anions have been the subject of many other theoretical studies and several relevant experimental studies. Reactions involving halogen anions at the interface between air and the concentrated salt solution comprising the aerosol particles have been proposed to be responsible for the release of reactive halogens into the atmosphere. Ice surface is different from liquid water surface. Liquid water and ice crystals have very different solubilities for foreign ions, and therefore the distribution of ions near the surface of crystalline ice may differ from that for liquid water. We observed the adsorption phenomena of cations and anions such as Halides on ice surface and the rearrangement of Hydrogen bonding network after adsorption of ions on ice surface. It was found that Positive (Na⁺) ion can easily attach on ice surface. The rearrangement of Hydrogen bonding network occurs after adsorption of ions on ice surface. Negative ions like Cl⁻, Br⁻ prefer H2 and H3 adsorption sites rather than H1 and H2 sites. We assumed that instead of F⁻, molecular HF formed on the ice surface which eventually migrates into the interior of ice surface.

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발표코드: **PHYS.P-265**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conformational and Vibrational analysis of Glucopyranose in aqueous solution: A combined study of quantum mechanical calculation and QM/MM-MD Simulations

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경북대학교 일반대학원 화학과 ¹경북대학교 화학과

The standard agent glucose has been the subject of numerous experimental and theoretical studies, especially in the aqueous environments which are present in most biochemical processes. The impact of the solvation process on the vibrational spectra of glucose in the mid-infrared region is investigated in this work. The association process of glucose in aqueous solution was studied by a combination of quantum mechanical calculations and QM/MM-MD simulations for glucose with 290 TIP5P water molecules. Conformations in which the water molecules created a favorable network completely around and under glucose were found to have low energy for both α and β anomers. Quantum mechanical calculation of the α/β anomeric ratio using MP2/cc-pVTZ level gave, $\sim 32/68\%$, highly favoring the β anomer in good agreement with the experimental $\sim 36/64\%$ value. An approximate hydroxymethyl population was obtained by noting average relative energies among the three conformational states, gg, gt, and tg. MD simulation shows that in both α (gg : gt : tg = 57.2 : 42.8 : 0.07 and β (gg : gt : tg = 56.48 : 43.19 : 0.33 (%) rotamer complexes the gg conformation was favored over the gt state, with the tg conformations all being of higher energy making little or no contribution to the rotamer population is in good agreement with Experimental homo nuclear J-coupling data. Our simulation shows experimental vibrational spectrum is closely related with gauche-gauche ($\omega = -60$) conformer.

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발표코드: **PHYS.P-266**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Proton Locations in the Collision-Induced Dissociation of Protonated Pentaglycine with Argon

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한국교원대학교 화학교육과 ¹Universite d'Evry ²한국교원대학교 화학과

A QM+MM direct dynamics chemical simulation was used to study gas phase collision-induced dissociation (CID) of protonated amino-pentaglycine with argon. The semiempirical model PM3 was used for intramolecular potential of peptides and analytic functions were used for intermolecular potential between argon and peptides. In order to study the effect of proton locations, collision induced fragmentations were carried out for 5 isomers of protonated amino-pentaglycine with the same skeleton structure but different protonation sites. More than 5,000 trajectories were run for each reaction using VENUS coupled with MOPAC. Simulations were performed with collisional energy of 350 kcal/mol and trajectories were terminated after 40 ps for each of peptides. The results were compared to each other as well as previous studies. Reaction ratio was 22.17% and 21.72% for the N-protonated isomers, and 7.13%, 7.18% and 6.77% for the O-protonated isomers. The most abundant ionic fragment was H4C1N1+.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Substituent Effect of Hetero Multi-Substituents on Electronic Transition Energy

이은혜 윤영욱 이상국*

부산대학교 화학과

Conjugated double bonded organic molecules are excellent candidates for testing free electron molecular orbital theory of π electronic states using 'a particle-in-box' eigenfunctions. The theory assumes that π electrons in a conjugated molecule can be separated from σ electrons and that the σ frame is frozen. In addition, all interelectronic interactions are neglected and the effective potential acting on each π electron is assumed to be given by 'a particle in-a-box' potential. The shift of the origin band of the multi-hetero-substituted benzyl-type radicals has been studied using a substituent effect on the electronic transition energy to rationalize the model developed for the shift of the electronic transition. We generated vibronically excited but jet-cooled multi-hetero-substituted benzyl-type radicals from substituted toluene precursors using a pinhole-type glass nozzle in a technique of corona excited supersonic expansion, from which visible vibronic emission spectra were recorded using a long-path monochromator. From an analysis of the spectra observed, we found the model developed for substituent effect on electronic transition energy of aromatic compounds explains well the observation. The orientation effect of substituents on the benzene ring agrees very well with those obtained from methyl, fluorine, and chlorine-substituted benzyl radicals. In this presentation, we will describe the model developed and compare the agreements with the observation for multi-hetero-substituted benzyl-type radicals.

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A new technique to predict Heat of Vaporization: Effective Fragment Potential MD Simulations

Manik Kumer Ghosh 최철호*

경북대학교 화학과

In this work, we have evaluated how accurate the effective fragment Potential (EFP) model is useful in studying condensed phase properties. Heat of vaporization has been predicted for ~15 organic solvents. The temperature and density dependent behaviors of EFP1 and EFP2 water have been examined. It shows that the box size does not affect heat of vaporization for both EFP1 and EFP2 models. The heat of vaporization of organic molecules can be predicted very accurately: the root-mean-square error is 0.88 kcal/mol. Not only this, EFP2 method can predict heat of vaporization in very short-MD simulation: ~10-15 ps. We have concluded that our sampling strategy yields a very accurate heat of vaporization of any organic solvents within short-MD simulations.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-269**

발표분야: 물리화학

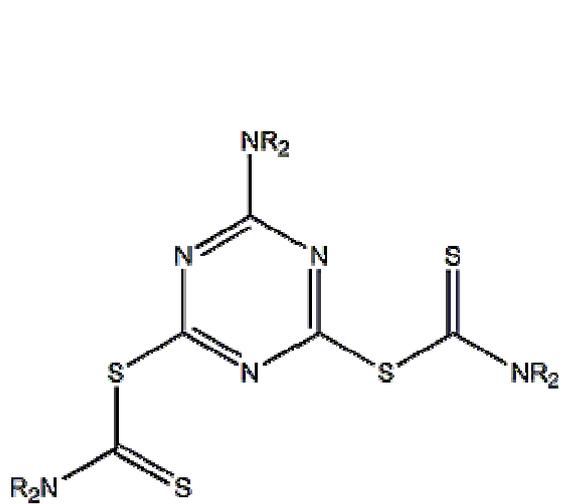
발표종류: 포스터, 발표일시: 수 16:00~19:00

1,3,5-triazine-2,4,6-triyl tris(dibenzylcarbamodithioate) and 6-(dibenzylamino)-1,3,5-triazine-2,4-diyl bis(dibenzylcarbamodithioate) Rotational barrier of Amide bond by Computational method

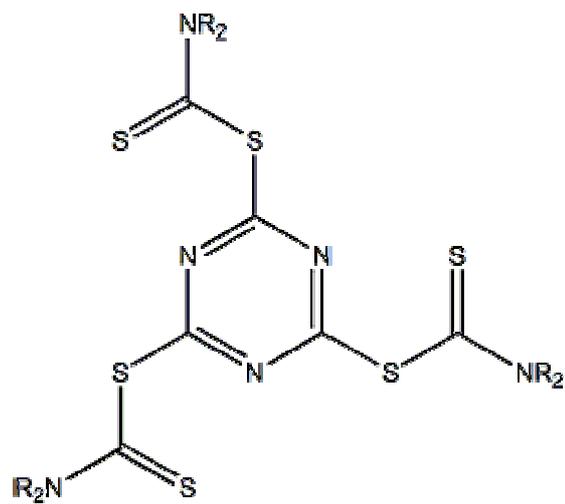
정태섭 이경구¹ 김영준² 곽경원*

중앙대학교 화학과 ¹군산대학교 화학과 ²충남대학교 화학과

An amide bond (peptide bond) is a covalent chemical bond formed between two molecules when the carboxyl group of one molecule reacts with the amino group of the other molecule. We calculated the free energy (ΔG_{\ddagger}) for rotation of C-N bond on dithiocarbamate at the molecular level using Density Functional Theory (DFT) method for some novel cyanuric chloride based compounds. Our results clearly show that calculated rotational barrier of our dithiocarbamates are approximately equal to experimental values by NMR. In our results, although there are almost never difference between two molecules, the C-N rotational barrier of 6-(dibenzylamino)-1,3,5-triazine-2,4-diyl bis(dibenzylcarbamodithioate) (compound 1) is slightly lower than 1,3,5-triazine-2,4,6-triyl tris(dibenzylcarbamodithioate) (compound 2). This can be explained electron donating effect of lone pair of an amine that is directly bonded 1,3,5 triazine ring in compound 1. The amine group of compound 1 can donate a lone pair for triazine ring, and then electron density of triazine ring is increased as compared with compound 2. This 'extra' electron density cascades down the dithiocarbamate group, finally affects electron density of thioketone group (C=S) in dithiocarbamate.

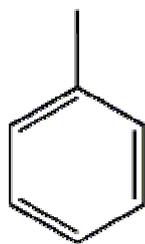


Compound 1



Compound 2

R=



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of the Hydrodynamic, Chloride ion and Oxygen Effects on Corrosion of Nickel in Bicarbonate Buffer Solution

임슬기 김연규*

한국의국어대학교 화학과

아르곤과 산소 분위기에서 변전위 분극법을 적용하여 bicarbonate 완충 용액에서 일어나는 Ni-RDE의 부식과 부동화 현상을 연구하였다. pH, Ni-RDE의 회전 속도, 용액에 녹아 있는 염화 이온의 영향을 조사했는데, pH와 Ni-RDE의 회전 속도의 변화는 Ni 전극에서 일어나는 산화 반응보다는 환원 반응에 큰 영향을 주었으며, 염화 이온은 부동화 막을 파괴하는 데에 큰 효과가 있음을 알 수 있었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-271**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrolysis of Formamide: A Combined Quantum Mechanical and Molecular Dynamic Simulations Study

백용수 Manik Kumer Ghosh 최철호*

경북대학교 화학과

Peptide bond hydrolysis is a key biochemical reaction in both intracellular and extracellular regions. But the reaction mechanism for the neutral hydrolysis of amides in water has not been yet established. Though there is some experimental evidence that uncatalyzed hydrolysis occurs in water in neutral pH, the corresponding reaction mechanism is controversial. In this work, we have investigated in detail the possible mechanism of the hydrolysis of formamide in aqueous solution. A combined quantum chemical calculations and quantum mechanical molecular dynamic (QMMD) simulations have been performed though this work. A both concerted and step-wise reaction mechanism has been considered.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mutation Effect on Amyloidogenic Human Protein β -2-microglobulin: Molecular Dynamics Simulations and Solvation Thermodynamics Analyses

홍주연 함시현*

숙명여자대학교 화학과

β 2-microglobulin (β 2-m) is a major component of amyloid fibrils deposited in patients suffering from dialysis-related amyloidosis. Recently, D76N and D59P mutants have been studied that are thermodynamically unstable and exhibit enhanced aggregation while W60C mutant is more stable and less prone to aggregate than wild-type. However, the structural and mechanistic features of different aggregation propensities of those mutants are still elusive. Here we carried out molecular dynamics simulations followed by solvation thermodynamics analyses to characterize the aggregation-prone structure of the wild type and its D76N, D59P, and W60C mutants. Compared to the native state structures determined by X-ray and NMR, the aggregation-prone structures are characterized by the exposure of the hydrophobic side-chains including proline cis-trans isomerization. Based on the solvation thermodynamic analysis, the aggregation-prone structures of D76N and D59P mutants exhibit greater hydrophobicity than those of wild-type and W60C mutant, which is in good agreement with the experimental observation. Understanding the structural and thermodynamic features of the aggregation-prone structures allow us to rationalize the experimentally observed higher aggregation propensity of the D76N and D59P mutants compared to the wild-type and W60C mutant.

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장소: 창원CECO

발표코드: **PHYS.P-273**

발표분야: 물리화학

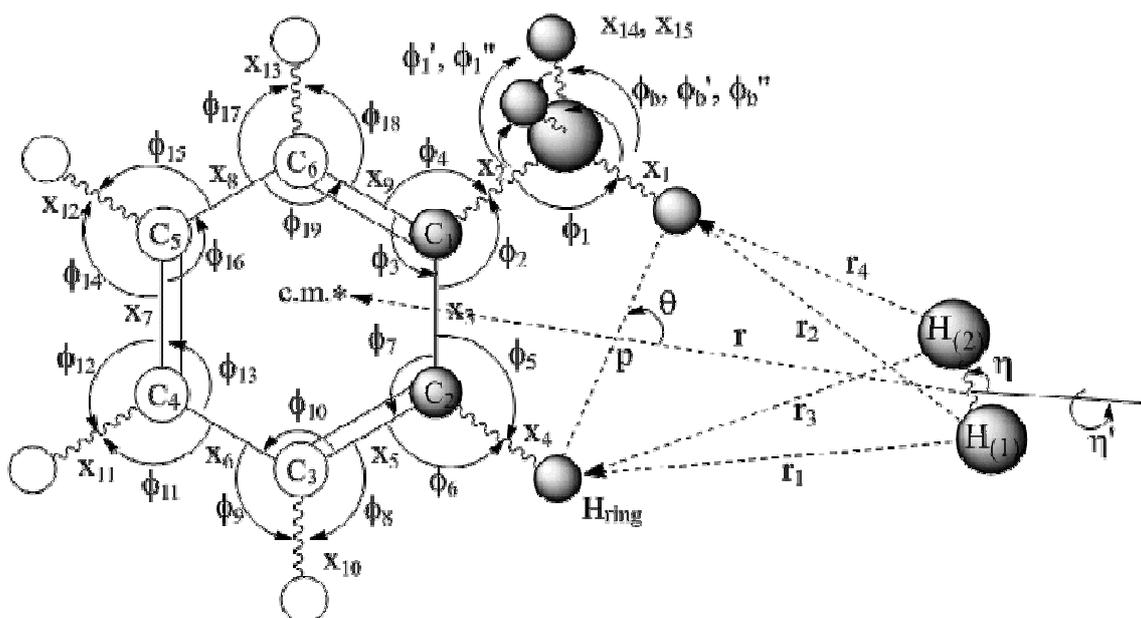
발표종류: 포스터, 발표일시: 수 16:00~19:00

Intermolecular energy flow and bond dissociation of vibrationally excited toluene in collisions with H₂ and D₂

이종백* Hyung Kyu Shin¹

전남대학교 화학교육과 ¹Dept of Chem, Univ of Nevada

Energy transfer and bond dissociation of C-H_{methyl} and C-H_{ring} in excited toluene in the collision with H₂ and D₂ have been studied by use of classical trajectory procedures at 300 K. Energy lost by the vibrationally excited toluene to the ground-state H₂/D₂ is not large, but the amount increases with increasing vibrational excitation from 5000 and 40,000 cm⁻¹. The principal energy transfer pathway is vibration to translation (V-T) in both systems. The vibration to vibration (V-V) step is important in toluene + D₂, but plays a minor role in toluene + H₂. When the incident molecule is also vibrationally excited, toluene loses energy to D₂, whereas it gains energy from H₂ instead. The overall extent of energy loss is greater in toluene + D₂ than that in toluene-H₂. The different efficiency of the energy transfer pathways in two collisions is mainly due to the near-resonant condition between D₂ and C-H vibrations. 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 H₂/D₂. 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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발표분야: 물리화학

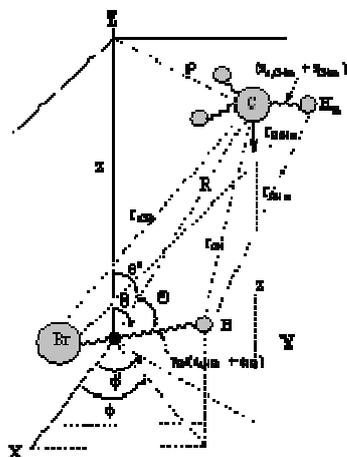
발표종류: 포스터, 발표일시: 수 16:00~19:00

Collision-induced Reaction Dynamics of $\text{CH}_3 + \text{HBr} \rightarrow \text{CH}_4 + \text{Br}$

이종백* Hyung Kyu Shin¹

전남대학교 화학교육과 ¹Dept of Chem, Univ of Nevada

The kinetics of the radical-polar molecule reaction $\text{CH}_3 + \text{HBr} \rightarrow \text{CH}_4 + \text{Br}$ has been studied at temperatures between 150 and 1000 K using classical dynamics procedures. Potential energy surfaces constructed using analytical forms of inter- and intramolecular interaction energies show a shallow well and barrier in the entrance channel, which affect the collision dynamics at low temperatures. Different collision models are used to distinguish the reaction occurring at low- and high-temperature regions. The reaction proceeds rapidly via a complex-mode mechanism below room temperature showing strong negative temperature dependence, where the effects of molecular attraction, H-atom tunneling and recrossing of collision complexes are found to be important. The temperature dependence of the rate constant between 400 and 1000 K is positive, the values increasing in accordance with the increase of the mean speed of collision. The rate constant varies from 7.6×10^{-12} at 150 K to 3.7×10^{-12} at 1000 K via a minimum value of $2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 400 K.



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장소: 창원CECO

발표코드: **PHYS.P-275**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Complexes of Cucurbiturils and Dioxane : A Computational Study

유인기 강영기*

충북대학교 화학과

To find an effective pathway for removing dioxane from mixtures, host-guest complex formation of cucurbit[n]urils ($n = 6, 7, \text{ and } 8$) with dioxane were studied using DFT calculations at the B3LYP/6-31G* level of theory. The equilibrium geometries, binding energies, and barrier energies at the portal of cucurbiturils were investigated. The results show that the CB[6]/dioxane complex is more stable than the other complexes, on the other hand the barrier to pass the portal of CB[6] was higher than the other complexes. In conclusion, while CB[7] removes most of dioxane from mixtures effectively, CB[6] does not make stable CB[6]/dioxane complexes. We confirmed these inclusion preferences experimentally by Headspace GC-MS method.

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장소: 창원CECO

발표코드: **PHYS.P-276**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

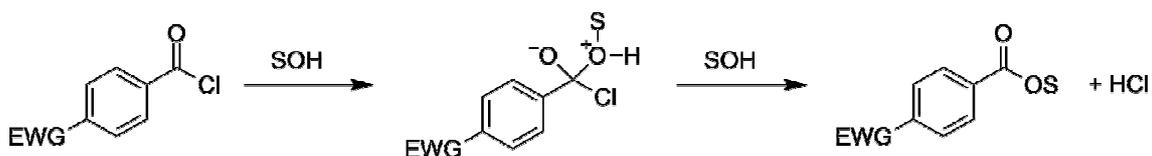
The Effect of Substituents on the Solvolytic Reactions of Benzoyl Chlorides

박경호* 양기훈¹ 경진범 Dennis N. Kevill²

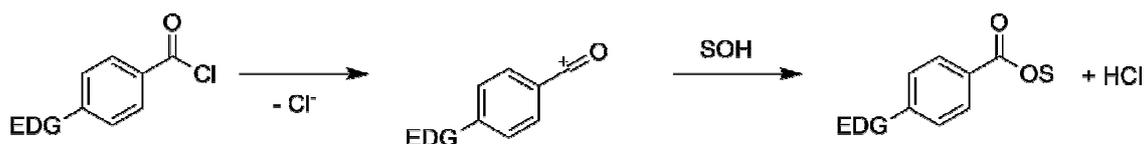
한양대학교 과학기술대학 응용화학과 ¹한양대학교 응용화학과 ²Northern Illinois University

The reactions of (4-trifluoromethylthio)benzoyl chloride was studied in usual solvolytic conditions, 25.0 oC, pure and hydroxylic binary solvents, and the conductivity method. Rate constants were analyzed by Grunwald-Winstein equations and compared with previously reported other benzoyl chlorides for confirming the effect of substituents. The solvolysis of (4-trifluoromethylthio)benzoyl chloride was showed different aspect compared with previously reported 4-methoxy and 4-methylthio derivatives, because para-substituent, 4-trifluoromethylthio group has electron withdrawal effect, so dual pathways were observed with several evidences, kinetic solvent isotope effect and thermodynamic parameters.

1. Bimolecular Pathway



2. Unimolecular Pathway



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장소: 창원CECO

발표코드: **PHYS.P-277**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvatochromic properties of coumarin dyes and their applications to amyloid aggregation probing

이휘인 이민영*

이화여자대학교 화학나노과학과

Solvatochromic fluorescence dyes such as ANS and bis-ANS have been widely used to probe protein aggregation. We explored two coumarin dyes, coumarin 6 (C6) and coumarin 7 (C7), as new solvatochromic dyes and used C6 and C7 to investigate the early stage of amyloid aggregation processes. The emission spectra of both dyes showed a significant spectral shift as bound to amyloid oligomers in comparison with the monomeric state in buffer. The sizes of amyloid oligomers were characterized by high resolution AFM as a function of incubation time. The steady-state and time-resolved fluorescence were employed to monitor the binding affinity of C6 and C7 to amyloid aggregates. The binding mode and association constant of the coumarin dyes to amyloid were analyzed on the basis of the molecular structure of oligomer aggregates.

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장소: 창원CECO

발표코드: **PHYS.P-278**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Elastic and diffusive motions in silver-containing Boger nanofluids

고문지 이민영*

이화여자대학교 화학나노과학과

A Boger fluid belongs to non-Newtonian and viscoelastic liquids in which the viscosity is independent of the shear rate. We prepared Boger nanofluids which consist of water, high molecular weight polyacryamide ($M_w = 18,000,000$), and silver nanoparticles. The shear viscosity and thermal conductivity of the Boger nanofluids were measured as a function of silver nanoparticle size and concentration. The translational diffusion coefficients of silver nanoparticles were measured using dynamic light scattering and by fitting the measured correlation functions to sum-of-exponential. The results were analyzed to distinguish the elastic and diffusive contributions and were described in terms of the local structures, viscoelastic properties, and particle characteristics of Boger nanofluids.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence energy and electron transfer involving lumiflavin chromophore in polymer media

이유민 이민영*

이화여자대학교 화학나노과학과

Flavins such as riboflavin (Vitamin B2), flavin mononucleotide (FMN), flavin adenine dinucleotide (FAD) play an important role in biological processes. This work attempts to explore lumiflavin (7,8,10-trimethyl-isoalloxazine), a basic unit of flavins, as a new fluorescence probe for the studies of light-induced energy and electron transfer processes. Using time-resolved fluorescence, we investigated the fluorescence resonance energy transfer (FRET) between lumiflavin and DQOCI and the photoinduced energy transfer (PET) between lumiflavin and tryptophan in poly(vinyl alcohol). Based on existing theoretical models, a comparative study between FRET and PET is presented for the first time by interpreting the fluorescence decay profiles of lumiflavin with respect to the quencher concentrations.

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장소: 창원CECO

발표코드: **PHYS.P-280**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydration/Dehydration Mechanisms in Aqueous Solution: A QM/EFP-MD Study

강은정 Manik Kumer Ghosh 최철호*

경북대학교 화학과

The hydration of carbon dioxide is the most important reaction in several biological and environmental processes. The reverse reaction: dehydration of bicarbonate ion also very important. Not only these hydration/dehydration reactions, simply intermolecular interaction between carbon dioxide and water molecules is of great interest due to importance of in different areas of science and technologies. But the detailed structural information during this process is still unknown. At first, we investigated and collected the structural information of carbon dioxide?water complexes in the aqueous solution. Then we studied the mechanism of hydration/dehydration reaction process in aqueous solution and detailed structural information during this process. Both ab initio cluster calculation and quantum mechanical effective fragment potential-molecular dynamic (QM/EFP-MD) simulations have been performed through this work.

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장소: 창원CECO

발표코드: **PHYS.P-281**

발표분야: 물리화학

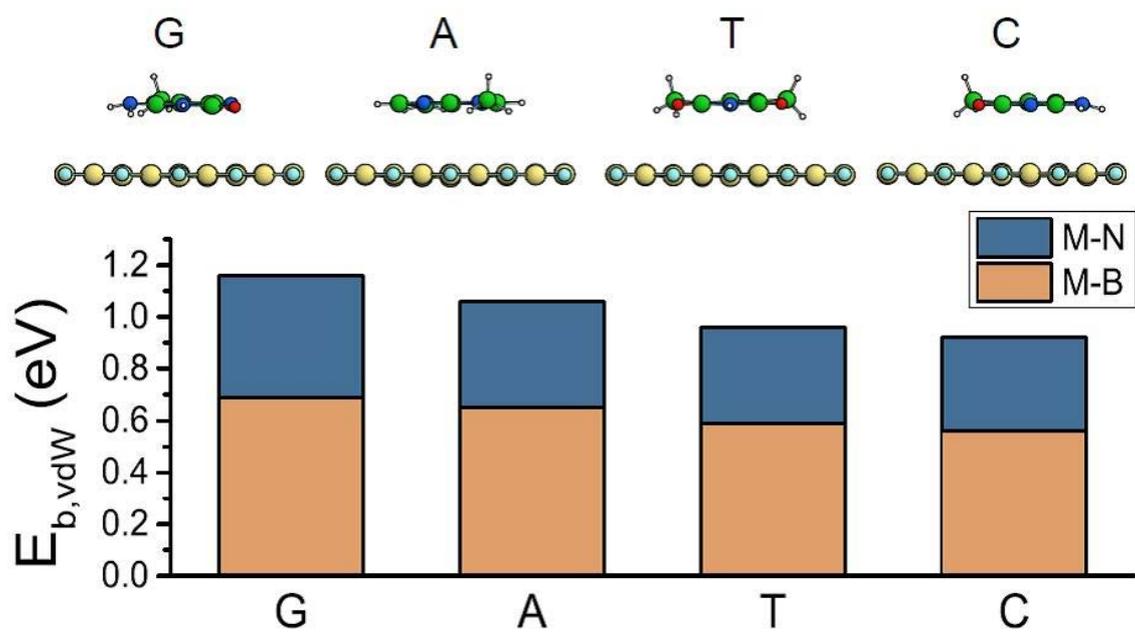
발표종류: 포스터, 발표일시: 수 16:00~19:00

Physisorption of DNA Nucleobases on h-BN and Graphene: vdW-Corrected DFT Calculations

이준호 조준형*

한양대학교 물리학과

We present a comparative study of DNA nucleobases [guanine (G), adenine (A), thymine (T), and cytosine (C)] adsorbed on hexagonal boron nitride (h-BN) sheet and graphene, using local, semilocal, and van der Waals (vdW) energy-corrected density-functional theory (DFT) calculations. Intriguingly, despite the very different electronic properties of BN sheet and graphene, we find rather similar binding energies for the various nucleobase molecules when adsorbed on the two types of sheets. The calculated binding energies of the four nucleobases using the local, semilocal, and DFT+vdW schemes are in the range of 0.54 ~ 0.75 eV, 0.06 ~ 0.15 eV, and 0.93 ~ 1.18 eV, respectively. In particular, the DFT+vdW scheme predicts not only a binding energy predominantly determined by vdW interactions between the base molecules and their substrates decreasing in the order of G>A>T>C, but also a very weak hybridization between the molecular levels of the nucleobases and the π -states of the BN sheet or graphene. This physisorption of G, A, T, and C on the BN sheet (graphene) induces a small interfacial dipole, giving rise to an energy shift in the work function by 0.11 (0.22), 0.09 (0.15), -0.05 (0.01), and 0.06 (0.13) eV, respectively. Reference- Jun-Ho Lee, Yun-Ki Choi, Hyun-Jung Kim, Ralph H. Scheicher, and Jun-Hyung Cho, J. Phys. Chem. C 117, 13435 (2013).



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장소: 창원CECO

발표코드: **PHYS.P-282**

발표분야: 물리화학

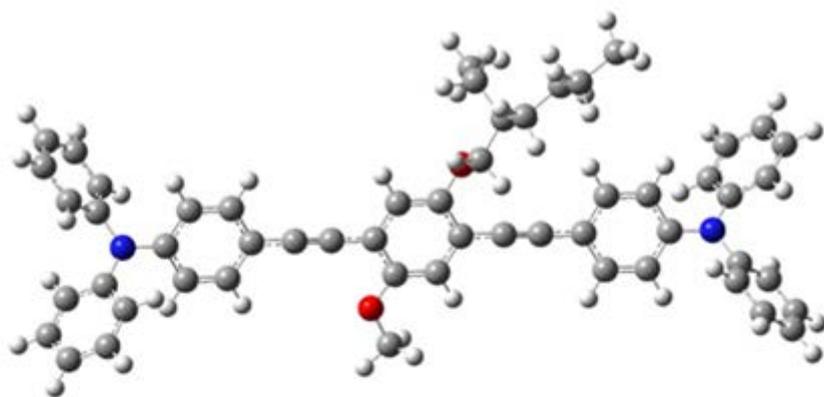
발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical study on the absorption maxima and the electronic properties of various molecular structures

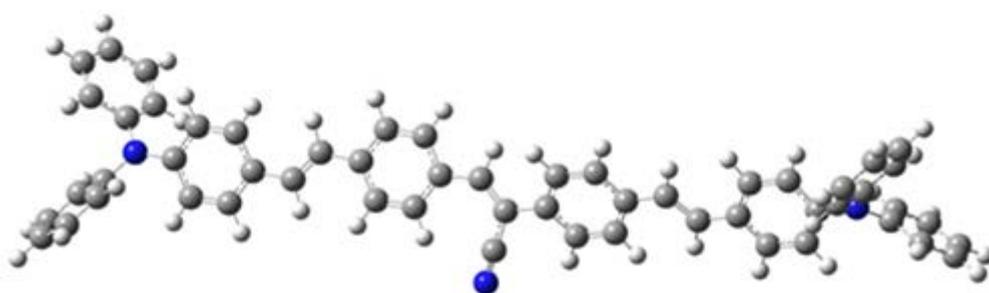
김종민 김승준*

한남대학교 화학과

벤치 마킹 테스트를 위하여 임의로 선택된 10 개 분자에 대하여 밀도 범함수 이론(DFT)과 시간 의존 밀도 범함수 이론(TDDFT)을 사용하여 UV/VIS 스펙트럼(Spectrum)을 예측하였다. 분자 구조는 B3LYP/cc-pVTZ 의 이론 수준까지 최적화하였으며, 분자 대칭 및 용매간의 상호작용에 대한 퍼텐셜 에너지를 고려하여 최대 흡수 파장(λ)을 예측하였다. 본 연구에서 최적화된 모든 분자 구조들은 진동주파수를 계산하여 최소 에너지(Local minimum) 구조임을 확인하였으며, 들뜬 상태의 진동 주파수로부터 최대 수직 전이(Frank-Condon factor) 효과를 고려하여 계산하였다. 이론으로 계산된 값과 실험값의 오차 퍼센트율을 구하고 선형 식을 세워 비교 및 경향성을 분석하였다. 이를 토대로 관심 있는 OLED 물질인 MW743 ((Z)-2,3-bis[4-(N-4-(diphenylamino)styryl)phenyl]-acrylonitrile, EMPA (N-diphenyl-[4-[2-[4-[2-[4-(N-phenylanilino)phenyl]ethynyl]phenyl]ethynyl]aniline]1-(heptyloxy)-4-(methoxy)benzene)들에 대한 UV/VIS 스펙트럼(Spectrum)을 예측하여 실험값과 비교 분석하였다.



EMPA



MW743



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-283**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photothermal Image Analysis for Capillary Electrophoresis

이재은 최중길*

연세대학교 화학과

This study demonstrates a photothermal image analysis for the capillary electrophoresis (CE). The Photothermal image analysis is a new detection method that combines the photothermal effect with the image analysis technique. The heat caused by the absorption of an excitation beam from the sample leads to the change in the aspect of a probe beam periodically. Since the probe beam is used as a reference indicating the signal of the photothermal effect due to the absorption of excitation energy at the sample, the detection of the signal is performed by observing the size or position changes of the probe beam. These changes are continuously monitored and analyzed in real time using a camera system and the signal amplitude is determined through FFT. It is possible to detect the changes of the probe beam by the heat generated from the sample flow in a capillary. A mixture of few different dye samples is separated in time by the CE and then detected by the photothermal image analysis. This new detection method is found to possess its advantage of wide applicability in various conditions with a high sensitivity.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **PHYS.P-284**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Monte Carlo Simulation Studies on the Field Effects in Diffusion-Influenced Reaction

김태준 김효준*

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One of long standing issues in diffusion-influenced reactions is the external field effect since it is common in a broad range of experiments. The external electric field can be a useful controllable factor. Similarly, the external magnetic field has been a valuable tool for various molecular studies. Even for a nonpolar particle, the ubiquitous gravitational force can affect its Brownian motion. However, it is not easy to analyze the field effects using the efficient lattice-based Monte Carlo simulations because the relation between the field strength and the direction probability is ambiguous. In this presentation, we report an explicit relationship between the two to extend the applicability of Monte Carlo simulations significantly.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural versus Energetic Approaches for Protein Conformational Entropy

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Conformational entropy is among the key factors that regulate protein folding, protein-protein interaction, and protein-ligand binding. Yet, its accurate estimation for complex bio-molecules remains a challenge in physical chemistry. The most popular quasiharmonic method is based on the conventional “horizontal” view of the free energy landscape, and formulates conformational entropy as accessible range of conformational space. Recently, an energetic approach has been proposed that instead focuses on the abscissa of the landscape, i.e., accessible range of the solvent-averaged effective energy. Here we demonstrate through applications to conformational ensemble of a folded protein that the conventional structural approach yields unreliable estimate of the conformational entropy due to inherent anharmonicities associated with the presence of multiple local energy wells, whereas the energetic approach retains efficacy since those energy wells probe similar values of the effective energy. The more robust energetic approach will be valuable for stability prediction and design of pharmaceuticals.

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Impact of Solvation Models on Structural Characteristics of Intrinsically Disordered Protein

정성호 함시현*

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Intrinsically disordered proteins are associated with functions of signaling and regulation as well as with a number of diseases such as cancer and neurodegenerative conditions. Molecular dynamics simulation is potentially a powerful tool to study those protein conformational disorders in full atomic details that would be difficult to gain from experimental measurements. However, the accuracy of the simulation critically relies on the quality of underlying potential energy functions or force fields. In particular, structural properties of intrinsically disordered proteins are expected to depend more sensitively on protein-water interactions because of their increased solvent exposure than folded globular proteins. Here, we investigate the impact of solvation models on structural characteristics of full-length amyloid-beta protein, an intrinsically disordered protein whose aggregation is linked to Alzheimer's disease. For this purpose, we performed extensive molecular dynamics simulations by combining AMBER ff99SB force field for protein with differing solvent water models as well as solvation procedures with different solvent box sizes. We find that the structural characteristics of amyloid-beta protein differ remarkably depending on the water model adopted as well as on the solvent box size. Our results demonstrate the significant sensitivity on the solvation procedure including the solvent force field in characterizing structural properties of intrinsically disordered proteins.

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Interaction of small hydrocarbon molecules with surface and bulk hydrogen on ZnO (000-1)-O terminated single crystal surface

MOTINABDUL

경북대학교 화학과

Bulk or subsurface hydrogen shows a very unique reactivity when it interacts with hydrocarbon species adsorbed on the surface. Compared with surface hydrogen, the reactivity of bulk hydrogen is quite different. It has been suggested that the difference in spatial orientation between surface and bulk hydrogen results in different reaction paths. When the surface of ZnO is exposed to atomic hydrogen at low temperatures, bulk diffusion of hydrogen takes place. We have studied the reaction of bulk hydrogen with CH₃OH and CF₃COOH. We will compare the reaction of bulk hydrogen with that of surface hydrogen.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Porous Silicon based Off/On Sensor for Acetylcholinesterase Inhibitor Determination

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공주대학교 화학과 ¹Dept. of Bioengineering, UC Berkeley, CA 94720, USA

Acetylcholinesterase immobilized p-type porous silicon material has been developed for sensation of acetylcholinesterase inhibitors, utilizing the fluctuation in the photoluminescence before and after reaction with inhibitor. Different pore diameter of porous silicon samples were prepared by electrochemical etching in HF based electrolyte solution and appropriate sample was selected suitable for enzyme immobilization with maximum trapping ability. Porous silicon showed strong photoluminescence with maximum emission at 593 nm and immobilization of acetylcholinesterase on porous silicon surface quenches the photoluminescence of porous material (Turn off sensor). This enzyme immobilized non-luminescent surface upon incubation with standard acetylcholinesterase inhibitors (neostigmine methylsulfate) for 30 minutes at 37 °C triggers the photoluminescence showing maximum emission at 593 nm (Turn on sensor). The dramatic change in photoluminescence of enzyme immobilized surface upon reaction with enzyme inhibitor can be used as a tool for detection of acetylcholinesterase inhibitors by utilizing photoluminescence response upon incubation with inhibitor. Surface modification was characterized by field emission scanning electron microscopy and photoluminescence measurements. We speculate that the sensor's ability to detect acetylcholinesterase inhibitors is due to conformational changes of the enzyme structure on inhibitor binding.

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Vibrational Relaxation of Cyanate or Thiocyanate Bound to Ferric Heme Proteins Studied by Femtosecond Infrared Spectroscopy

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부산대학교 화학과

Femtosecond vibrational spectroscopy was used to measure vibrational relaxation time (T_1) of anion bound to ferric myoglobin (Mb) and hemoglobin (HbIII) in D₂O solution at 293 K. The anti-symmetric stretching (ν_1) mode of NCS in thiocyanate ion (NCS⁻) bound to ferric Mb (MbNCS) and Hb (HbNCS) has two bands near 2000 and 2040 cm^{-1} , red-shifted by 20 ? 60 cm^{-1} from that of NCS⁻ ion in D₂O solution. In contrast, the ν_1 mode of NCO in cyanate ion (NCO⁻) bound to Mb (MbNCO) and Hb (HbNCO) shows one band near 2160 cm^{-1} , almost the same location as that of NCO⁻ in D₂O solution, suggesting that the bonding characteristics of NCO⁻ changes barely upon binding to the heme Fe of Mb and Hb. The T_1 of the ν_1 mode of NCS in MbNCS and HbNCS is 7.2 ± 0.2 and 6.6 ± 0.2 ps, respectively. Both T_1 's are smaller than that of NCS⁻ in D₂O solution, 18.3 ps. The T_1 of the ν_1 mode of NCO in MbNCO and HbNCO is 2.4 ± 0.2 and 2.6 ± 0.2 ps, respectively, which is larger than that of NCO⁻ in D₂O solution, 1.6 ± 0.2 ps. Smaller T_1 of the ν_1 mode of NCS bound to heme proteins suggests that the intramolecular vibrational relaxation (VR) is the dominant relaxation pathway for the excess vibrational energy in the ν_1 mode of NCS in MbNCS and HbNCS. On the other hand, longer T_1 of the ν_1 mode NCO bound to heme proteins suggests that the intermolecular VR is the dominant relaxation pathway for the excess vibrational energy in the ν_1 mode of NCO⁻ in D₂O solution, implies that intramolecular VR becomes more important in vibrational energy dissipation of the ν_1 mode of NCO in MbNCO and HbNCO. Faster VR in the ν_1 mode of NCO than NCS in the corresponding ligand bound to heme proteins suggests that intramolecular VR is more efficient in NCO⁻ than NCS⁻ bound to heme.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

DFT study of the role of intramolecular hydrogen bonds in two representative phenolic antioxidants in their activities against radical compound

장효원* 이진호¹

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Amide derivatives of trihydroxyphenylacetic acid and gallic acid were compared in their antioxidant activities by measuring the radical scavenging activity adopting diphenyl picrylhydrazyl radical. We choose one specific compound for each acid, among them gallic acid derivative were observed to surpasses phenylacetic acid derivative in their activity. This experimental observation was tried to be simulated quantum chemically using DFT calculations in this work. Through the reaction path forming a complex molecule composed of antioxidant and radical, several local minima were located, each stabilized by proper hydrogen-bonds between two combining molecules. From each local minimum, hydrogen-transfer reaction path from antioxidant to radical, and the accompanying activation energy was determined and compared to the values for other path and complex, accordingly. Hopefully, these activation energetics could be shown to support the existing experimental observations.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

DFT study of nitrogen-nitrogen bond activation during the model catalytic cycle synthesizing hydrazine-hydrogen from ammonia using iridium pincer complex

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Catalytic hydrazine decomposition is important process such as monopropellant thrusters, gas generators and hydrogen production for electric fuel cells. In this study, the previously studied catalytic role of iridium pincer complex for N-H and C-H bond activation is extended to N-N bond activation and tested for hydrogenation of hydrazine to ammonia reaction. Specifically, a hypothetical reaction pathway composed of 7 elementary steps connecting reactant of hydrazine and hydrogen molecule to product of two ammonia is proposed by DFT calculation. The highest activation barrier is located 89 kJ/mol above the reactant and the rate determining step has 178 kJ/mol barrier corresponding to N-N bond breakage, which is compared to the uncatalyzed barrier of 375 kJ/mol. The extent of N-N bond activation by the catalyst is compared to the uncatalyzed case. In addition, we note that the substrate-catalyst complex exhibits 4 to 7 coordinated geometries during the catalytic actions.

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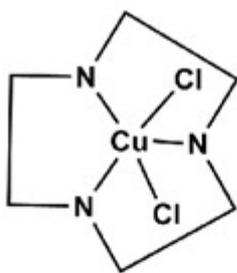
발표종류: 포스터, 발표일시: 수 16:00~19:00

The ligand effect and cooperative role of metal ions on the DNA cleavage efficiency of mono and binuclear Cu(II) complexes containing macrocyclic ligands

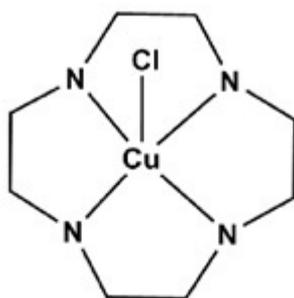
문지혜 장윤정 이동진¹ 김석규*

영남대학교 화학과 ¹경일대학교 화학공학과

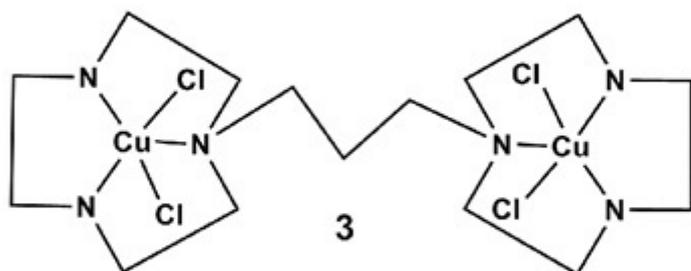
Two binuclear Cu(II) complexes of N-functionalized macrocycle ligands have been synthesized and compared their ability to hydrolyze the cleavage of supercoiled plasmid DNA (pBR322) with structurally related non-functionalized mononuclear Cu(II) complexes. The binuclear Cu complex of symmetrical ligand (3) showed significantly enhanced double-strand cleavage activity compared to other three complexes at the same $[Cu^{2+}]$ concentration. Surprisingly, binuclear complex with unsymmetrical macrocyclic ligand (4) did not give rise to double-strand DNA cleavage. The linear DNA formation induced by mononuclear complex (2) is realized via a non-random double-stranded scission process. The differential cleavage activity is discussed in relation to the dimer formation, effective cooperation and coordination environment of metal centre. The hydrolytic cleavage by the copper complexes without H_2O_2 is supported by the evidence from anaerobic reaction, free radical quenching, and NBT assay. Conversely, both the binuclear complexes (3) and (4) cleave supercoiled DNA very efficiently to form III (linearized DNA) in the presence of the hydrogen peroxide, indicating nuclearity is a crucial parameter in oxidative cleavage. The radical scavenger inhibition study and NBT assay suggest the involvement of hydrogen peroxide and superoxide ion in the oxidative cleavage of DNA by binuclear complexes.



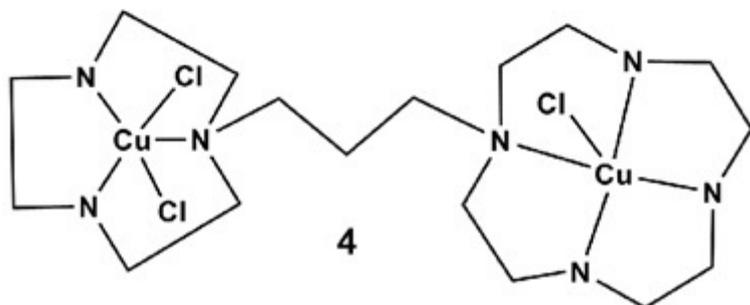
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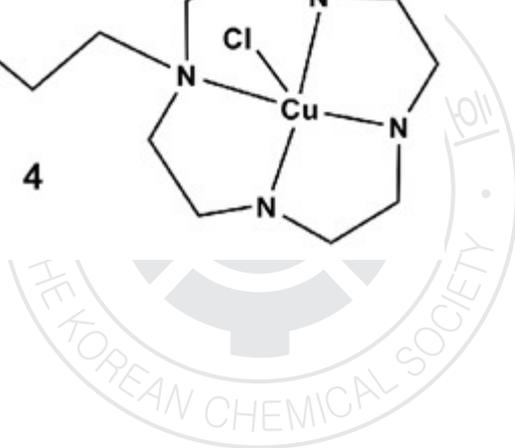
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일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Direction of intercalation of a *bis*-Ru(II) complex to DNA probed by a minor groove binding molecule, 4',6-diamidino-2-phenylindole

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The direction of intercalation to DNA of the planar dipyrido[3,2-*a*:2',3'-*c*]phenazine ligands (dppz) of a bis-Ru(II) complex, namely; [Ru(1,10-phenanthroline)₂dipyrido[3,2-*a*:2',3'-*c*]phenazine]²⁺ linked by a 1,3-*bis*(4-pyridyl)propane, to DNA was investigated by probing the behaviour of 4',6-diamidino-2-phenylindole (DAPI) bound deep in the minor groove. The *bis*-intercalation of DPPZ resulted in a slight blue shift and hyperchromism in the DAPI absorption band, as well as a large decrease in DAPI fluorescence intensity, which was accompanied by an increase in the dppz emission intensity. A reduced intensity of positive induced circular dichroism (CD) and linear dichroism (LD) were also observed. These spectral changes suggest that the insertion of the dppz ligand caused a change in the binding mode of DAPI, which probably moved to the exterior of DNA from the minor groove. At the surface of DNA, DAPI binds at the phosphate groups of DNA by an electrostatic attraction. Consequently, this observation indicates that the dppz ligand intercalates from the minor groove.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation of Poly[d(A-T)₂] Specific Z-DNA by a Cationic Porphyrin

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Typical CD spectrum of the right-handed poly[d(A-T)₂] was reversed when *trans*-bis(N-methylpyrimidium-4-yl)diphenyl porphyrin (*trans*-BMPyP) was bound, suggesting that the helicity of the polynucleotide was reversed to the left-handed form. The formation of the left-handed Z-form poly[d(A-T)₂] was confirmed by ³¹P NMR, in which a single ³¹P peak of B-form poly[d(A-T)₂] was split into two peaks, which is similar to the conventional B-Z transition of poly[d(G-C)₂] induced by the high ionic strength. The observed B-Z transition is unique for poly[d(A-T)₂]. The other polynucleotides, including poly[d(G-C)₂], poly(dG) · poly(dC) and poly(dA) · poly(dT) remained as the left-handed form in the presence of the same porphyrin. This observation suggests that the porphyrin array that was formed along the poly[d(A-T)₂] provides a template to which left-handed poly[d(A-T)₂] is associated with an electrostatic interaction.

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발표분야: 물리화학

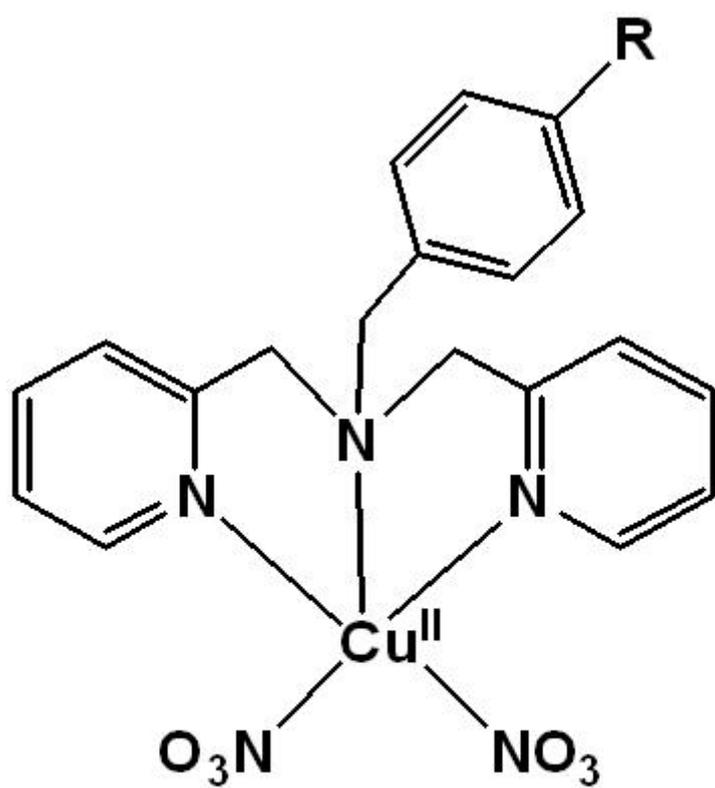
발표종류: 포스터, 발표일시: 수 16:00~19:00

Real-time Detection of DNA Cleavage Induced by Copper Complexes

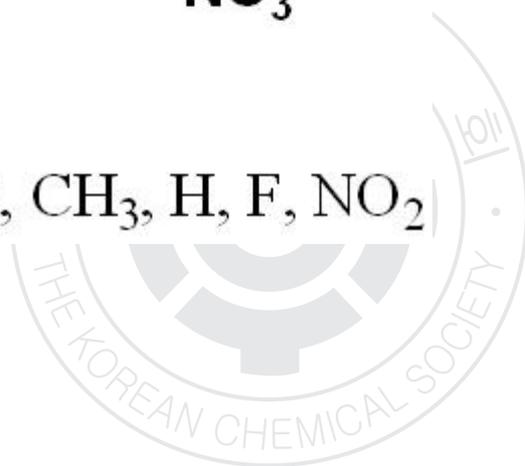
WANGWEI 정맹준¹ 김석규*

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The efficiency of 4-R-Benzyl-dpa (dpa: dipicolylamine) Copper complexes (R=CH₃O, CH₃, H, F, NO₂) in oxidative DNA cleavage was examined by electrophoresis and linear dichroism (LD). Among the five Cu complexes, the 4-MeOBdpa+Cu, 4-MeBdpa+Cu showed the highest efficiency in super-coiled DNA (scDNA) cleavage in electrophoresis. The LD signal at 260nm decreased gradually with increasing time. The decrease in LD magnitude was explained best by the sum of two single exponential curves. This suggests that the cleavage reaction involves two first order kinetic processes; an increase in flexibility due to scission of one of the strands and shortening in the DNA stem due to cut of both stands of double stranded DNA (dsDNA). In agreement with the electrophoresis data, the Bdpa+Cu complex exhibited the highest efficiency with the singlet oxygen radical found to be the essential reactive oxygen species. The order of efficiency in both scDNA and dsDNA was as follows: 4-MeBdpa+Cu > 4-MeOBdpa+Cu > Bdpa+Cu > 4-FBdpa+Cu > 4-NO₂Bdpa+Cu.



$\text{R} = \text{CH}_3\text{O}, \text{CH}_3, \text{H}, \text{F}, \text{NO}_2$



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, DNA binding and cleavage of divalent transition metal complexes

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Abstract: Complexes of dipyriddyamine based ligand with benzo quinoline moiety containing divalent metal ions Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) have been structurally characterized and their electrochemical properties has also been studied. The interaction of the five metal complexes to calf thymus DNA has been investigated with aid of UV absorption and linear dichroism studies, and the mode of CT-DNA binding for the complexes have been proposed. The experimental results show that they can efficiently induce considerable oxidative DNA cleavage in the presence hydrogen peroxide and dioxygen. The Zn(II) does not show any appreciable cleavage activity, Cd(II) and Ni(II) are moderately active, while Cu (II) and Co(II) shows formation of a significant quantity of linear DNA resulting from double-strand breaks (dsb). Mechanistic studies reveal the involvement of $\cdot\text{OH}$ and $^1\text{O}_2$ as the reactive species in the scission process under an aerobic medium. A mechanism involving either the Fenton or the Haber – Weiss reaction is proposed for the DNA cleavage mediated by these complexes. The Cu (II) and Co(II) complexes can also cleave the double stranded CT-DNA in the presence of activator most probably *via* an oxidative mechanism, whereas the activity of the other complexes is negligible under similar reaction conditions. The kinetic aspects of double-stranded CT-DNA cleavage with both Cu (II) and Co(II) are detailed.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Spectroscopic Study on the Interactions of Porphyrin with G-quadruplex

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영남대학교 화학과

TMPyP(*Meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin) is known to have a high affinity for G-quadruplex DNA. However, there is still some controversy over the exact binding site(s) and mode(s) of TMPyP to G-quadruplex DNA. In this study, the binding properties of TMPyP to thrombin-binding aptamer (TBA = d(G)_nTT(G)_nTGT(G)_nTTG_n, where *n* = 2, 3, and 4), which forms a quadruplex in the presence of K⁺ ion, was investigated by various optical spectroscopies namely, UV, CD and time-resolved fluorescence spectroscopy. Upon binding to the G-quadruplex, a large red-shift and hypochromism in the Soret absorption region of TMPyP were observed, suggesting a strong interaction between TMPyP and the G-quadruplex. A positive induced CD signal in the Soret region was apparent for *n* = 2 and 4, whereas bisignate band was observed for *n* = 3, indicating that the binding mode of TMPyP to these G-quadruplex depends on the number of the G-quartet. For all cases, the fluorescence decay time of ~ 5 ns for DNA-free TMPyP exhibited two decay times. This observation suggested that the binding mode of TMPyP to G-quadruplex is heterogeneous.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction of MnTMPyP with Triplex Helical DNA

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영남대학교 화학과 ¹삼척대학교 식품영양학과

Interaction of MnTMPyP with various triplex DNAs(PolydC · PolydG · PolydC, PolydT · PolydA · PolydT, PolyC · PolydI · PolydC) studied absorption, Circular dichroism(CD) and Linear dichroism(LD). A positive CD-signal observed for interaction of PolydC · PolydG · PolydC with MnTMPyP. In the case of PolyT · PolydA · PolydT low mixing ratio have only one positive signal where as two Positive signals observed for high ratio. PolydC · PolydI · PolydC case have one positive signal at low ratio and weak negative, at high mixing ratio LD spectrum of triplex DNAs also produced different kind of LD signals.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

여러 종류의 친환경 지방산 첨가에 의한 아이오노머의 동적 기계적 성질 및 형태학

김영민¹ 고헌환¹ 김준섭² 유정아^{3,*}

조선대학교 신재생에너지융합학과 ¹조선대학교 첨단부품소재공학과 ²조선대학교 응용화학소재공학과 ³조선대학교 화학교육과

아이오노머의 구조적인 특성과 그와 상관된 물성으로 학계 및 산업계에서는 아이오노머의 응용분야에 대한 많은 연구가 진행되고 있다. 하지만 아직 이온성 고분자의 사용 범위는 일반 고분자와 비교해 산업계에서의 이용은 미미한 실정이다. 기존의 가소제나 첨가제의 단점을 보완하고 장점은 더욱 부각시킬수 있는 대체제로 이용을 위하여 본 실험을 진행하였다. 대두, 우지, 미강 지방산등의 친환경 지방산을 첨가한 아이오노머를 만들어 물리적 성질 및 형태학적인 분석을 시도하고자 하였다. 술폰산을 2.7% 포함한 P(S-co-SA)Na 아이오노머에 일정한 중량비의 대두,우지, 미강 지방산을 첨가하여 DMA 를 이용하여 동적 기계적 성질을 측정하였다. 순수한 P(S-co-SA)Na 아이오노머와 각각의 지방산을 첨가한 아이오노머의 matrix 와 cluster T_g 를 비교하여 보면 지방산을 첨가하였을 때 cluster T_g 가 비교적 큰폭으로 낮아짐을 알 수 있다.

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발표코드: **PHYS.P-300**

발표분야: 물리화학

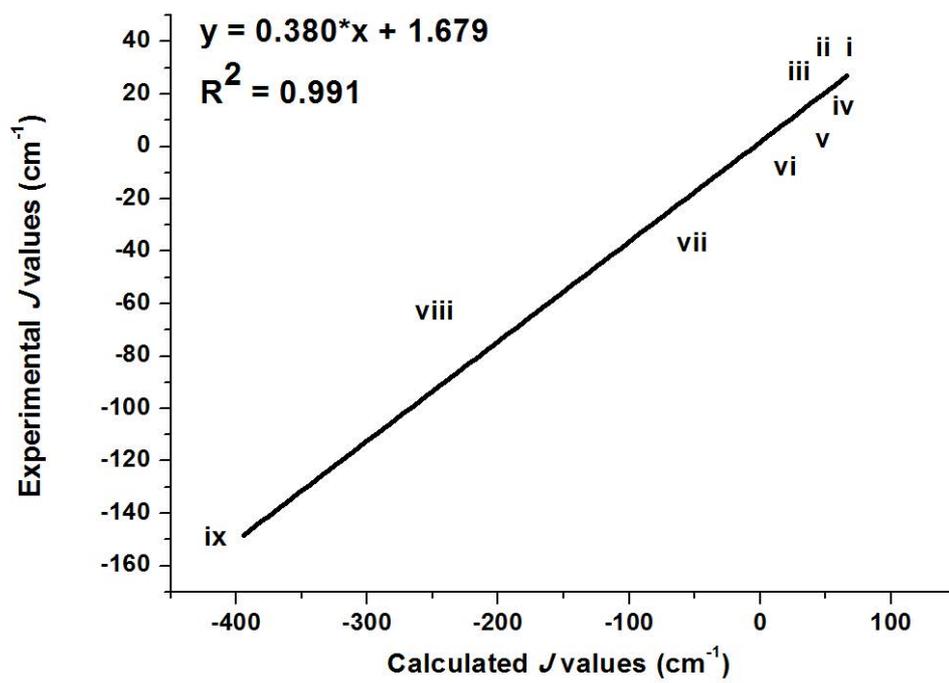
발표종류: 포스터, 발표일시: 수 16:00~19:00

Scaling approach for Intramolecular Magnetic Coupling Constants for Stable Organic Diradicals: A DFT Study

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성균관대학교 화학과

The intramolecular magnetic coupling constant (J) of 9 diradicals (i-ix) coupled with an aromatic ring were investigated by means of unrestricted density functional theory calculations [B3LYP/6-311++G(d,p)]. For those diradicals, the remarkable linear relationship was found between the calculated and experimental J values on the basis of results of the linear regression analysis. In this study, we suggest that the value of slope (0.380) of linear regression line can be used as scaling factor for estimating the accurate J values. By applying this scaling factor to the calculated J values, we can predict the reliable J values of four DTDA diradicals (x-xiii) coupled with an aromatic ring for the first time. It also found that certain scaling factors have a restricted application depending on the length of a coupler. In conclusion, this approach, which uses a scaling factor, can be used to estimate the accurate J values for diverse diradical systems coupled with a particular coupler using DFT calculations.



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The Grunwald-Winstein Relationship in the Solvolysis of β -substituted Chloroformate Ester Derivatives: The Solvolysis of Alkyl Chloroformates

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Solvolysis rate constants of 2-phenylethyl- (1) and 2,2-diphenylethyl chloroformate (2), together with the previously studied solvolyses of α - and β -substituted chloroformate ester derivatives, are reported in pure solvents and binary mixtures at 40.0 °C. The linear free energy relationship (LFER) and the sensitivities to changes in solvent nucleophilicity (N_T) and solvent ionizing power (Y_{Cl}) of the solvolytic reactions is analyzed using the Grunwald-Winstein equation. The kinetic solvent isotope effects (KSIEs) and the activation parameter values for the solvolyses of both substrates are also determined in additional. These results are supported well the bimolecular pathway with same aspects. Furthermore the small negative values for the entropies of activation of solvolysis of 1 and 2 in the highly ionizing aqueous fluoroalcohols were consistent with the ionization character (mechanism) of the rate-determining step, and the KSIE values of 1.78 and 2.10 in methanol-*d* indicate that one molecule of solvent acts as a nucleophile and the other acts as a general-base catalysis. It is found that the β -substituents in chloroformate is not the important factor to be decided the solvolysis reaction pathway.

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Understanding structural properties affecting Amyloid β ($A\beta$) Aggregation

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Amyloid β ($A\beta$) is made up of 40-42 amino acids and is generated by proteolytic cleavage of the amyloid precursor protein. The formation of the $A\beta$ fibrils has been known as a key process in Alzheimer's disease, but the mechanism has not been clearly understood. In the $A\beta$ fibril structure, residues 1-17 have been known to be disordered and residues 18-26 and 31-42 forming β sheets connected by the turn structure. Recently, new structural model of $A\beta$ fibril was reported and mutations of phenylalanine residues to leucine/isoleucine residues were reported to make $A\beta$ aggregation accelerated. We have performed systematic simulations on two popular structural models of the $A\beta$ fibrils for the wild type, F(19,20)I and F(19,20)L mutants using AMBER force field with the implicit solvation model. Our results showed that the steric zipper contacts might be favorable interactions in the aggregation process and the structural flexibility of I/L residues might play the role as an enhancer for aggregation. The relative high barrier for the isomerization between two structural models implies that the β -sheet-turn- β -sheet topology of the monomer could play a vital role. It can be argued that different topologies suggested by the two structural models are favored in the different stages of aggregation: the early onset of the nuclei and the elongation process.

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Theoretical approaches on the hydrogen-bonding effect of $H_2O_n-H_2O_m$ ($n=1-4$, $m=1-4$) dimers

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Hydrogen polyoxide, H_2O_n ($n=1-4$) 이중합체(dimer)에 대하여 분자 구조 변화에 따른 수소결합(H-bonding) 효과를 연구하기 위하여 순 이론적 계산 (ab initio), 밀도 범함수 이론 (DFT) 등 양자역학적 방법을 사용하여 분자 구조를 최적화하고 결합에너지 및 진동주파수를 계산하였다. 분자 구조는 B3LYP, CAM-B3LYP, MP2 의 양자역학적 방법들을 사용하여 최적화하였으며, 최적화된 모든 분자 구조들은 진동주파수를 계산하여 최저에너지(true local minimum) 구조인 것을 확인하였다. 보다 정확한 결합에너지(E) 계산을 위하여 CCSD(T) 이론수준에서 한 점(single-point) 에너지를 계산하였으며, 영점 진동에너지(ZPVE) 보정과 바탕집합 중첩 에러(BSSE) 보정을 하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Spectroscopic investigation of the interaction and binding site of gallic and ellagic acids with bovine serum albumin

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인천대학교 화학과

The interaction of tannic acid derivatives, gallic and ellagic acids, with the protein, bovine serum albumin (BSA) has been studied using fluorescence spectroscopic methods. Gallic and ellagic acids, natural dietary phenolic substances, show a variety of biological activities including antioxidant, anti-inflammatory, and anti-fibrosis, which are in part due to interactions with biomolecules such as proteins or DNA. The interaction of gallic and ellagic acids with BSA was characterized by examining the quenching of intrinsic fluorescence of BSA. The binding parameters including the binding constants and the number of binding sites were determined using the modified Stern-Volmer equation as well as the Scatchard-type analysis, and the nature of binding interactions was discussed. Site marker displacement experiments were also conducted to reveal binding sites of BSA for gallic and ellagic acids.

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Physisorption of the Various Gases (CO, CO₂, NO, SO) on Graphene and g-BN sheet on the DFT Study

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그래핀(graphene)의 탄소(C)를 붕소(B)와 질소(N)로 치환한 g-BN(B₁₆N₁₆H₁₄)과 그래핀(C₃₂H₁₄)의 흡착 물성을 비교하기 위하여 대기 오염의 주범인 CO, CO₂, NO, SO 기체들의 물리흡착(physisorption) 에너지를 계산하여 비교하였다. 각각의 분자구조는 밀도 범함수 이론(DFT) 가운데 B3LYP 와 CAM-B3LYP 방법을 사용하여 최적화 하였으며, 최적화된 모든 분자 구조에서 진동 주파수를 계산하여 최저 에너지 (true local minimum) 구조인 것을 확인하였다. 물리흡착 에너지에 대한 보다 정확한 계산을 위하여 진동주파수를 이용하여 영점 진동에너지(ZPVE)를 보정하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of laser wavelength and energy density on Ni nanoparticles by pulsed laser ablation in deionized water with or without SDS

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In the past decade, pulsed laser ablation in liquids (PLAL) environment has proven to be efficient method for preparing various nano materials. PLAL has been a successful nanofabrication tool, allowing the adjustable fabrication design by experimental parameters such as the laser wavelength and the presence of surfactants. However, in case of the fabrication of Ni nanoparticles by PLAL, there were few studies on the dependence of size distribution of Ni nanoparticles on the laser energy density and wavelength. In this experiment, we use a pulsed nanosecond Nd:YAG laser in deionized water with Ni plate. It produces nano-structured Ni particles at different laser wavelength (532nm, 1064nm) and energy density (3.2 J/cm² , 10.5 J/cm² and 19.9 J/cm²) with and without sodium dodecyl sulfate(SDS) addition as a surfactant. Laser power is fixed by 100mJ/pulse. In this study, the mean diameter and the width of size distribution of the nanoparticles were influenced by the laser energy density and wavelength. Based on the observations, we propose that the wavelength and energy density dependence of the laser ablation processes can be explained by the amount of energy absorbed to the metal target and the space homogeneity of ablated plume. The consequences of ablation mechanism are also discussed. In addition, structural and morphological characterizations of synthesized Ni nanoparticles were conducted by cyclic voltammetry (CV) using multi-walled carbon nanotube (MWCNT), UV-vis spectroscopy and high-resolution transmission electron microscopy (HR-TEM) .

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Transient Optical Property of Fluorescence of Graphene Oxide(GO) Depending on Concentration

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엘투케이플러스 기업부설연구소 ¹한국표준과학연구원(KRISS) 양자연구부 분광그룹 ²한국표준과학연구원 미래융합기술부 의료융합측정표준센터

The origin of fluorescence from Graphene Oxide has been interesting in application of Graphene Oxide, which could be very potential for low-cost opto-electronics, biological applications, membranes, and transport barrier composites. Recently, the origin of fluorescence of Graphene Oxide is proposed through the tuning of PL from 400 nm 800 nm could be realized by gradual reduction of the GO suspension and the electron-hole recombination from the bottom of the conduction band and nearby localized states to wide-range valance band as origin of the fluorescence. Herein, we could see the shift of fluorescence of Graphene Oxide depending on concentration in water solution and polymer matrix. We have characterized transient optical properties that transient spectroscopy was performed with the TCSPC by utilizing tunable ultrashort pulses generated from Orpheus and Pharos combinations and the pump-probe technique via Ti:sapphire femtosecond laser with 800nm wavelength.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Picosecond Dynamics of Photoexcited HNO-bound Myoglobin in D₂O Solution Probed by Femtosecond Vibrational Spectroscopy

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Like nitric oxide (NO), nitroxyl (HNO), a reduced form of NO, plays many biologically important roles including neurological function and vascular regulation. Although HNO is unstable in aqueous solution, it is exceptionally stable on binding to ferrous myoglobin (Mb) to form MbHNO. Various experimental and theoretical investigations has been carried out to unveil the structure of the active site and binding characteristics of MbHNO that can explain its functioning mechanism and the origin of its unusual stability. However, the binding dynamics of HNO to Mb, as well as the photochemical and photophysical processes associated with binding, have not been fully established. Herein, femtosecond vibrational spectroscopy was used to probe the photoexcitation dynamics of excited MbDNO in D₂O solution at 294 K with a 575-nm pulse. Time-resolved spectra were described by three vibrational bands near 1380 cm⁻¹, in the expected N²O stretching (ν_{N^2O}) mode of MbDNO, and all three bands showed instantaneous bleach that decays on a picosecond time scale. The three bands were assigned based on isotope shifts upon ¹⁵N substitution and ab initio calculation of the vibrational frequency on a DNO-bound model heme. These three bands likely arise from Fermi interactions between the strong ν_{N^2O} mode and the weak overtone and combination modes of the N atom-related modes. The immediate appearance of the bleach in these bands and the picosecond decay of the bleach indicate that most of the photoexcited MbDNO undergoes either picosecond geminate rebinding of DNO to Mb subsequent to its immediate deligation, rapid electronic relaxation accompanied by picosecond thermal relaxation of heme, or both.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Triarylamine-Functionalized Ru Dyes with Different Conjugation Lengths for Highly Efficient Dye Sensitized Solar Cells

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Since highly efficient dye-sensitized solar cells (DSSCs) based on ruthenium (Ru) complex, extensive efforts have been focused on development of new sensitizers to boost the power conversion efficiency. Functionalization of photo-sensitizer with extended π -electron delocalization is one of promising means to increase molar extinction coefficients, to shift the absorption bands to match the solar spectrum, and to enhance redox reversibility and photo-stability. Electron-rich molecules such as triphenylamine and carbazole provide good hole-transporting properties for photovoltaic applications. On the basis of this concept, we have designed new Ru dyes with an alkoxy-substituted triphenylamine group that are bridged from bipyridine through extended π -conjugation of one or more styryl groups, and investigated their properties as a photo-sensitizer in DSSCs. The effects of ligands with different conjugation linkage length on the photophysical properties and on the performance of DSSCs based on the new dyes have been studied.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Conformational Preferences of Helix Foldamers of γ -Peptides Based on 2-Aminocyclohexylacetic Acid

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The conformational preferences of helix foldamers having different sizes of the H-bonded pseudocycles have been studied for di- to octa-peptides based on 2-aminocyclohexylacetic acid (γ Ac_{6a}) with a cyclohexyl constraint on the C β -C γ bond using density functional methods. The conformational analyses on the γ Ac_{6a} peptides with homochiral (3*S*,4*S*) configuration reveal that the (*P*)-2.5₉-helices are most preferred for the di- γ Ac_{6a} peptides in the gas phase, which are also preferred in water considering the negligible difference in electronic energy between 9- and 14-helix for di- γ Ac_{6a} peptides. As the peptide sequence becomes longer, the (*P*)-2.5₁₄-helices are most preferred for the tetra- to octa- γ Ac_{6a} peptides both in the gas phase and in water due to the larger helix propensities and helix dipole moments of 14-helice. The mean backbone torsion angles and helical parameters of the 14-helix foldamers of oligo- γ Ac_{6a} peptides are consistent with those of X-ray structures for oligopeptides of (*S*)-2-((1*S*,2*S*)-2-aminocyclohexyl)butanoic acid and tetrapeptide of γ 2,3,4-aminobutyric acid despite the different substituents on the backbone. In particular, we found that the difference of the conformation preferences of between γ Amc₆ and γ Ac_{6a} oligopeptides could be decided by the only different positions of cyclohexyl constraints such as on the C α -C β bond and on the C β -C γ bond despite the same formula, and the similar mean backbone torsion angles and helical parameters.

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Topological Entanglements and Dynamics of a CNT in Polymer Melts

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서강대학교 화학과

We investigate the topological constraints and dynamics of carbon nanotubes (CNTs) and polymers in polymer nanocomposites by using molecular dynamics (MD) simulations. Topological entanglement between a CNT and polymers has a great effect on the dynamic behavior of polymers. The topological entanglement also would be responsible for the enhancement of mechanical properties of the polymer nanocomposites. We observe the dynamics of CNTs as the degree of entanglement increases. We quantify the degree of the topological entanglement of the polymer around the CNT by calculating the winding number of the polymer per CNT. We also try to elucidate the effect of stiffness of CNT on the topological entanglement and on the dynamics of the CNT.

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화학적 기상 증착에 의한 실리콘 표면에서 박막형성에 관한 연구

이경민* 김창민*

경북대학교 화학과

화학적 기상 증착은 화학 반응을 수반하는 증착 기술로서 모든 도체 박막의 증착에 사용될 수 있는 기술로써 넓은 면적에 빠른 속도로 박막을 형성할 수 있는 장점이 있다. 이 연구는 UHV 조건에서 화학적 기상 증착 과정에 따른 구리 박막의 성장 메커니즘을 규명하는 것을 목표로 하며 AES, LEED, TPD 를 사용하여 연구하였다. O₂(g)에 의해 산화된 Si(111) 표면 위에 -OH 를 형성한 후 (hfac)CuI(COD)와 H₂ 를 precursors 로 사용하여 박막을 형성하였다

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Semi-empirical simulation of absorption spectra for isotopomers : in case of formaldehyde molecules

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안정한 동위원소가 의학, 산업, 기초과학 분야 등에서 널리 사용되고 있다. 동위원소를 이용하기 위해서 동위원소 분리 기술이 점점 발전하게 되었다. 동위원소를 분리하는 여러 방법중 하나인 분자 레이저 동위원소 분리법(MLIS)은 특정 동위원소를 포함하는 분자만 흡수하는 파장의 레이저를 조사하여 동위원소를 분리하는 방법이다. MLIS 를 위해서는 각각의 동위원소를 포함하는 분자의 흡수선을 모두 알 필요가 있다. 하지만 현실적으로 넓은 범위에서 아주 적은 비율로 존재하는 동위원소의 흡수선을 실험적으로 알아내는 것은 매우 어렵다. 그렇기 때문에 MLIS 에서 계산을 통해 동위원소가 포함된 분자의 흡수선을 예측하는 것은 매우 중요한 일이다. 이번 발표에서는 진동분광학에서 널리 사용되고 있는 scaling factor 를 전자분광학과 회전분광학의 영역까지 확장하여 적용하였으며, 계산값과 실험값을 비교하였다. 계산에는 CO, NH₃, HCN, formaldehyde, phenol 의 다섯 가지의 분자가 사용되었다. Turbomole 프로그램을 이용하여 여러 계산 수준에서 전자전이와 진동전이, 회전전이에 관한 값들을 계산하였고, 이것을 실험적으로 측정된 값들과 비교하여 scaling factor 를 구하였다. 같은 분자에서 동일 계산수준으로 계산한 경우, 포함하고 있는 동위원소가 다르더라도 scaling factor 가 거의 같게 나오는 결과를 얻을 수 있었다. 동위원소를 포함하고 있는 여러 가지 종류의 formaldehyde(H¹²CH¹⁶O, H¹³CH¹⁶O and D¹²CH¹⁶O)에서 scaling factor 를 구한 뒤 각각 평균하여 각각의 계산 수준별 scaling factor 값을 결정하였다. 이를 이용하여 formaldehyde(H¹²CH¹⁶O)의 스펙트럼을 예측하였고, 직접 실험을 통하여 얻은 formaldehyde 의 스펙트럼과 비교하여 의미있는 결과를 도출하였다.

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Vibrational Predissociation of Hetero Dimer Clusters of Aniline: Molecular Structure and Time Resolved Analysis

Madhusudan Roy 김국기 송재규 박승민*

경희대학교 화학과

Here we have reviewed molecular structures of aniline water, aniline methanol, aniline ethanol, aniline pyrrole and aniline benzene hetero dimer clusters cations with IR. Most of the cases we have found similar molecular structures reported by different groups previously; more electronegative component of the solvent or pi electron of benzene ring makes one hydrogen bond to one NH of aniline. But little different structure from the previously reported for aniline pyrrole cation was found; here two different hydrogen bond found which makes this cation very stable. Moreover in this research time resolved analysis of this clusters are performed exciting all the available vibrational modes. For all clusters the dissociation time decreases with increasing the photodissociation energy.

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Molecular engineering of donor-acceptor co-polymers for bulk heterojunction solar cells

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군산대학교 화학과

We report a computational modeling investigation, based on DFT and TD-DFT calculations, on the structural, electronic, and optical properties of different donor-acceptor co-polymer system. The donor moieties that are considered are the derivatives of thienocyclopentathiophene, fluorene, and thienobenzothiophene. For the acceptor moieties, we considered thieno[3,4-b]pyrrole-4,6-dione; thieno[3,4-b] thiophene-4,6-dione; tetrafluoro-1,3- dihydrothieno[3,4-c]thiophene and its non- fluorinated counterpart; the use of various electron-donating substituents within the fused π -conjugated polymer system; and the substitution of selenium for sulfur in 3-fluorothieno[3,4-b]thiophene moiety. Among the donor-acceptor combination, the best in terms of molecular energy levels, energetic driving force, maximum absorption, calculated open-circuit voltage, reorganization energies, ionization potential, and electron affinity is poly[(bisthieno(bisthieno[3,2-b:2',3'-d]thiophene)- alt-(5-alkyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione)] and poly[(4,8-dimethyl[1,3] oxazolo[5,4-f][1,3]benzoxazole)- alt-(thieno[3,4-d]pyrimidine)].

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Fabrication of NaTi₂O₄ Photoanode for Dye-Sensitized Solar Cells

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Photoelectrochemical characteristics of sodium titanate nanobelts were reported as a function of photoanode in dye sensitized solar cell. NaTi₂O₄ nanobelts were synthesized by hydrothermal method using Ti(OBu)₄ as a precursor molecule in a concentrated aqueous NaOH solution. The formation mechanism of NaTi₂O₄ nanobelts in the synthetic process has been comparatively studied on the control of pH, reaction time and concentration of precursors, etc. The optical property and morphology have been investigated with Ultraviolet-visible spectroscopy, transmission electron microscope, scanning electron microscope, and X-ray diffraction spectrometer. NaTi₂O₄ nanobelts were used for photoelectrode, based on their optical and morphological characteristics. After transparent film of NaTi₂O₄ nanobelts is formed on the fluorine-doped tin oxide (FTO) glass by doctor blade method, the photoelectrochemical results were discussed on the structure of photoanode of dye sensitized solar cells.

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Fabrication of Cu₂O-WO₃ p-n Junction Film to Enhance the Anodic Photocurrent

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서강대학교 화학과

The transparent WO₃ films with the thickness of ca. 200 nm were fabricated on FTO by a facile spin coating method. Cu₂O films with different morphologies were prepared on FTO and WO₃/FTO by electrochemical deposition of a copper precursor solution with different pHs (pH 7, 9 and 11) [1, 2]. The morphologies of as-obtained films were characterized by scanning electron microscopy ; the films composed of nano-sized particles were uniform. The crystallinity of films was characterized by XRD. Compared with that of bare WO₃/FTO film, the anodic photocurrent of Cu₂O-WO₃/FTO prepared at pH 7 was enhanced by the construction of p-n junction.

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Synthesis and Characterization of Anodized TiO₂ Nanotubes Arrays/ZnO Composite Photoanode

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TiO₂ nanotubes arrays (TNTA) synthesized by electrochemical anodization of Ti foil using ammonium fluoride and glycerol (electrolyte) at constant anodization potential of 60 V for 10 h. Titania nanotube arrays have superior electron transport properties compared to titania nanoparticulate film based electrode. Photoelectrochemical properties of TNTA can be further tuned by optimizing the geometrical parameters such as wall thickness tube length and pore diameters for better photoelectrochemical properties. However solar efficiencies of TNTA achieved to date are still lower than the theoretical predicted values due to recombination of electron and holes. Coupling of TNTA with other materials having suitable band gap and band edge positions is an appropriate strategy for the separation of photogenerated charge carriers. Here in this work we have electrodeposited ZnO in the TNTA and loading amount has been controlled by varying the electrodeposition parameters for ZnO. Composite electrode has been investigated for photoelectron chemical characterization.

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Photocatalytic Study of Anatase TiO₂ Film : Comparative Photoactivity with Different Facets

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서강대학교 화학과

It has been reported that the specific facet of TiO₂ have higher reactivity in term of coordination, anatase titanium dioxide has been widely investigated because of many promising properties in photocatalytic reaction. For example, TiO₂ is inexpensive, abundant and environmental-friendly material. It has relevance to photoelectrochemical water splitting ability. In this study, we prepared film with the {100} and {001} facets to study photocatalytic properties comparatively. We focused on single crystal particles and films with different facets. We synthesized particles via facile hydrothermal approach and used HF as capping reagent. We made monolayer film with the specific facets by rubbing method that is useful to arrange micro particles. After that, we can have done secondary growth on pre-formed oriented crystal monolayer while disturbing self-crystallization which is the key to achieving orientation control during film growth. Through this study, we can know which film with different facets have high photo-reactivity.

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Synthesis of Single-Crystalline Monoclinic BiVO₄ on FTO glass by the Seed Layer Assisted Growth Method

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1-D single crystalline nano-structures are important in the field of photo-electrochemical semiconductor because they can provide photogenerated charges via direct electrical pathways and their reduced grain boundaries. This structure also results in excellent charge transport properties. Among various semiconductors, BiVO₄ is a promising material to achieve efficient water photoelectrolysis with visible light illumination. In this study, we report BiVO₄ film on the FTO by hydrothermal method. Using seed layer by spin-coating, BiVO₄ film with various morphologies was grown on the seed layer. We demonstrate growth of single-crystalline monoclinic BiVO₄ on FTO. The structure and optical properties of BiVO₄ film have been well characterized and displayed a strong photo response in the visible region.

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Fabrication of TiO₂ Paste with Nano-sized of β -NaYF₄ : 18% Yb³⁺, 2% Er³⁺ Upconverting Nanoparticles and its Application to Dye-Sensitized Solar Cells

신우진 강영수*

서강대학교 화학과

Up-conversion is a process where low-energy photon is converted into a high-energy photon [1]. Up-converting phosphors can convert near-infrared light into visible light. Converted visible light is effectively absorbed by a dye which is the most commonly used N-719 for DSSC (dye-sensitized solar cell). Currently the most promising up-converting nanoparticles such as β -NaYF₄ are the outstanding candidates for application. It emits around 550 nm after absorb near-infrared. β -NaYF₄ is made of using Y(NO₃)₃·4H₂O, Yb(NO₃)₃·5-6H₂O, Er(NO₃)₃·4H₂O, NaF and trisodium citrate by a hydrothermal method. Nano-sized β -NaYF₄ doped with Yb³⁺, Er³⁺ is fabricated with TiO₂ paste. These mixture is expected to enhance the efficiency of DSSC

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Quantitative and Qualitative Analyses of Reactive Oxygen Species on Photofunctional Polymer for Biomedical Application

손현아 김용록*

연세대학교 화학과

Reactive oxygen species (ROS) have widely been studied for the applications of photodynamic therapy, wastewater purification, stereospecific synthesis of organic compounds. The photo-induced ROS initially consists of two types of oxygen molecules. They are defined as super oxide anion radical and singlet oxygen molecules which are generated from Type I reaction and Type II reaction, respectively. In recent years, ROS generating materials such as photofunctional polymers, photofunctional metal, and photofunctional ceramic have extensively been applied to bio-medical materials and environmental disinfection materials. However, The quantitative and qualitative analyses of ROS generated from the materials are not yet fully investigated in details. In this study, photo-induced ROS generated from the photofunctional polymer were quantitatively and qualitatively investigated by various spectroscopy methods of steady-state and time-resolved NIR spectroscopies.

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Multi-Functional Magnetic Nanoparticles for Cardiovascular Disease

LIJING 김용록*

연세대학교 화학과

We fabricated the multifunctional magnetic nanoparticle (MFMN) conjugated with photosensitizer and thrombus targeting protein. The fabricated MFMN was characterized with transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), UV-Vis absorption spectroscopy, and fluorospectroscopy. To confirm the singlet oxygen generation from the MFMN, singlet oxygen phosphorescence were measured with time and wavelength-resolved singlet oxygen phosphorescence spectroscopy. Thrombolytic efficacy of the MFMN was evaluated by enzyme-linked immunosorbent assay (ELISA) in-vitro and flowmetry in a mice embolic model to check the application possibility as a new and effective thrombolysis reagent.

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Fabrication of (012) Orientated Hematite Film and Its PEC Performance

강명종 강영수*

서강대학교 화학과

To enhance the optoelectronic properties of hematite as photoanode for solar water splitting, hematite films were orientated on (012) plane by rubbing methods and secondary growth of organized microcrystal. (012) orientated hematite film has showed enhanced photoelectrochemical effects with maximum photocurrent of 0.8mA/cm² at 0.23 V vs. Ag/AgCl. This is due to existance of surface hydroxyl group and short bond length between O and Fe atom.

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Enhanced Water Oxidation via Facet-engineering and Cocatalysts Deposition on BiVO₄ Photoanode

이동호 강영수*

서강대학교 화학과

BiVO₄ is a promising semiconducting material for solar water oxidation, because of its relatively narrow band gap energy (2.4eV) and low valence band edge providing sufficient overpotential for water oxidation. To further improve the photoreactivity of BiVO₄ as an anode, two approaches were carried out. On the photoreactive {040} facet controlled film, oxidation and reduction cocatalysts were deposited on the surface using photo-assisted electrodeposition. Depositions of oxidation and reduction catalysts on crystal facets were examined by SEM and photocurrent densities were measured under 1 sun to see the photoelectrochemical properties of these new photoanodes. Further characterization is required to confirm the photo-deposited cocatalysts using XPS and HRTEM. Finally, water oxidation ability will be checked measuring oxygen evolution using GC.

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Controlling Morphosynthesis of Semiconductor Nanomaterials for Photoactivity Enhancement

van thanh khue 강영수*

서강대학교 화학과

Taking advantages of selective adsorption of each particular crystal facet of semiconductor nanomaterials, the morphology-controlled synthesis of various shapes was done by using surfactants or foreigner chemical species that benefit to 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 -Fe₂O₃ 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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Photophysical properties of precursor solution based CIGS films

손소형 한노수 박용진 박승민 송재규*

경희대학교 화학과

Due to the high absorption coefficient and suitable band gap, $\text{CuIn}_x\text{Ga}_{1-x}\text{S}_2$ (CIGS) thin films are the viable candidates as the alternative of the silicon solar cells. In addition, the printable CIGS thin films are more affordable process than the traditional films prepared by the vacuum process. In this regard, the photophysical properties such as the lifetime and energy levels were investigated in the solution-processed CIGS thin films on Mo substrates. The band gap was changed as a function of the thickness, which is attributed to the interaction between Mo substrate and CIGS absorber. The configurations of the CIGS films also changed the open circuit voltage of the solar cells, which was related to the variation of the band gap. The efficiencies of the different configurations are explained by the defect states, which determine the lifetime of the CIGS films. Moreover, the CIGS solar cells on another substrate (ITO) were compared in terms of efficiencies, energy levels, and lifetimes.

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Generation of Circular Polarized Laser Pulses Using a Photoelastic Modulator

홍아람 김남준*

충북대학교 화학과

We developed a pulse technique to generate right- and left-handed circular polarized laser pulses alternatively using a photoelastic modulator (PEM). We synchronized the firing of a 10 Hz nanosecond laser with the modulation of PEM using a frequency divider and digital delay generators. Using this technique, we successfully obtained the circular dichroism (CD) spectra of (R)-(-) and (S)-(+)-10-camphorsulfonic acid (CSA) in aqueous solution. The dependences of CD values on the laser power and the concentration of sample were also investigated.

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Ultraviolet-ultraviolet hole burning spectroscopy of adenine complexes with an alkali metal cation stored in a quadrupole ion trap

박광식 김남준*

충북대학교 화학과

We obtained ultraviolet (UV) photodissociation and UV-UV hole burning (HB) spectra of adenine complexes with alkali metal cations (M^+A , $M = K$ and Na) stored in a quadrupole ion trap (QIT) at 9 K. The UV photodissociation spectrum exhibits well-resolved vibronic peaks in the wavenumber region of $35900\sim 36700\text{ cm}^{-1}$. All of those vibronic peaks are assigned as a single conformational isomer from the UV-UV HB spectrum. By comparing the UV photodissociation spectrum of M^+A with those of M^+7MA (7-methyladenine) and M^+9MA (9-methyladenine), we concluded that the adenine in K^+A is not 9H- but 7H-tautomer. Theoretical calculations are performed to support this conclusion.

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PEAA 아이오노머와 PMMA 아이오노머의 블렌드 및 동적 기계적 성질

김영민 ¹고광환¹ 유정아² 김준섭^{3,*}

조선대학교 신재생에너지융합학과 ¹조선대학교 첨단부품소재공학과 ²조선대학교 화학교육
과 ³조선대학교 응용화학소재공학과

실온에서 유연하고 변형이 잘 되는 PEAA 아이오노머에 투명하고 단단한 PMMA 를 블렌드 하였을때 상호보완되어 새로운 형질의 아이오노머가 형성되거나 하나의 고유의 성질은 유지한채 다른 아이오노머는 가소제 혹은 첨가제 역할을 하게 되는지에 대한 연구를 하였다. PEAA 아이오노머와 PMMA 아이오노머를 각각 8:2, 5:5, 2:8 의 중량비로 블렌드 하였다. 각각의 비율로 블렌드한 아이오노머 혼합체와 고유의 아이오노머의 동적 기계적 성질을 비교하기 위해 DMA 를 이용하였다. PEAA 아이오노머에 PMMA 아이오노머의 함량이 높아질수록 PMMA 아이오노머의 고유의 성질이 뚜렷하게 나타났고 이는 두 아이오노머의 상분리로 각각의 고유 성질을 나타내는 것으로 보인다. 두 아이오노머가 육안으로는 잘 섞여 있는듯 보이나 결과로 보아 고유의 성질에는 영향을 미치지 않고 각각의 함량에 따라 개개의 특성만을 보여 주는 것을 알 수 있다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-331**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Orbital Interaction and Electron Density Transfer in $\text{Pd}^{\text{II}}([\text{9}]\text{aneB}_2\text{A})\text{L}_2$ Complexes : Theoretical Approaches

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경상대학교 화학교육과 ¹경상대학교 화학과 ²한국기초과학지원연구원 하이테크소재연구부

The geometric structures of Pd-complexes $\{\text{Pd}([\text{9}]\text{aneB}_2\text{A})\text{L}_2$ and $\text{Pd}([\text{9}]\text{aneBAB})\text{L}_2$ where A = P, S; B = N; L = PH_3 , $\text{P}(\text{CH}_3)$, Cl^- \}, their selective orbital interaction towards equatorial or axial (soft A...Pd) coordination of macrocyclic [9]aneB₂A tridentate to PdL₂, and electron density transfer from the electron-rich trans L-ligand to the low-lying unfilled a_{1g}(5s)-orbital of PdL₂ were investigated using B3P86/lanl2DZ for Pd and 6-311+G** for other atoms. The pentacoordinate endo-[Pd([9]aneB₂A)(L-donor)₂]²⁺ complex with an axial (soft A--Pd) quasi-bond was optimized for stability. The fifth (soft A--Pd) quasi-bond between the ?-donor of soft A and the partially unfilled a_{1g}(5s)-orbital of PdL₂ was formed. The pentacoordinate endo-Pd([9]aneB₂A)(L-donor)₂]²⁺ complex has been found to be more stable than corresponding tetracoordinate endo-Pd complexes. Except for the endo-Pd pentacoordinates, the tetracoordinate Pd([9]aneBAB)L₂ complex with one equatorial (soft A-Pd) bond is found to be more stable than the Pd([9]aneB₂A)L₂ isomer without the equatorial (A-Pd) bond. In particular, the geometric configuration of endo-[Pd([9]anePNP)(L-donor)₂]²⁺ could not be optimized.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Well-aligned ZnO Nanotubes and its applications

김도훈 강영수*

서강대학교 화학과

The well-aligned ZnO nanotubes are fabricated on the Si(100) substrate by etching the ZnO nanorods which is formed by hydrothermal growth method. $\text{Zn}(\text{NO}_3)_2$ and Hexamine are used for the reaction precursors and the reaction occurred in 93 °C for 3 h. The ZnO seed layer should be formed before the hydrothermal reaction is taking place. The crystallinity of film was characterized by X-ray diffraction. And the morphologies of the ZnO nanotubes are characterized by scanning electron microscopy and transmission electron microscopy. The ZnO nanotubes has high surface area so they can be applied in many way such as formation of high-efficient junction with other chemical materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-333**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Study for Geometric Structures and Characteristic of Cyclic Polythiophene Derivatives

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거제중앙고등학교 ¹경상대학교 화학교육과

Cyclic polythiophene derivatives $[(-SC_4H_2-CC-)_n]$, their derivatives substituted with the functional group ($-NH_2$, $-CONH_2$, $-COOH$), and their complexes combined with some carbon dioxides were optimized at the HF/3-21G* levels. Geometric structures, bond lengths, atomic charges, HOMO-LUMO energy gaps, and binding energy (BE) were analyzed. With increasing n ($4 \leq n \leq 12$), the structures of the derivatives turn to be planar and HOMO-LUMO energy gap (ΔE_{H-L}) gradually decrease. At $n \geq 14$, the structures of the derivatives curved with varying curvature and the energy gap of HOMO-LUMO (ΔE_{H-L}) increases. In the derivatives with substituted functional group ($-NH_2$, $-CONH_2$, $-COOH$), the geometric structures are more complex than the corresponding cyclic polythiophene derivatives, respectively. The atomic charges (QS) of the sulfur atom increase : derivative-COOH > derivative-CONH₂ > derivative-NH₂. The HOMO-LUMO energy gaps (ΔE_{H-L}) of derivative-NH₂, derivative-CONH₂, derivative-COOH are 8.01~8.57, 7.32~7.56, and 7.67~7.81 eV respectively. The structures of cyclic polythiophene derivatives with the carbon dioxide were optimized through hydrogen bond. Among the complexes, the structure of derivative combined with the carbon dioxide is more stable than the others. The binding energies (BE) of derivative-NH₂, derivative-CONH₂, derivative-COOH are -1.38 ~ -1.25, -1.51 ~ -1.47, and -1.78 ~ -1.28 eV, respectively.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid-state NMR, IR, and X-ray investigation of triarylboronic anhydrides(I)

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Two triarylboronic acid anhydrides, 2,4,6-triphenylboroxine and 2,4,6-tris(4-fluorophenyl)boroxine, were investigated by B-11 and C-13 solid-state NMR and FT-IR in this study. These samples were collected on the way to get pure forms of the corresponding arylboronic acids in the present work. We report B-11 MAS and static NMR spectra obtained at two magnetic fields of 9.4 and 21.1 T. C-13 spectra of 2,3,4-triphenylboroxine and phenylboronic acid are completely different, and the as-received commercial sample was found to be mostly the anhydride form of phenylboronic acid. This phenomenon was also detected in the FT-IR spectra. X-ray crystallographic structures of the samples under study are reported. DFT calculations of the B-11 NMR parameters are performed.



Scheme. Interconversion of phenylboronic acid and its anhydride

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-335**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interpolation of quasidiabatic potential energy matrix and its application on nonadiabatic dynamics of green fluorescent protein chromophore

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포항공과대학교 화학과

Theoretical studies on the nonadiabatic dynamics are crucial for understanding the photochemical processes in various chemical systems. However, a prohibitively high computational cost needed for the potential energy surface (PES) construction makes the related simulations practically difficult for large, and therefore realistic, systems. Here, a method for conducting nonadiabatic molecular dynamics simulation using the interpolated quasidiabatic potential energy matrix is presented. As a demonstration, the excited state dynamics of the green fluorescent protein chromophore is studied, with a large number of trajectories. A method for describing the nonbonded interactions between the excited state molecule and external environment will also be discussed.

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장소: 창원CECO

발표코드: **PHYS.P-336**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

DFT study on reaction mechanism of Transamidation of Carboxamides with Amines catalyzed by L-proline

Li Jun 이해황 김찬경*

인하대학교 화학과

The transamidation reaction between carboxamides and amines catalyzed by L-proline was studied theoretically by using the density functional method of B3LYP with 6-31++g* basis set using Gaussian 09 package. The results indicate that the energy barrier for the overall process without catalyst is very high (47.89 kcal/mol). In the presence of catalyst, the reaction proceeds through a multi-step mechanism but the energy barrier is much lower than the reaction without catalyst. The reaction mechanism in the presence of solvent is also considered in this work. This shows that L-proline functions as an efficient catalyst.

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장소: 창원CECO

발표코드: **PHYS.P-337**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

QSPR studies on Ozonolysis Rate Constants using MSEP method

Li Jun 매방¹ 박병호 김창곤 이해황 김찬경*

인하대학교 화학과 ¹인하대학교 물리화학부/화학과

In this work, ozonolysis rate constants of 39 aromatic compounds were studied using QSPR method developed in our lab. All the molecular structures were optimized using the B3LYP/6-31G(d) method and verified as minima from the vibrational frequency calculations. Molecular descriptors were derived from these structures using the molecular surface electrostatic potential method (MSEP). Linear correlations were tried using in-house package. The regression coefficient (R^2) for 4 descriptor model is 0.902 and increases to 0.941 when one additional descriptor was added to the model. This work shows that our MSEP model developed for QSPR study on high energy density materials (HEDM) can also be used to predict reaction rates with considerable accuracy.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **PHYS.P-338**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Modeling Studies on Uptake of Hydrogen Molecule by Graphene

김창곤 박병호 이해황 박수진 김찬경*

인하대학교 화학과

To describe the physisorption phenomenon for carbon nanomaterials accurately, detailed first-principle calculations on the interactions of molecular hydrogen, H_2 , with model system of single- and multilayered graphenes have been carried out. Unlike earlier works on this subject, the present work could expect to provide more useful and reliable information on the physisorption. In the present work, the two-layered ONIOM approach implemented in the Gaussian 03 and 09 packages was used due to the size of the system. The low-level was treated with the DFT method of PW91 functional (DFT-PW91) with the 6-31G(d) basis set because the PW91 functional at least partly recovers the dispersion interaction. The core high-level region was treated using the MP2 level with the Dunning's correlation consistent basis set, cc-pvTZ to take into account the dispersion energy.

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발표코드: **PHYS.P-339**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Computational Study of Hydrogen Adsorption on Pristine Graphene Sheet

박병호 김창곤 이해황 박수진 김찬경*

인하대학교 화학과

Alike earlier works on this subject, this studies are aimed to investigate hydrogen storage capability of pristine graphene sheet using unit cell approaches. We used $n \times n$ unit cell ($n=1, 2, \dots, 8$) and add hydrogen molecules on the graphene sheets. Physisorption orientations were also investigated, and it suggests favorable structures. It was predicted that ideal distance between two layers is about 6.5 \AA . The GGA (generalized gradient approximation) calculations were performed using the Perdew-Burke-Ernzerhof function, including the Grimme dispersion correction term. The basis functions were used DNP (Double Numerical plus Polarization) function. The convergence tolerance of energy is 1.0×10^{-5} Hartrees and the maximum force is 0.002 Ha/\AA . The maximum displacement is 0.005 \AA . And C-C bond lengths were fixed at 1.418 \AA because the bond length of the graphite is 1.418 \AA . Value for the global orbital cutoff is 3.700 \AA . All the calculations were performed by using the material studio DMol³ code.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-340**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Studies on the Mechanism of Pyridinolysis of Y-Substituted Phenoxy Hydrogen Isothiocyanophosphonate

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인하대학교 화학과

The kinetics and mechanism of the pyridinolysis ($\text{XC}_5\text{H}_4\text{N}$) of phenoxy hydrogen isothiocyanophosphonate ($\text{Y-C}_6\text{H}_4\text{O(P=O)(H)NCS}$) in acetonitrile are investigated at room temperature 25.0°C . The Hammett and Brønsted correlations, physical and thermodynamic parameters as well as molecular orbital overlapping indicate the nucleophilic attack and leaving group (-NCS) departure strategies. These are interpreted to indicate a mechanistic behavior for the reactions whether these are following concerted or a stepwise route during expulsion of the isothiocyanate (NCS) leaving group from the intermediate or TS. The positive and negative ρ_X , and β_X values imply the characteristics of the nucleophilic attack. In addition the steric effects of the ligands play an important role in determining the pyridinolysis rates of isothiocyanophosphonates.

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장소: 창원CECO

발표코드: **PHYS.P-341**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Three-dimensional wave-packet propagation for the non-adiabatic dissociation dynamics of *F-H-Cl*

안희선 백경구*

강릉원주대학교 화학과

In order to study the detail initial dynamics of a proton-coupled electron-transfer process, the ultrafast dynamics initiated by the photo-excitation to the charge-transfer state of *FHCl* is investigated theoretically. Adiabatic potential energy surfaces (PESs) of the ground (*F-H-Cl*) and the excited charge-transfer state (*F⁺-H-Cl*) are constructed within three nuclear degrees of freedom, the stretching of *F-H* and the *H-Cl* bonds and the bending of *F-H-Cl*. The ab initio calculations for the adiabatic PESs used the multi-reference configuration interaction plus Davidson correction (MRCI+Q) method with the aug-cc-pVTZ basis sets. Then, the three-dimensional (3D) diabatic PESs and the diabatic coupling term between them are constructed by using a heuristic procedure, based on the smoothness of the PESs. The non-adiabatic effect between the ground and the charge-transfer states was treated by using the (diabatic) potential coupling term. The early-time dissociation dynamics of the charge-transfer electronic state are investigated by the time-dependent quantum mechanical wave-packet propagations. The characteristic of the population transfer at the non-adiabatic region and the branching ratio between the two dissociation (*F/Cl*) channels are studied with special emphases on the effects of the initial vibration levels and the isotope substitution (*H/D*). The implications on the branching between the proton-transfer and the electron-transfer channels are discussed. Analyses also include the differences and the similarities between the current results with 3D full-space and those of our previous work with the restricted collinear 2D space.

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장소: 창원CECO

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Vibrational spectrum of tetrahydropyran cation by vacuum ultraviolet mass-analyzed threshold Ionization spectroscopy

강충만 강도원 김홍래* 권찬호*

강원대학교 화학과

Vibrational spectrum of tetrahydropyran cation in the ground electronic state was obtained using the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopic technique. From VUV-MATI spectrum, which is essentially the vibrational spectrum of tetrahydropyran cation, the ionization energy was determined by extrapolation of the MATI onset position to the zero-field limit. Vibrational analysis of the bands in VUV-MATI spectrum was performed by utilizing vibrational frequencies and Franck-Condon factors calculated at density functional theory (DFT) level.

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발표코드: **PHYS.P-343**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure determination and vibrational assignment of biphenyl derivatives on metal surface by density functional theory (DFT) calculations

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강원대학교 화학과

Spectra of biphenyl derivatives adsorbed on silver nanoparticles have been measured by surface-enhanced Raman scattering (SERS). Assignments for the vibrational peaks observed in the SERS spectra have been performed utilizing density functional theory (DFT) calculations. Based on excellent agreement between the experimental and the calculated results achieved, structures of 4,4'-biphenyl dicarboxylic acid (BPDC), 4,4'-biphenyldithiol (BPDT), 4,4'-bis(mercaptomethyl) biphenyl (BMBP) on silver were defined their adsorption behaviors were also characterized. In addition, absence of C-H stretching bands in the SERS spectrum of BPDC supports parallel orientation of biphenyl ring against the Ag surface and broadened, red-shifted ring stretching bands suggest that adsorption should take place through interaction of π -systems of the phenyl ring with Ag. While, only absence of the C-H stretching band with very small Raman scattering cross-section for BPDT seemed not pertinent in judging the definitive orientation of molecule. Also, absence of S-H stretching band in the SERS spectrum of BMBP indicates that the molecule has been adsorbed on metal surfaces via two thiol groups.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of SERS substrates through size control of silver nanoparticles by citrate reduction

이진철 엄소영 김홍래 권찬호*

강원대학교 화학과

Silver nanoparticles for high sensitive SERS substrate were systematically synthesized by using citrate as reduction agent. The synthetic parameters such as the concentration ratio for citrate against silver nitrate and the reduction time and temperature were optimized to give the large enhancement of the SERS signal determined. It was found that size control of silver nanoparticles was possible by changing the synthetic parameters. The size and shape of nanoparticles synthesized under various conditions were clarified by TEM studies.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Photodissociation dynamics of H atom production from benzene and benzaldehyde-d_α at 205 nm

박성만 권찬호* 김홍래*

강원대학교 화학과

Photodissociation dynamics of H atom production from benzene and benzaldehyde-d_α at 205 nm has been investigated by the spectrum of the H atom products. The spectrum of H atom was measured by laser-induced fluorescence (LIF) from the 3s, 3d to the 2p state (Balmer- α line) induced by two photon absorption from the 1s state. From Doppler profile analysis in the spectra, translational energy releases are determined for H atom dissociation channels of C₆H₄COD + H, C₆H₅CO + D, C₆H₅ + H and C₆D₅ + D. In addition, quantum chemical calculations have been performed to construct potential energy surfaces for the ground and the excited electronic states leading to the individual product channels and utilized to comprehend the photodissociation dynamics.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Expression, purification and NMR Structural Studies of syndecan-4 as cell surface receptor

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한국의국어대학교 화학과

Syndecans as cell surface receptors participate in biologically important cell-cell and cell-matrix interactions. They have a common basic structure including modified extracellular domains and conserved transmembrane and cytoplasmic domains. One of them, syndecan-4 may affect tissue development and repair as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4 (Syd4-TM) consists of 25 hydrophobic amino acids and is involved in formation of dimer or oligomer of syndecan that are crucial for transduction of signals. However, a lot of efforts to elucidate the structure and function of Syd4-TM still have been hindered by insufficient yields and low solubility. Thus, we demonstrated an optimized method for recombinant expression and purification of three kinds of Syd4-TM like wild type Syd4-TM (wSyd4), mutant Syd4-TM (mSyd4), and Syd4-eTC. A mutant Syd4 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 Syd-TM 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-TM 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 monomerization.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **PHYS.P-347**

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Structural and functional Characterization of modified LPcin with Enhanced Antimicrobial Activities

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한국의국어대학교 화학과

Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113-135 region of Component-3 of protease-peptone. LPcin has been designed and modified to enhance their antibacterial activity using mutation, sequence shuffling for better amphipathic characteristics to improve interacting with bacterial membrane. Three different analogs of LPcin, LPcin-yk2 which has mutant amino acids, LPcin-yk1 and LPcin-yk3 that has shorter mutant amino acids are recently developed by using peptide engineering techniques in our lab. In order to comprehend the correlation between the structure of LPcin analogs and bacterial membrane surface, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using many biophysical techniques. We tried to express and purify as large as amounts of LPcin and three different LPcin analogs to study the structure. We finally optimized and succeed to overexpress in the form of fusion protein in Escherichia coli and purified. In order to identify their characteristic structure of the purified peptides in membrane environment, we performed NMR spectrometry with samples mimicking membrane environments. For identifying antimicrobial mechanisms and dynamics, we use various 1D and 2D NMR techniques using bicelle samples. In here, we will present the optimizing processes for high-yield expression, purification and solution and solid-state NMR experiments for investigating anti-bacterial mechanisms.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Dimer Assemblies and Their Plasmonic Properties

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단국대학교 화학과

Assembly of nanoparticles is appealing way for fine control of surface plasmon resonance frequency rather than manipulating shape of nanoparticles. Therefore, the nanoparticle assembly has been widely studied. The core-satellite assembly system we reported is good at fine control and observation of strong surface plasmon coupling (*ACS Nano* 2012, 6, 7199; *J. Phys. Chem. Lett.* 2013, 4, 1371). However, the core-satellite assembly gives structural complexity, which is challenging to predict the origin of spectral property by calculation. Therefore, we develop the simplest dimer assembly system based on desilicization to reduce the structural complexity for calculation that gives fundamental understanding of surface plasmon coupling or Fano resonance.

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Core-Satellite Plasmonic Photocatalysts

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유기 오염물질을 분해하여 정화하는 방법을 개발하는 일은 환경적으로 매우 중요한 일이며 많은 연구가 진행되고 있다. 특히 반도체 입자인 TiO_2 와 태양광을 이용하여 유기 오염물질을 광분해 하는 연구가 진행되고 있으며 이처럼 태양광을 받아 광분해를 일으킬 수 있는 TiO_2 와 같은 입자를 광촉매라고 부른다. 하지만 TiO_2 의 큰 bandgap 때문에 광분해를 하기 위해 필요한 태양광은 자외선 영역으로 국한되며 그로 인한 효율의 한계가 발생 하는 문제점이 있다. 이러한 문제점을 해결하기 위하여 금속 나노입자 표면에 TiO_2 shell 을 씌우거나 반대로 TiO_2 표면에 금속을 코팅하는 방법으로 가시광선 영역에도 촉매 반응을 유도하는 방법이 새롭게 연구되고 있다. 금속 나노입자의 경우 가시광선 영역의 빛을 흡수할 수 있으며 주변에 강한 전자기장을 형성한다. 우리는 금속 나노입자에 의해 흡수된 빛이나 생성된 전자기장을 이용하여 TiO_2 가 가시광선 영역에서도 광촉매 반응을 일으킬 수 있게 된다는 것을 확인하고자 금속 나노입자 표면에 TiO_2 shell 을 씌우고 메틸렌 블루를 가시광선 영역에서 광분해하여 촉매 반응을 확인하였다. 나아가 이렇게 씌워진 TiO_2 shell 표면에 금속 나노입자를 흡착시켜 코어-위성 형태의 조립체를 만들어 hot spot 에서의 촉매 효율의 증가 정도를 확인하고자 한다.

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Structure and Tautomerism of 2-amino-4(5H)-thiazolone derivatives as 11 β -HSD1 inhibitors in the Gas Phase and in Solution: A DFT Study

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한국화학연구원 신약플랫폼기술연구그룹 ¹충북대학교 화학과 ²한국화학연구원 신물질연구본부/신약플랫폼기술팀

Generating the favorable tautomeric states of drug-like molecules in solution is important for success in both ligand- and structure-based drug designs. The structure and tautomerism of 2-amino-4(5H)-thiazolone derivatives as 11 β -HSD1 inhibitors have been studied using B3LYP/6-31+G(d), M06-2X/6-31+G(d), and ω B97X-D/6-31+G(d) model chemistries with the implicit CPCM and SMD solvation methods in the gas phase and in solution. In the gas phase, the imino tautomers are computed to be more stable than the amino tautomers, whereas the amino form of a novel 2-amino-4(5H)-thiazolone derivative is found to be the predominant tautomer in the gas phase and in solution. The macroscopic pK_a value and the amino/imino tautomeric equilibrium constant (pK_T) of a novel 2-amino-4(5H)-thiazolone derivative are estimated to be 2.65, which is in good agreement with the experimental value of 2.33 ± 0.13 , and 3.99 at 25 °C using the statistically weighted free energies of its cationic and neutral forms in the gas phase and their solvation free energies in water at B3LYP/6-31+G(d) level of theory, respectively.

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Unusual solvatochromic effect on fluorescence quantum yield of a novel dye derived from resveratrol

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서울대학교 화학부 ¹서울대학교 생물물리 및 화학생물학과 ²서울대학교 자연과학대학 생물물리 및 화학생물학과

Resveratrone is a highly fluorescent organic compound photochemically derived from resveratrol, which is a natural product abundant in nuts, berries, and grapes. It has many desirable traits as a biocompatible fluorophore, including a large Stokes' shift, high fluorescence quantum yield, large two-photon absorption cross-section, and no cytotoxicity. We found that there exists a strong correlation between the fluorescence quantum yield of resveratrone and its pKa in alcoholic solvents in the form of a linear solvatochromic shift. We suggested that such a remarkable behavior may result from the higher fluorescence quantum yield of resveratrone anion relative to that of the neutral form, which was verified by DFT calculations.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Anomalous Light-induced Agglomeration of Nanoparticles

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서울대학교 생물물리 및 화학생물학과 ¹서울대학교 생물물리 및 화학생물학부 ²서울대학교
화학부

We discovered a highly anomalous light-induced phenomenon of nanoparticles on a substrate under an optical microscope. Upon irradiation of light, a large (possibly > 10 μm in diameter), doughnut-shaped agglomeration of nanoparticles was found to take place, regardless of the type of nanoparticles. We found that this phenomenon is highly correlated with the microscope mounting medium, which typically contains light-absorbing materials. Using atomic force microscopy and wide-field or confocal fluorescence microscopy, we obtained AFM and fluorescence images of nanoparticles and analyzed the agglomeration-formation process to propose the origin of this remarkable phenomenon.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical study of covalently linked carbocyanine dyes with remarkable resistance against photo-bleaching

박재완 권지웅¹ 황지희² 김성근*

서울대학교 화학부 ¹서울대학교 생물물리 및 화학생물학과 ²서울대학교 생물물리 및 화학생물학

Although the carbocyanine dyes are widely used in the fields of fluorescence microscopy and spectroscopy, the finite lifetime of their fluorescence states has prevented long-time observation of the event of interest. Here, we discovered that the photo-stability of a carbocyanine dye can be considerably enhanced when it is covalently linked with another one. Using fluorescence correlation spectroscopy and computational method, we investigated the photophysical characteristics of covalently linked carbocyanine dyes in our effort to achieve unprecedented photo-stability of organic dyes.

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Investigating Structural Dynamics of Biomolecules by using Cryogenic Electron Microscopy

조준범 이효철*

한국과학기술원(KAIST) 화학과

Probing structural changes of biomolecules during a reaction is important point to understand mechanism and function of those molecules in the reaction. Here, we suggest novel method to observe reactions including biomolecules such as proteins using cryogenic electron microscopy. Compared to conventional transmission electron microscopic technique, cryogenic electron microscopy has an advantage in biological molecules due to their structural preservation in their native states. In addition, time-resolved cryogenic electron microscopy that provides information about intermediate structures during certain reaction also has been already demonstrated. Here we propose a novel sample system including reaction channel so that we can probe the reaction steps after vitrifying the whole channel. Our ultimate goal is to observe multiple portions of the vitrified channel and to get structural information of reaction intermediates from each portion. Combining newly developed sample system with biomolecules, we can draw a statistical distribution of structural parameters of target molecules during the reaction.

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A Computational Investigation of Alkyl Side Chain Impact on the Intermolecular interaction and Photovoltaic Properties of Small Molecule

서동균 곽경원* 이경구¹

중앙대학교 화학과 ¹군산대학교 화학과

Push-pull-push small molecules are promising donor materials for organic solar cells. We investigate the electronic structure of DPP(TBFu)₂ with different configuration of side alkyl chains attached to the backbone of small molecule. The total C number of the side chains in each molecule was kept at 16. These alkyl chains are crucial component for intermolecular interaction as well as to increase the solubility of molecule in organic solvent. Previously, detailed computational study and comparison of the effect of different alkyl chains on the properties of these copolymers were not elucidated. Herein, various alkyl side chains were introduced and their effects to the molecular and electronic structure were investigated with Molecular Dynamics simulation and Density Functional Theory.

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Terahertz spectrocalculation with Solid State Chemistry by Density Functional Theory

여학민 이경구¹ 곽경원*

중앙대학교 화학과 ¹군산대학교 화학과

Experimental study of Solid state chemistry as Ceramic and amorphous materials was improved consistently, but comparison of analytical and theoretical study has some limited field yet. However, in recent years, rapid development of THz spectroscopy tool provide many advantages to analysis solid state sample without destruction. For these reasons, It is possible to observe vibrational modes of supramolecular complexes of small molecules by combination of THz spectroscopy and DFT calculation. We conducted solid-state DFT calculations using DMol3 program package and Crystal09 program to confirm the structure and to predict and compare the data of spectra in THz region of melamine, aflatoxin, and zearalenone.

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Spectroscopic Analysis of Amide Bond rotation in Diethylamide Derivatives with a Theoretical Approach

김성수 민지은 안상두 장석규 곽경원*

중앙대학교 화학과

Enantiomerization in Aromatic amides has been reported in recent years. We investigate the rotational barrier to Ar-CO and N-CO for taking the conjugation of Ar-CO and N-CO bond into account in Diethylamide Derivatives. In this work, the variable-temperature NMR (VT-NMR) experiment was performed in Diethylamide Derivatives for explaining the increased conjugation of Ar-CO bond and decreased conjugation of N-CO bond as we increased the substituted benzene moiety connected to the amide derivatives. For supporting this conjugative effects on Diethylamide Derivatives, computational calculations with DFT at the 6-311G(d) basis set were also applied. Potential Energy Scan methods through this calculation determine not only the ground and transition states but also the Gibbs energy difference. Therefore, we are able to compare experimental and theoretical methods.

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Analysis of Intensity and Sensitivity of Single- and Multiple-Channel RF Head Coils in 3.0-T MRI System

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High-resolution anatomical and functional images can be acquired using high- and ultra-high-field magnetic resonance imaging (MRI) systems. An increase in the main magnetic field strength results in high resolution but suffers from the disadvantage of field nonuniformity in the radio frequency (RF). To overcome this RF field inhomogeneity, a parallel RF transmission system and sensitivity encoding are widely used. Our experimental results showed that the best signal intensity was in the transmit and receive mode head coil, except for the T2-weighted fast field echo (FFE). The best signal-to-noise ratio (SNR) was in the 32-channel head coil. In general, multiple-channel coils have been known as more efficient materials in terms of the SNR. However, they may not be as important in experiments where intensity is an important factor. Therefore, a suitable coil should be selected using a pulse sequence.

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Numerical Studies on Signal Behaviors of iMQC MR imaging Depending on Relaxation Times at 14 T

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As a new method for contrast enhancement in MRI, the intermolecular multiple quantum coherences (iMQCs) MR imaging has recently attracted considerable attention mostly because of the intrinsic sensitivity of the iMQCs to changes the magnetization and susceptibility structures.¹⁻³ Relaxation times (T1 and T2) play an important role in creating and determining susceptibility structures of the matters for MRI detection. In this study, we have experimentally and numerically investigated the relaxation time dependence on the intensity profiles and/or contrasts of the intermolecular double quantum coherences (iDQCs) MR images by fixing and varying T1 and T2, respectively and vice versa.

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Very Fast Synthesis of Silver Cyanide by Pulsed Laser Ablation in N,N-dimethylformamide

이슬기 최명룡*

경상대학교 화학과

Silver cyanide (AgCN) micro-rods were prepared by a pulsed laser ablation method in N,N-dimethylformamide (DMF). AgCN was synthesized in a harsh experimental condition, i. e., high temperature (several thousand K) and pressure (several GPa) produced by plasma plume. A possible mechanism of forming the AgCN micro-rods via a fast reaction between silver cations from silver nitrate as a precursor and cyanide anions formed from DMF through a recombination process is proposed in this poster. The structural, morphological and optical properties of the AgCN micro-rods were characterized by various techniques, such as X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), transmission electron microscope (TEM), energy-dispersive X-ray spectroscopy (EDS), gas chromatography (GC), and Fourier transform infrared and Raman spectroscopy.

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pH-Dependent Dispersivity of the Halloysite Solution

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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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Photoluminescence Imaging of Eu(III)-doped Indium Hydroxide and Oxide nanostructures

김원주 손영구*

영남대학교 화학과

Eu(III) was doped into indium hydroxide and oxide cubes and wires. Their structural and spectroscopic properties were examined by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis absorption (UV-Vis) and photoluminescence spectroscopy. We will discuss the results during the poster presentation.

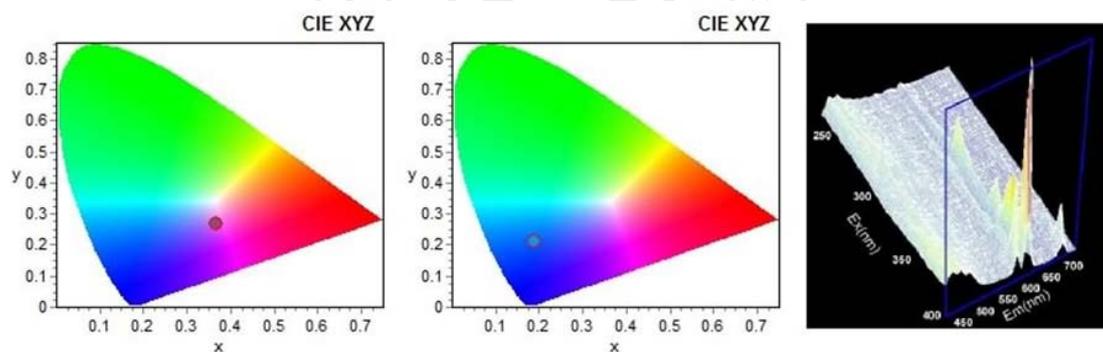


Figure. CIE color coordinates for Eu(III)-doped indium hydroxide and oxide wires (left two), and 3D-photoluminescence profile of Eu(III)-doped indium hydroxide wire.

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A Combined AFM-TIRFM Study of Annexin V-Induced Pore Formation on Supported Lipid Bilayer

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연세대학교 화학과 ¹국민대학교 생명나노화학과

We have studied the morphology changes of artificial phospholipid membranes by binding of Annexin V (A5), an anionic phospholipid binding protein, using combined AFM and TIRFM techniques. There have been previously numerous reports that suggest the calcium ion channel activities of water-soluble A5 on membrane at mildly acidic pH conditions, either by undergoing a massive conformation change into a transmembrane protein, or by forming A5 clusters that can be inserted into membrane. In this study, we found that the A5 binding on supported lipid bilayer at mildly acidic pH's induced the formation of nano-sized pores rather than the typical protein ion channels. We have characterized closely the sizes and shapes of individual pores as well as their behaviors upon the changes in the pH and calcium ion concentrations. Finally, we discuss about the relationships between our A5-induced nano-pores and the previously reported calcium ion channel activities of A5.

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Studies of gadolinium oxide nanoparticles coated with various ligands as MRI contrast agents

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Ahmad**

경북대학교 화학과

나노입자는 다양한 분야에 걸쳐 연구가 되고 있다. 그 중 영상의학분야 역시 많은 관심을 받고 있다. MRI 조영제로써 뛰어난 효과가 검증되어, 기존의 조영제를 대체할 만한 가능성을 계속 시험하는 중이다. 이 연구에서는 산화 가돌리늄 나노입자에 다양한 생체적합적 리간드를 코팅하여, 리간드에 따른 차이점을 살펴 보고자 한다. 산화 가돌리늄에 코팅되는 리간드는 D-glucuronic acid, PEG diacid 250, PEG diacid 600, 세가지 종류로 코팅한다. 이를 확인하기 위해 HRTEM, XRD, FT-IR, TGA, DLS 를 사용하였고, 농도를 확인하기 위해 ICP-AES 로 측정하였다. 그리고, MRI 조영제로써 사용할 수 있는지 여부를 확인하기 위해 Relaxivity, Cytotoxicity test 를 시행하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-365**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, magnetic properties, map images, and water proton relaxivities of D-glucuronic acid coated Ln_2O_3 nanoparticles ($\text{Ln} = \text{Ho}$ and Er)

김성준 이강호* 김초롱 Badrul Alam Bony Xu Wenlong tirusew tegafaw Md. Wasi Ahmad

경북대학교 화학과

T_2 MRI contrast agents can not be synthesized by using molecules but nanoparticles because appreciable magnetic moments at room temperature are needed. Recently, some of lanthanide (Ln) oxide nanoparticles have shown decent magnetic moments at room temperature and even at ultrasmall particle diameters. In this study, we explored D-glucuronic acid coated Ln_2O_3 nanoparticles ($\text{Ln} = \text{Ho}$ and Er) with ultrasmall particle diameters. They showed decent magnetic moments at room temperature and as a result, appreciable transverse water proton relaxivities (r_{2s}) at 1.5 tesla MR field. Clear dose-dependent contrast enhancements in R_2 map images were observed in both samples. These results showed that D-glucuronic acid coated Ln_2O_3 nanoparticles ($\text{Ln} = \text{Ho}$ and Er) would be potential T_2 MRI contrast agents at high MR fields.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

NEXAFS analysis on the surface electronic states of MZO films

전소현 서현진 유정훈 이진수 부진효*

성균관대학교 화학과

Metal doped ZnO (MZO, M = Li, Ag, Al) films were prepared by RF magnetron sputtering on glass substrates with MZO ceramic targets. For the doping sources contained in each MZO targets, we used LiCl, AgNO₃, Al(OH)₃ powders by mixing the powders into pure ZnO powder with a various rate (0~10 wt.%), respectively. The dependence of film properties including microstructure, optical and electronic on coating parameters such as, target composition was investigated. As metal doping amounts and a kind of dopant in the target were changed, the crystalline and the transmittance as well as optical band gap were changed. Electrical resistivity was also changed with changing metal doping amounts and a kind of dopant. To investigate these phenomena in details, valence band structure of the MZO films were also investigated by XRD, XPS and NEXAFS analysis.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Viscosity dependence of 10-23 deoxyribozyme reaction kinetics: single-molecule vs. ensemble measurements

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10-23 deoxyribozyme is a single-stranded DNA enzyme that catalyzes the cleavage of specific RNA sequence. Our previous single-molecule study using total internal reflection fluorescence microscopy identified a series of distinct reaction steps that include enzyme-substrate binding, substrate cleavage, half-substrate dissociation and full-substrate dissociation. In this study, we measured the rates of individual reaction steps by varying solvent viscosity and found that they were significantly affected by viscosity. On the other hand, polyacrylamide gel electrophoresis showed little viscosity dependence for the enzymatic turnover rate, which shows that single-molecule measurement can reveal kinetic factors that are averaged and often hidden in an ensemble measurement.

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발표코드: **PHYS.P-368**

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Efficient measurement of DNA lengths by STED nanoscopy

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서울대학교 화학부 ¹서울대학교 생물물리 및 화학생물학부

By employing STED (stimulated emission depletion) nanoscopy and dynamic molecular combing, we attempted to make a precise length measurement of DNA. Two kinds of plasmid with different number of DNA repeat sequence were extracted from E. coli and digested by Xho I restriction enzyme. DNA was stretched on cover glass whose surface was treated with siliconizing fluid, which gave a much better result than the conventional silanization method. We were able to readily discriminate different DNAs whose lengths were apart by as little as 200 nm. This method is highly suited for efficient and precise measurement of DNA lengths, with a possible application for early diagnosis of genetic diseases that arise from different DNA repeat sequences.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

High-concentration limit of detecting single molecules by the combination of ALEX-FRET and STED nanoscopy

배소현 김남두 강주연 권지용¹ 임영빈¹ 김성근*

서울대학교 화학부 ¹서울대학교 생물물리 및 화학생물학과

Following our previous work to combine ALEX-FRET and STED nanoscopy to reduce the effective focal volume for single-molecule detection that permits a maximum concentration of 5 nM in organic solvent, we applied this new technique to aqueous solution considering that most biological molecules exist in aqueous solution. ssDNA was labeled by ATTO 647N or DY-510XL dyes, and the fluorescence signal was enhanced in Trolox solution. We confirmed that we can detect a single DNA molecule at 5 nM concentration even in aqueous solution and still clearly discriminate low vs. high FRET DNA pairs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Monte Carlo Study of the Water Meniscus Confined between an Atomic Force Microscope Tip and a Surface

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Water condenses between an atomic force microscope (AFM) tip and a surface to form a nanoscale liquid meniscus. It is well known that this nanoscale meniscus produces a significant adhesion force on the tip. Utilizing a grand canonical Monte Carlo simulation of lattice gas model, we investigated the behavior of water meniscus and capillary force between the tip and surface. We studied the onset and broadening of meniscus by changing the tip curvature and tip-liquid interaction. The tip-liquid interaction is characterized in terms of the wettability of the tip. As the tip curvature increases (the tip is sharper), both the meniscus width and the capillary force decreased. On the other hand, as the tip-liquid interaction decreases (the tip becomes more hydrophobic), the meniscus width and capillary force decreased.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

REMPI, UV-UV hole-burning and IR-dip spectroscopic studies of jet cooled phenacetin

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경상대학교 화학과 ¹서울대학교 화학부

Phenacetin (PA) is one of the typical synthetic fever reducers as similar to Acetaminophen (AAP), a major ingredient of Tylenol. PA and AAP are both derivatives of acetanilide, substituted by ethoxyl group and hydroxyl group in the para position of acetanilide, respectively. In this work, we present the conformational investigations and photochemistry of jet-cooled PA using one color resonant two-photon ionization (REMPI), UV-UV hole-burning and IR-dip spectroscopy. Moreover we calculated the optimized structures of PA by density functional theory (DFT). Here, we report the structural information of PA by comparing the experimental data and that from the calculations.

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발표코드: **PHYS.P-372**

발표분야: 물리화학

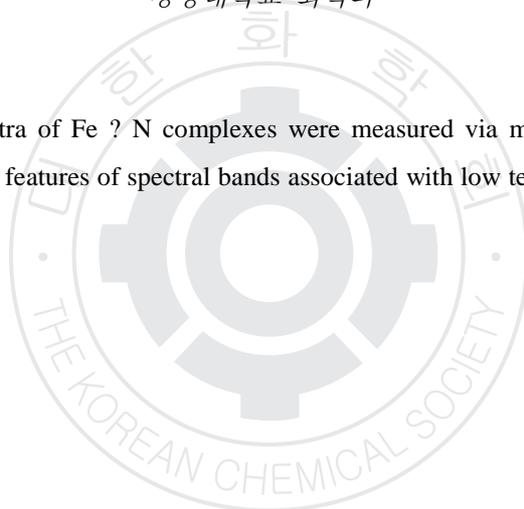
발표종류: 포스터, 발표일시: 수 16:00~19:00

Matrix Infrared Spectroscopy and Theoretical Study of Iron Dinitrogen Complexes : Fe(N₂),Fe(NN)_x (x=1-5)

이지훈 민아름 안아름 문철주 최명룡*

경상대학교 화학과

In this work, infrared spectra of Fe ? N complexes were measured via matrix isolation spectroscopic techniques, providing sharp features of spectral bands associated with low temperature (< 10 K) and high vacuum (



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study of magnetic and fluorescence properties of D-Glucuronic acid Coated HoEuO₃ Nanoparticles

Xu Wenlong Badrul Alam Bony tirusew tegafaw 김초룡 김성준 Md. Wasi Ahmad 이강호*

경북대학교 화학과

In this report, we synthesized a water-soluble and biocompatible D-Glucuronic acid coated Eu³⁺ doped Holmium oxide nanoparticle. They were characterized with XRD, FT-IR, TGA, Fluorescence spectrophotometer, HRTEM, SQUID magnetometer and MRI instrument. There is no appreciable cytotoxicity up to 500 μM (Ho) concentration. The synthesized nanoparticles were monodisperse with average diameter (davg) of 2 nm. The Eu³⁺ doped Holmium oxide nanoparticles were found to be paramagnetic and emitted strong red fluorescence. From in vivo MRI experiment we found that the negative contrast had been enhancement on mouse liver and kidneys after the injection of nanocolloid. Hence, it can be used as a MRI-optical dual imaging contrast agent.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Silica-Coated Magnetic Nanoparticles

tirusew tegafaw Badrul Alam Bony Xu Wenlong 김초룡 김성준 Md. Wasi Ahmad 이강호*

경북대학교 화학과

In recent years, magnetic nanoparticle materials have been intensively studied because they often exhibit very interesting properties, which cannot be achieved by their bulk counterparts. In this present work, we synthesized different magnetic nanoparticles were coated with a silica shell by the stober process. The surfaces of silica-coated magnetic nanoparticles are hydrophilic, and are readily modified with other functional groups. The functionalization could introduce additional functionality, so that the magnetic particles are potentially of use in biolabeling, drug targeting, and drug delivery. They were characterized with XRD, HRTEM, FT-IR, TGA, and SQUID magnetometer.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis of mixed lanthanide oxide nanoparticles for dual modal contrast agent

Badrul Alam Bony Xu Wenlong tirusew tegafaw 김초룡 김성준 Md. Wasi Ahmad 이강호*

경북대학교 화학과

We accomplished a novel and an efficient one-pot synthesis of biocompatible D-glucuronic acid coated ultrasmall Tb^{3+} : Ho_2O_3 nanoparticles for dual modal contrast agent. Aqueous suspensions of 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. Remarkable features, like relaxivities and fluorescence of Ho_2O_3 nanoparticles, enhanced because of adding Tb^{3+} nanoparticles. Moreover, the toxicity of Ho_2O_3 nanoparticles was also minimized in addition to Tb^{3+} nanoparticles. The efficiency of D-glucuronic acid coated ultrasmall Tb^{3+} : Ho_2O_3 nanoparticles as T_2 MRI contrast agent and fluorescence imaging agent were proved through in vitro T_2 MR Images and fluorescence images respectively, which can be an efficient and novel addition to biomedical applications.

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발표코드: **PHYS.P-376**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Iodine Compound Coated Gd₂O₃ Nanoparticle as a Potential T₂ MRI-CT dual Contrast Agents

Md. Wasi Ahmad Xu Wenlong Badrul Alam Bony tirusew tegafaw 김초룡 김성준 이강호

*

경북대학교 화학과

Magnetic resonance imaging (MRI) is widely used in modern clinical medicine as a diagnostic tool, and provides noninvasive and three-dimensional visualization of biological phenomena in living organisms with high spatial and temporal resolution. The surface modified Gd₂O₃ nanoparticles has a higher relaxation rate compared to currently commercialized MRI contrast agent. The performance of nanoparticles for biomedical applications is highly dependent on the nature and quality of surface coating materials. Therefore, considerable attention has been paid to magnetic nanoparticles as MRI contrast agents with efficient targeting ability and cellular internalization ability, which make it possible to offer higher contrast and information-rich images for detection of disease. In this study, the coating of iodine compound on the surface of Gd₂O₃ nanoparticles were confirmed by FT-IR, TEM, XRD, TGA and MRI instrument. These analyses also demonstrated the strong attachment of iodine compound on the surface of Gd₂O₃, forming a protective layer on the nanoparticles. The relaxometric properties, cytotoxicity and the MRI signal of iodine coated Gd₂O₃ nanoparticles were examined.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantum Chemical Calculations of 3-Cyanoindole-(H₂O)_n (n=1-10) Clusters

안아름 최명룡*

경상대학교 화학과

Indole is an aromatic heterocyclic organic compound, consisting of a six-membered benzene ring fused to a five-membered nitrogen-containing pyrrole ring. It is also a popular component of fragrances and precursors many pharmaceuticals. In this study, theoretical calculations of 3-cyanoindole (3-CI) and its water clusters with their size up to 10 water molecules are conducted to aid in the spectroscopic analysis in this laboratory. We calculated the 3-Cyanoindole-(H₂O)_n (n=1-10) clusters using density functional theory (DFT) with a 6-311++G(d,p) basis set and obtained several low minimum energy structures of each 3-Cyanoindole-(H₂O)_n cluster, including global and low-lying energy local minimum isomers. We further carried out the excited state calculations for the corresponding 3-Cyanoindole-(H₂O)_n (n=1-10) cluster using time dependent-DFT (TD-DFT). The excited state structures and transition energies of 3-Cyanoindole-(H₂O)_n (n=1-10) clusters obtained in this work can be helpful to accommodate the experimental observations.

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발표코드: **PHYS.P-378**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

PLASTICIZATION EFFECTS ON THE DYNAMIC MECHANICAL PROPERTIES OF SODIUM NEUTRALIZED PS-BASED IONOMERS WITH A DERIVATIVE DIMER ACID

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조선대학교 첨단부품소재공학과 ¹조선대학교 신재생에너지융합학과 ²조선대학교 화학교육과 ³조선대학교 응용화학소재공학과

The effects of the addition of sodium salts of derivative dimer acid(methyl ester, isooctyl ester, isotridecyl ester) on the dynamic mechanical properties of poly(styrene-co- sodium styrenesulfonate) (PSSANA) and poly(styrene-co- sodium methacrylate) (PSMANA) ionomers were studied using DMA, TGA techniques. In the case of PSSANA ionomer system, two glass transitions(T_g s) were observed at ca. 140 °C, 260 °C, respectively. In the case of PSSANA ionomers containing the isooctyl ester, the positions of loss tangent peaks shifted to lower temperatures from ca.140 °C to ca 90 °C and from 260 °C to 170 °C, respectively. This finding suggests that the isooctyl ester might act as plasticizer, at least to some, in the PSSNa ionomer. In addition, it is imply that the isooctyl ester might be very effectice plasticizer.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

NMR structure refinement using STAP and flat-bottom potential without NOE data

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The low-quality structure refinement is one of important challenges in protein structure prediction. Many studies have been conducted for protein structure refinement; especially refinement of structure derived from NMR spectroscopy is accelerated. In this study, we demonstrate that statistical torsion angle potential (STAP) can drive to refine NMR structures without NOE data. Because NOE data have an ambiguity and uncertainty, we used flat-bottom potential instead of NOE data. The materials of flat-bottom potential are distance and dihedral angle derived from given structures. Instead of the NOE restraints, they prevent a structural dislocation during the refinement process. A simulated annealing protocol was used to optimize energy of structures. The protocol was tested on 134 NMR structures in Protein Data Bank (PDB) that are coexisting in X-ray structures. Among them, 50 structures of training set used to find the optimal “width” parameter in the flat-bottom potential functions. Validations of the “width” for 84 structures, most of 12 quality assessment scores of refined structure are significantly improved.

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Rotamer Prediction using Statistical Torsion Angle Potential

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To understand protein functions, an accurate protein structure is prerequisite. Particularly, side-chain motion affects protein-protein interaction and protein-molecule interaction in tertiary protein structure. Since determination of rotamer prediction is experimentally difficult, we used computational method with well-defined knowledge-based potentials. Statistical Torsion Angle Potential (STAP) with Φ - χ_1 , Ψ - χ_1 and χ_1 - χ_2 combinations and simulated annealing protocol were used to predict these populations. The computational predictions of χ_1 and χ_2 rotamer populations were performed for 10 target proteins. Order parameters which were used to evaluate accuracy of side-chain were good agreement with those in experimental results. This study can be used to characterize the χ_1 and χ_2 conformations of exposed residues and to understand side-chain motions.

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Synthesis of Electrospun RuO₂/ReO₃ composite Nanofibers and their Electrochemical properties

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대학교 화학나노과학과*

Transition metal oxides constitute a very interesting class of materials because of the variety of functional properties and phenomena. Ruthenium oxide (RuO₂) is a great material as electrodes in electrochemical devices because of their high electrical conductivity, chemical stability, and characteristics. Also, rhenium oxide (ReO₃) is the interesting material as a sensor for electroactive species and they have high electrical conductivity. Generally nanostructures have more improved electrochemical and catalytic ability than large scale structure. Thus, it is a task of great significance to synthesize nanofibers in nanoscale. Electrospinning is the facile synthetic technique for RuO₂/ReO₃ composite nanofibers to make uniform fibers of nanoscale. We have prepared nanofibers from mixed solution of ruthenium precursors and rhenium precursors by electrospinning and then obtain RuO₂/ReO₃ composite nanofibers successfully after calcination. We characterized the morphology and structures of RuO₂/ReO₃ composite nanofibers by scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectrum and transmission electron microscopy (TEM). Additionally, capacitance measurements and hydrogen peroxide detection is performed by using RuO₂/ReO₃ composite nanofibers and the results show high capacitance and sensitivity of hydrogen peroxide reduction.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical analysis of experimental artifact caused by photobleaching in single-molecule measurements

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Accurate measurement of chemical kinetics for a slow reaction by the single-molecule fluorescence techniques is challenging due to the finite lifetime of fluorescent molecules resulting from photobleaching. In this study, we propose a simple mathematical model describing the effect of photobleaching on the observed single-molecule kinetics. According to our model, intrinsic kinetic rates can be obtained by simply subtracting the inverse of fluorophore lifetime from the inverse of the observed average reaction dwell-time. This model was verified in several simulations as well as in our study of enzyme kinetics of 10-23 deoxyribozyme and its RNA substrate by total internal reflection fluorescence spectroscopy. This new model allows kinetic measurement of diverse biochemical reactions that are too slow to be directly measured because photobleaching takes place before the reactions themselves.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigations of the Core/Shell Model of Nanoconfined Aqueous Solution in AOT Reverse Micelles

이주용 박광희 이경구¹ 곽경원² 조민행*

고려대학교 화학과 ¹군산대학교 화학과 ²중앙대학교 화학과

IR probes have been extensively used to monitor local electrostatic and solvation dynamics. Particularly, their vibrational frequencies are highly sensitive to local solvent electric field around an IR probe. Here, we show that the experimentally measured vibrational frequency shifts can be inversely used to determine local electric potential and field distributions and solute-solvent electrostatic interaction energy. In addition, the upper limits of their fluctuation amplitudes are estimated by using the vibrational bandwidths. Applying this method to a core/shell model has often been used to describe water confined to the interior of reverse micelles.

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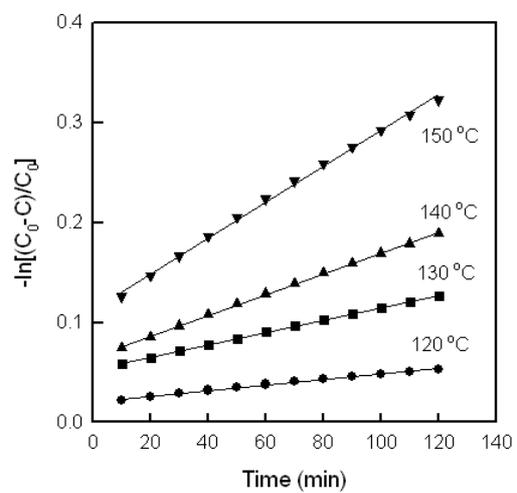
발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermogravimetric investigation of volatility of dimer acid and dioctyl phthalate in plasticized poly(styrene-co-sodium styrenesulfonate) ionomers

고광환 김영민¹ 김준섭² 유정아^{3,*}

조선대학교 첨단부품소재공학과 ¹조선대학교 신재생에너지융합학과 ²조선대학교 응용화학소재공학과 ³조선대학교 화학교육과

The loss of plasticizers from plasticized polymers is interesting from the point of view of processibility of polymer materials and optimization of the process as well as for the evaluation of lifetime of plasticized polymer products in use. The process of volatilization of dimer acid(DA) in plasticized Na-sulfonated polystyrene (PSSNa) ionomer was studied by the method of isothermal thermogravimetry in the temperature range of 120 °C-150 °C. The rate constants of the process of plasticizer volatilization were calculated and the dependence of rate constant on the initial concentration of plasticizer in plasticized PSSNa. The activation energy of the process was calculated from the exponential dependence of the rate constant of volatilization on temperature.



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Property of Upconversion Substrate made by Pulsed Laser Deposition

김범진 김형민* 박찬량^{1,*}

국민대학교 생명나노화학과 ¹국민대학교 화학과

Upconversion Substrates ($\text{NaY}_{0.77}\text{Yb}_{0.20}\text{Er}_{0.03}\text{F}_4$) were prepared by pulsed laser deposition. Deposition film emits green upconversion in infrared excitation at 980 nm. But atmospheric annealed upconversion film emits red upconversion. Due to observing this phenomenon, we obtain fluorescence of upconversion film by controlling temperature. Total peak intensity is decreased when the temperature is increased. When cooling this down, peak around red wavelength range (640 nm ~ 700 nm) is increased significantly. This implies that the property of host is changed. In order to confirm this, we use various equipment to analyze.

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A combined SERS and DFT study of hydroxy derivatives of flavone adsorbed on silver colloids

이승장 서성욱 조한국 정병서*

인천대학교 화학과

Surface-enhanced Raman scattering (SERS) spectra of several hydroxy derivatives of flavone, 3-hydroxyflavone, 7-hydroxyflavone, and 5,7-dihydroxyflavone (chrysin), were obtained on silver colloids, and compared to discern the effects of differing position of OH groups in hydroxyflavones on the adsorption geometry and interaction with the metal surface. The SERS spectra were also measured at different pHs to gain information on pH-dependent behavior of the spectral variation and adsorption geometry. Normal mode assignments of the observed bands in the FT-Raman and SERS spectra were aided by density functional theory (DFT) calculations. The adsorbate-metal interaction is modelled as an adduct of hydroxyflavone with a single Ag atom or with a small Ag cluster. The interaction of adsorbates with metal nanoparticles as well as the adsorbate conformation was discussed, based on the combined results of the FT-Raman and SERS spectra and DFT calculations.

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Single-molecule study for the effect of DNA methylation on the kinetics of Type II restriction enzyme reaction with DNA

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서울대학교 화학부 ¹서울대학교 생물물리 및 화학생물학과

DNA methylation plays a great role both in eukaryotic and prokaryotic cells. In eukaryotes, it suppresses gene regulation, whereas in prokaryotes, specifically in bacteria, it protects the cell from invasion of foreign genes. Many studies have been carried out for the effect of DNA methylation at the ensemble level, but in this study, we investigated the effect of DNA methylation on DNA-protein interaction by single-molecule fluorescence to understand the interaction at the molecular level. We measured the association and dissociation rates of native vs. methylated DNA and found that they converge to the corresponding ensemble rates. We were able to differentiate the kinetics of association, conformational change, and dissociation and found that our result was consistent with the fact that DNA methylation interrupts the DNA- protein interaction, especially at a specific kinetic step.

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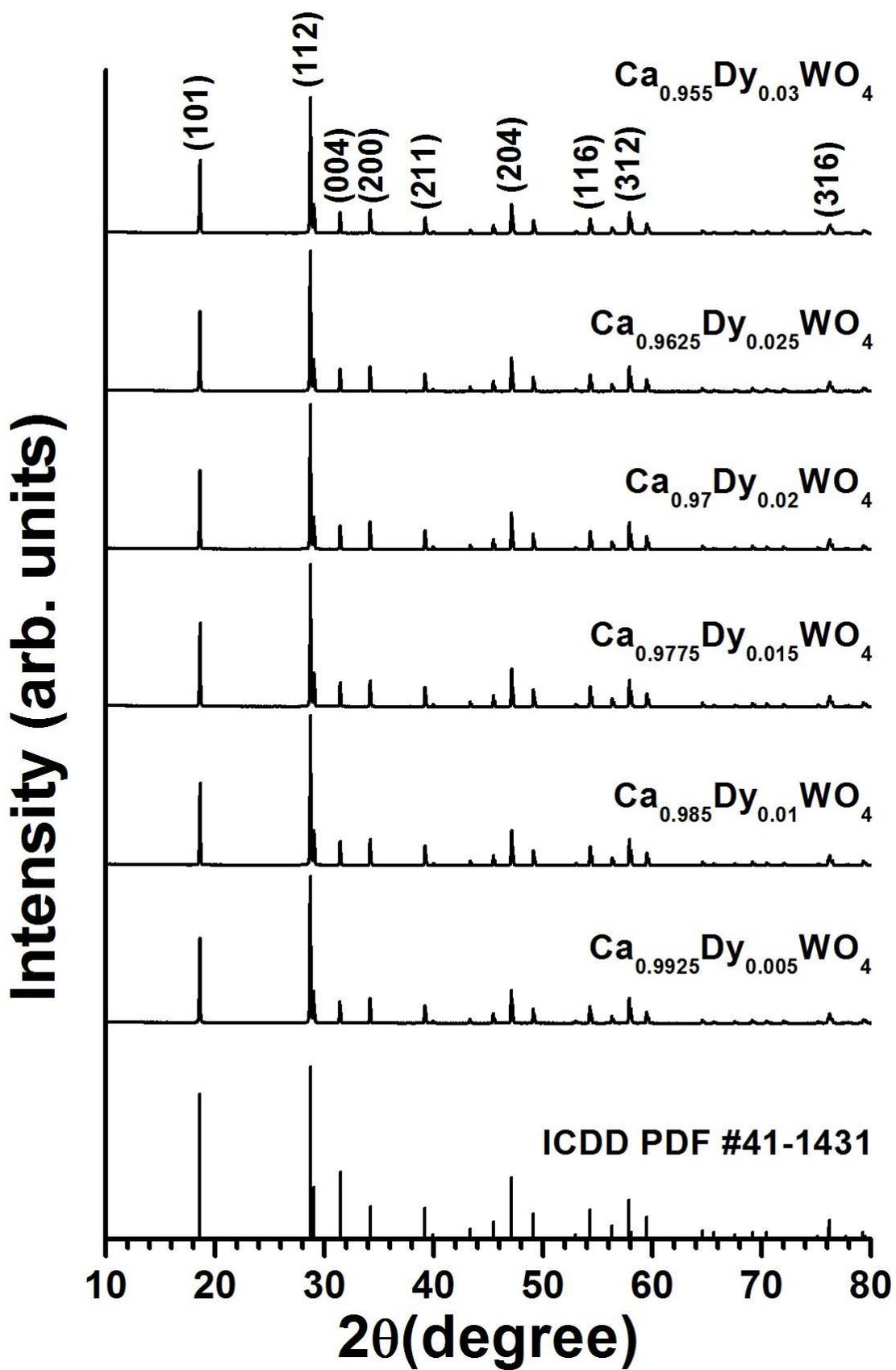
발표종류: 포스터, 발표일시: 수 16:00~19:00

Point Defects and Spectroscopic Studies of Yellow Phosphors $\text{CaWO}_4:\text{Dy}^{3+}$ and $\text{CaWO}_4:\text{Dy}^{3+},\text{Na}^+$

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신라대학교 신소재공학과

Two different types of yellow phosphors $\text{CaWO}_4:\text{Dy}^{3+}$ and $\text{CaWO}_4:\text{Dy}^{3+},\text{Na}^+$ were synthesized with various concentrations of Dy^{3+} ions by using a solid-state reaction. The former type contains both substitutional and vacancy point defects, while the later has only substitutional ones. X-ray diffraction (XRD) results show the (112) main diffraction peak centered at $2\theta=28.72$ deg. (Figure 1), and indicate that there is no basic structural deformation caused by the Dy^{3+} (and Na^+) ions or the vacancies in the host crystals. The photoluminescence (PL) emission and photoluminescence excitation (PLE) spectra revealed the optical properties of trivalent dysprosium ions. Delicate characteristics of point defects are reflected in the photoluminescence of yellow phosphors. The FT-IR spectra make clear that some of the ungerade vibrational modes have shifted positions and different shapes spreading over wide range of frequencies, caused by different masses of Dy^{3+} (and Na^+) ions or vacancies from Ca^{2+} ions. Raman spectra also exhibit subtle differences of point defects in $\text{CaWO}_4:\text{Dy}^{3+}$ and $\text{CaWO}_4:\text{Dy}^{3+},\text{Na}^+$ in the gerade normal modes.*Corresponding author (S. -W. Cho, Silla University)



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Fabrication of Three-dimensional Networks of Carbon Nanotube Coated with PolyAniline for Supercapacitor Application

안도연 이해원*

한양대학교 화학과

Carbon nanotube has been applied to a lot of applications because of its unique structural, mechanical, electrical properties. And Fabrication of three-dimensional network of carbon nanotubes was achieved by growing carbon nanotubes between silicon pillars. This unique structure shows highly dense and uniform structure which has a strikingly large surface area. On the other hand, Polyaniline presents high conductivity and thus have been widely applied to supercapacitors. But the poor cyclability limit their application for supercapcitors. In this study, three-dimensional network of carbon nanotubes was coated with polyaniline using in-situ polymerization method. By doing so, we were able to fabricate the unique nano structure of electrode with strikingly high surface area in ordered arrays. This structure of polyaniline coated 3D CNT Networks showed increase in specific capacitance and life cycle compared to the previous instance.

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Correlation of the Rates of Solvolysis of 2,4-Dinitrobenzenesulfonyl Chloride Using the Extended Grunwald-Winstein Equation

최호준 구인선*

경상대학교 화학교육과

The specific rates of solvolysis of 2,4-dinitrobenzenesulfonyl chloride have been determined in binary aqueous solvent mixtures at 25.0 °C. Comparison of the specific rates of solvolyses of 2,4-dimethoxybenzenesulfonyl chloride in terms of linear free energy relationships (LFER) are helpful in mechanistic considerations, as is also treatment in terms of the extended Grunwald-Winstein equation. It is proposed that the solvolyses of 2,4-dinitrobenzenesulfonyl chloride in binary aqueous solvent mixtures proceed through an dissociative S_N2 pathway rather than through an addition-elimination pathway.

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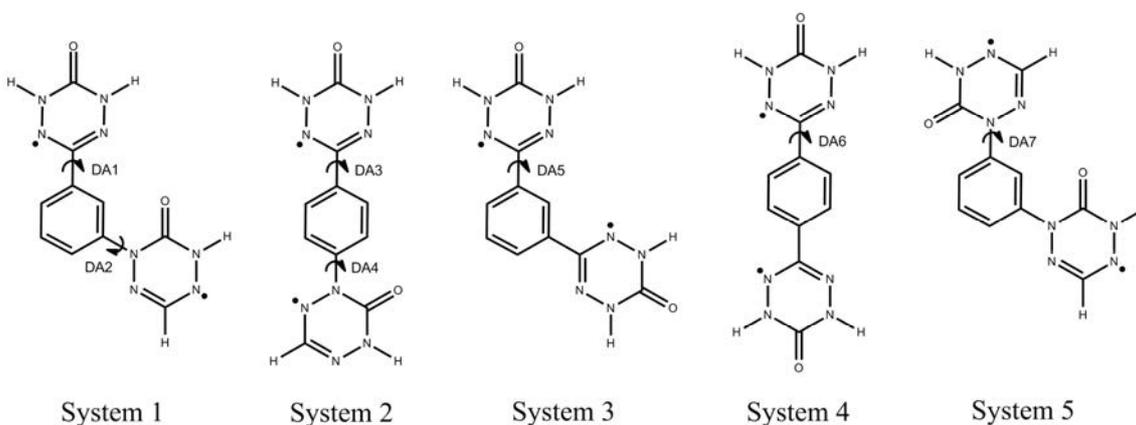
발표종류: 포스터, 발표일시: 수 16:00~19:00

A DFT Study on Magnetic Coupling in Oxoverdazyl-Benzene-Oxoverdazyl Diradical Systems

박영근 고경철 문종훈 김선경 조대흠 이진용*

성균관대학교 화학과

The intramolecular magnetic coupling constant (J) values of diradical-based magnet models (S1-S5) were studied using unrestricted density functional theory. The model systems were designed with series of oxoverdazyl radicals (o-Ver(N) and o-Ver(C)) linked through a benzene coupler. They were divided according to either connectivity of the radical (C or N) or geometrical topology (meta- and para-) of benzene coupler. Reasonable relationship was found between spin density distribution and sign of J value. With our results we determined ferro/antiferromagnetic interactions. J values were also calculated along the twisting movement by the scan of dihedral angles between the radical and the coupler. An overall trend was found as absolute value of J decreased over increasing torsion angles.



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A Highly Selective and Sensitive Fluorescent PET (Photoinduced Electron Transfer) Chemosensor for Zn²⁺

문종훈 김선경 박영근 조대흠 이진용*

성균관대학교 화학과

Control of dihedral angles in binaphthyl groups can be key for developing chiral catalysts, liquid crystals, chiroptical devices and other intelligent chiral material. Binaphthyl groups are unique and versatile frameworks for chiral recognition and asymmetric synthesis. However, no study has investigated the dihedral angle by the reversible molecular recognition process, which can be easily monitored by circular dichroism (CD) spectra and selective fluorescence changes. We report herein unique binaphthyl-pyrene system 1, whose dihedral angles were reversibly modulated after adding Zn²⁺. This is the first example in which metal ion recognition induced significant changes in dihedral angles that induced unique “off-on” fluorescence enhancement at 545 nm. We performed density functional theory (DFT) and time-dependent DFT (TDDFT) calculations with the M06/6-31G* method. The experimental CD observation was explained by the conformational changes upon Zn²⁺ binding, and the fluorescent sensor behavior was understood by oxidative photoinduced electron transfer (PET) based on quantum calculations.

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Synthesis and Characterization of Luminescent Polymer Nanoballs Incorporated with Eu(III) Complexes: Application to Detection of Some Cations in Water

강명현 강준길*

충남대학교 화학과

Luminescent polymer nanoballs were synthesized by self-organization process via two steps. First, a solution of a mixture of Eu(III) complex and polymer dissolved in THF solvent was gradually diluted with water and then the volatile THF solvent was gradually evaporated from the mixture. The polymers used in this work were poly(methylmethacrylate) (PMMA). The size of Eu(III)-encapsulated polymer nanoball was controllable by adjusting the concentration of the complex and the volume ratio of water to THF. The morphology of the fabricated polymer nanoball was confirmed by FE-SEM. The photophysical properties of polymer nanoballs were investigated by excitation and luminescence spectra. Also we observed that some cation gave rise to emission quenching. The cation quencher used in this work were Cu^{2+} , Cd^{2+} and Hg^{2+} . The emission quenching of Eu-(III)-encapsulated polymer nanoball was investigated as a function of cation concentration.

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Understanding of the metal-binding site in L-Arabinose isomerases through modeling and simulations

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조선대학교 약학과

L-Arabinose isomerase (AI) catalyzes the isomerization of L-arabinose to L-ribulose at elevated temperatures in the presence of divalent metal ions. The metal ion as the manganese (Mn^{2+}) plays a key role in the ligand binding and the structure stability at elevated temperature as $60^{\circ}C$ to $74^{\circ}C$. However, the structure study by X-ray has been performed at a low temperature and it is a limitation of the experimental method. In this work, we have modeled the two types of the structures; one is only with Mn^{2+} ion and the other is a complex system with Mn^{2+} ion and ligand as L-arabinose. Based on the X-ray study of the thermophilic *Geobacillus Kaustophilus* Arabinose Isomerase (GKAI) with Mn^{2+} ion, the molecular dynamic simulation (MD) was run at various temperatures. We have analyzed the surrounding of the active binding site with the metal ion and proposed the interaction of the water-metal ions-ligand.

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Synthesis and luminescence properties of Eu(II) complexes with Schiff base, o-N2O2

함아리 강준길*

충남대학교 화학과

Blue europium(II) complex with Schiff base was synthesized using the Eu_2O_3 solution. The Schiff base, o-N2O2H2 (2,2'-(1E,1'E)-(1,2-phenylenebis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol), used in this work as chelating ligand was synthesized from salicylaldehyde and o-phenylenediamine. The synthesized Schiff base ligand and Eu(II) complexes were confirmed with EA, ICP and TGA. The Eu(II) complexes excited at UV produced blue luminescence. The excitation spectra measured by monitoring the blue emission proved that the energy transfer took place effectively via the Schiff base ligand. Specific emission bands were observed around 400 ~ 450 nm region. In this presentation, the energy transfer between the o-N2O2 and the europium(II) ion will be precisely discussed.

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Photocatalytic activity test of TiO₂-SiO₂ composite particles by acid-catalyzed sol-gel method

유정훈 이진수 부진효*

성균관대학교 화학과

Titanium dioxide, among the transition metal oxide semiconductors widely used in photo-catalysis, is the most suitable photocatalyst due to its high photocatalytic efficiency and chemical and physical stability under the reaction conditions. Combined TiO₂/SiO₂ nano-particles were prepared by acid-catalyzed sol-gel method using titanium tetraisopropoxide (TTIP) and Tetraethyl orthosilicate (TEOS) as precursors at 600 °C. The structural properties of the prepared TiO₂/SiO₂ nanocomposited particles showed that polycrystalline particles are included anatase and rutile phase at XRD data. Also, the XRD intensity was decreased at increasing of TEOS precursor concentration. Photocatalytic activity of the TiO₂/SiO₂ (7:3) composited particles showed decomposition of ~95 % of methylene blue solution in 30 min.

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Chemical Charge Doping in Graphene by Sulfuric Acid Optically Separated from Native Mechanical Strain

안광현 이대응 류순민*

경희대학교 응용화학과

그래핀(graphene)의 라만 스펙트럼은 전하밀도(charge density)와 기계적 변형(strain)에 민감하여 연구에 널리 활용되고 있다. 그러나 실제 시료에서 관찰되는 두 물리량의 복잡한 변이를 정량 분석하기 위해서는 기계적 변형뿐만 아니라 전하밀도의 영향에 대한 신뢰도 높은 검정곡선이 필요하다. 이를 위해 본 연구에서는 황산 수용액을 통한 p-형 화학도핑(chemical doping)을 이용하여 전하밀도의 변화가 유발하는 라만 스펙트럼의 변이를 조사하였다. 분자의 효율적인 계면 확산을 위해 산화반응을 이용하여 그래핀의 기저면에 나노공(nanopore)를 만든 후, 액상에서 라만 스펙트럼을 측정하였다. 황산 농도를 증가(감소)시켰을 때 G 와 2D 피크의 진동수는 상호간에 일정한 비율로 증가(감소)하여 정공의 밀도가 증가(감소)하는 것을 알 수 있었다. 관찰된 전하밀도에 의한 G 와 2D 피크의 진동수 변화는 전기적 방법을 이용한 기존 결과보다 높은 재현성을 보여 신뢰도 높은 검정곡선으로 활용될 수 있을 것이다. 또한 본 연구를 통해 알게 된 황산 분자의 2 차원 계면 확산 현상을 자세히 소개하고자 한다.

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Observation of Raman G-band splitting in ABC trilayer graphene with a broken inversion symmetry

박광희 류순민*

경희대학교 응용화학과

이중층 그래핀(graphene) 표면에 전하를 주입하면 반전 대칭(inversion symmetry)이 깨지고 라만-비활성 진동 모드가 라만-활성화되면서 라만 G 피크가 갈라진다는 것이 알려져 있다. 삼중층 그래핀은 그래핀이 적층되는 방식에 따라 ABA(Bernal), ABC(Rhombohedral) 그래핀으로 나뉘며 ABC 그래핀은 ABA와는 달리 반전 중심을 가지고 있다. 본 연구에서는 기계적 박리법으로 만들어진 ABC 그래핀에서 반전 대칭이 깨질 때 일어나는 라만 스펙트럼의 변화를 탐구하였다. ABA 그래핀과는 달리 이중층 그래핀과 ABC 그래핀에서는 저진공 열처리 또는 요오드 흡착반응을 한 후에 G 피크가 갈라짐을 관찰하였다. 이로부터 위의 반응들이 복층 그래핀의 하단 또는 상단 표면에 잉여 전하를 유발하여 반전 대칭을 깨트린다는 사실을 유추하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-399**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of In₂O₃coated single-walled carbon nanotubes

박태희 이종택 박현준 이상훈 이휘건*

한양대학교 화학과

We investigated field emission (FE) properties of indium oxide (In₂O₃)-coated single-walled carbon nanotubes (SWNTs) prepared by a successive ionic layer adsorption and reaction process. The turn-on field had a lower value and FE currents were increased by three times compared with pristine SWNTs. Uniformity and brightness were increased after deposition from a FE display pattern. X-ray photoelectron spectroscopy (XPS) data suggested that the work function value of SWNTs was reduced after In₂O₃ deposition, resulting in increasing FE characteristics. Life time stability tests also revealed that In₂O₃ films protected SWNT tips during FE under exposure to O₂.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-400**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Modification of 3D Network of CNTs by Stages for Detecting Oral Cancer Biomarker

오은결 이해원* 이수범 서정은

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Oral cancer (oral squamous cell carcinoma, OSCC) is the sixth most common cancer in the developed world. Salivary biomarkers of oral cancer like CA125, Cyfra21-12, TPS3 significantly altered in OSCC patient as compared with healthy controls. Existing methods to detect biomarkers for early diagnosis such as ELISA, antibody array, commercial multiplexed bead platforms have some limitations. To overcome some limitation, 3D network of CNTs was used because of highly enhanced surface area and net-like structure enabling to give high chance for capturing biomarkers. Here, surface of 3D Network of CNTs was modified by biotin, streptavidin, biotinylated capture antibody to detect CA125 (cancer antigen 125), oral cancer biomarker. Each modification stages were examined by SEM and optical microscope to confirm that surface modified 3D network of CNTs can detect CA125. Detection CA125 in 3D Network of CNTs was possible by surface modification by stages.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-401**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Study of Hydrogen Adsorption on Graphene and Fullerene Surface

백지혜 김용호*

경희대학교 응용화학과

graphene 은 전기 전도도, 열 전도성, 탄성 등이 뛰어나 차세대 신소재로 각광을 받고 있으며 뛰어난 전기전도성을 이용해 고속 트랜지스터 소자에 응용되는 등 구리와 실리콘을 대체할 수 있는 나노전자소자의 유망물질로 고려된다. 또 fullerene 은 탄소 원자 5 각형 또는 6 각형으로 이루어진 원형과 유사한 모양의 탄소 동소체이며 전이금속, 유기물질 등을 도핑하여 optical 및 switching devices, 수소 저장물질로서 응용되고 있다. 본 연구에서는 DFT 이론을 바탕으로 graphene 과 fullerene 의 표면에 수소 흡착에 따른 potential surface energy 를 계산하였다. H 와 D 의 반응속도는 다차원 터널링 근사를 고려한 변분법적 전이상태이론으로 계산하여 반응속도론적 동위원소효과를 얻었고 터널링효과를 계산하였다. graphene 의 반응은 2 층의 graphite 과 두 층간의 pi-pi interaction 이 반응동역학에 미치는 영향에 대하여 연구하였고 다양한 크기의 fullerene 과 POAV 에 따른 반응을 비교하여 관찰하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-402**

발표분야: 물리화학

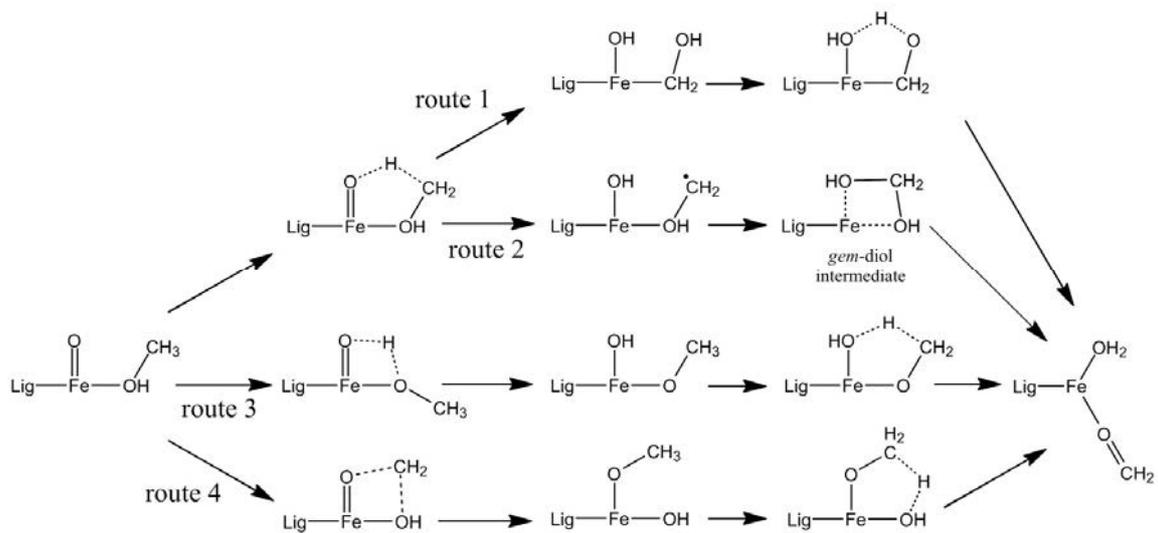
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reaction Mechanism and Large Tunneling Effect of the Alcohol Oxidation by High-Spin Iron-Oxo Complex of Non-heme Ligand: A Theoretical Study

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경희대학교 응용화학과

The alcohol oxidation to corresponding carbonyl compound by high-spin iron-oxo complex is one of the most important reactions. Several possible mechanisms have been proposed for this reaction and large kinetic isotope effect for the hydrogen transfer was found in the alcohol oxidation by high-valent iron-oxo complexes of heme and non-heme ligand. In this work, the mechanistic insight of methanol oxidation by high-spin $[(\text{bpg})\text{Fe}^{\text{IV}}=\text{O}]^+$ complex was studied. We found that this reaction is proceeded via dual hydrogen abstraction mechanism with a rate-determining C-H activation and the $\text{Fe}^{\text{IV}}/\text{Fe}^{\text{III}}$ reduction is the driving force of the C-H activation. Besides that, the variational transition state theory including multidimensional tunneling approximations was used to calculate rate constants to accurately predict the KIEs for the methanol oxidation based on the quantum mechanically generated intrinsic reaction coordinates of the H-transfer. At 298 K, the calculated and experimental KIE are 18.5 and 20.0, respectively, which are in good agreement within the limit of experimental error. Tunneling is found to be very significant for the C-H activation and the representative tunneling path (RTP) is very different from the MEP. The RTP appears at 2.5 kcal/mol below the top of the adiabatic energy barrier at 298 K and does not significantly depend on temperature above the range of 273 to 310 K.



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장소: 창원CECO

발표코드: **PHYS.P-403**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

3D Network of CNTs Inserted Microfluidics Chips for the Fast Detection

이수범 이해원*

한양대학교 화학과

For the point-of-care diagnosis, the fast and accurate detection of disease markers is important. The reaction, occurs in a test-tube, takes several hours which is not suitable for the point-of-care. In a microfluidics system, consistent flow and the micro reaction chamber boost up the reaction time. 3D Network of CNTs have a net like structure which generates more friction and resistant during flow and it boost up the reaction time. The experimental results, modified the surface of CNTs with biotin and flowed streptavidin solution into the reaction chamber, shows that the 3D Network of CNTs reached the saturation point within 1 min in a microfluidic system when 3D Network of CNTs went through the same reaction in a test tube did not reach the saturation point after one hour

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-404**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A theoretical study of small molecules as donor and acceptor materials for OPV applications

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경기대학교 화학과

Small molecules have been designed for donor and acceptor materials for organic photovoltaic (OPV) applications. These materials consist of thiophene and various electron accepting units. DFT level of theory were employed for the investigation. Upon charge transfer, however, these materials are subject to the so-called broken-symmetry, due to the symmetric molecular structure and hence unrestricted HF calculations were conducted for ionic radical states. It turned out that the wavefunctions for cationic state were delocalized mainly over thiophene units while those for anionic state were dominated by electron accepting units. IPs and EAs for these materials are computed to be compatible with those of well-studied materials, suggesting that these materials can be applied for OPV applications.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-405**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New gas sensor using 3-D Single-Walled Carbon Nanotubes network suspended on ZnO Nanorods

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한양대학교 화학과

Gas sensors can be classified into a chemical type operated by gas adsorption and a physical type operated by ionization. The chemical types of gas sensor usually utilize an electrical response by the adsorption of gas molecules on the surface of the active layer, which leads to a large change in its electrical resistance. But most of these sensors (except for the CNTs-based sensors) need high working temperatures, for example 300~500 °C. Meanwhile, structures with large surface area may be required for distinguishable detection, which cause problems like high power consumption and pre-heating time. On the other hand, ionization sensors as a physical type gas sensor work by fingerprinting the ionization characteristics of distinct gases. However, this kind of instrument has high power consumption and risky high-voltage operation, and thus cannot be used on site. In this experiment, we fabricated a gas ionization sensor based on 3-dimensional (3D) single-walled carbon nanotube (SWNT) networks suspended between ZnO nanorods by using a chemical vapor deposition method. ZnO nanorods were grown on the pyramid-like protrusions of a textured Si substrate. The breakdown voltages and stability of the 3D SWNT networks were measured and compared to those of a SWNT film synthesized on Si substrate. Our results show that 3D SWNT networks on ZnO nanorods enable ionization gas sensors to be sensitive, selective, and highly stable devices.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-406**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the MCM41 confinement effect on the structure and dynamics of lithium borohydride by using solid-state NMR

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한남대학교 화학과 ¹caltech

The structural and dynamical properties of lithium borohydride confined in on ordered porous silica (MCM41) were studied by using ¹H, ⁷Li, and ¹¹B solid-state NMR. The physicochemical properties of metal hydrides modified at the nano scale. The lithium borohydride, a material with high hydrogen content, could be readily incorporated into porous silica (MCM41) by using a simple chemical impregnation technique (solvent infiltration). This method has the advantage that impregnation can be performed under milder conditions as compared to the melt infiltration scheme. We were able to confirm infiltration effect with the solid-state MAS NMR experiments. Observed starting at 323 K, a four-line pattern superimposed on the broad line became visible. This pattern can be assigned to mobile borohydride species which means that the mobility of the borohydride increased by the confinement at LiBH₄. As drying time increased, the line split was more evident even at low temperature, which means penetration efficacy increased. We concluded that nano scale confinement of lithium borohydride in the porous silica strongly enhanced the mobility of borohydride anion and lithium cation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-407**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SERS Hot Spot Formation with Thiol Functionalized Cucurbit[n]uril

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포항공과대학교 화학과

We developed a new strategy for the generation of surface-enhanced Raman scattering (SERS) hot spots by anchoring a suitable target molecule in a close proximity to the metal surface/nanoparticle using the host-guest chemistry of cucurbit[6]uril (CB[6]). Two kinds of nano structures were prepared; the aggregation of Ag nanoparticles and Ag nanoparticles on an Ag substrate. The role of thiol-CB[6] is a linker which connects Ag nanoparticles or Ag nanoparticle and a bulk Ag surface with reproducible gap distance forming strong Ag-S bonds. Gap distance between Ag nanoparticles is close enough for a strong SERS signal. The structure of these nanostructures was investigated by transmission electron microscopy (TEM), atomic force microscopy (AFM), IR, UV-Vis spectroscopy, and X-ray photoelectron spectroscopy (XPS). IR and XPS measurements confirm the vertical geometry of thiol CB[6] on metal surface indicating that CB[6] pore is open. These open CB[6] pore can interact with several guest molecules very selectively generating very strong SERS signal of guest molecules. P-toluidine molecules were used as a guest molecule and a Raman report molecule. This system provides reproducible SERS hot spot having chemical selectivity via host-guest interaction of CB[6].

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-408**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Eu(III)-Incorporated Silica Nanoparticles for a Red LED

정용광 강준길*

충남대학교 화학과

The powdered complex and the complex-incorporated silica particles were fabricated with 365-nm UV-LEDs. The PL properties of the fabricated LEDs operated at 3.0 V were investigated as a function of time. Figure 5 shows the intensity decay of the red emission. The intensity of the red emission from the powder-casted LED was decreased rapidly by 80 % as soon as the LED was on. The powdered complex was significantly degraded by the heat emitted from the pumping UV-LED, of which the junction temperature was higher than 150 °C. Contrary, for the CS and the IS complexes, the intensity was maintained without loss after slightly down at the initial stage, while for the OS complex the intensity was gradually decreased. These results indicated that the silica matrix capping the complex well protected the complex from the thermal degradation. Figure 6a shows PL spectra of the fabricated LED devices. The PL spectra consisted of two strong bands. The sharp band and its satellite, peaking at 360 nm and 410 nm, respectively, were due to an emission from the pumping InGaN diode, and the low-energy bands, appearing in the 590 ~ 700 nm region, were due to the emission from Eu(III). The relative intensity between the two strong bands was dependent on an amount of the casted phosphor. The CIE 1931 chromaticity of the three devices is shown in Figure 6b. The chromaticity index (x, y) varied from (0.5467, 3382) for the IS-fabricated LED and (0.5505, 0.3342) for the CS-fabricated LED to (0.4682, 0.3437) for the OS-fabricated LED. This blue-shift of the x-index was dependent on the relative intensity of the 410-nm satellite band to that of the red emission.

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장소: 창원CECO

발표코드: **PHYS.P-409**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structures and bonding properties of Gold-Arg-Cys complexes: DFT Study of Simple Peptide-Coated Metal Surface

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We present structures, bonding characteristics and infrared spectra of gold surface(111)-Arg-Cys complex calculated by periodic plane wave DFT technique. We examine the detailed features of bonding between gold surface and dipeptide. The dipeptide is revealed to form covalent bond via the -SH group with several gold atoms, and also weaker(noncovalent) interactions via the guanidine side chain lying more or less parallel to the gold surface. The S-H bond dissociates as a result of the S-(Au)_n bond formation, with the proton binding over several gold atoms. The calculated infrared spectra agree well with experimental observations reported by Petoral and Uvdal[Colloids and Surfaces B, 2002, 25, 335]

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-410**

발표분야: 물리화학

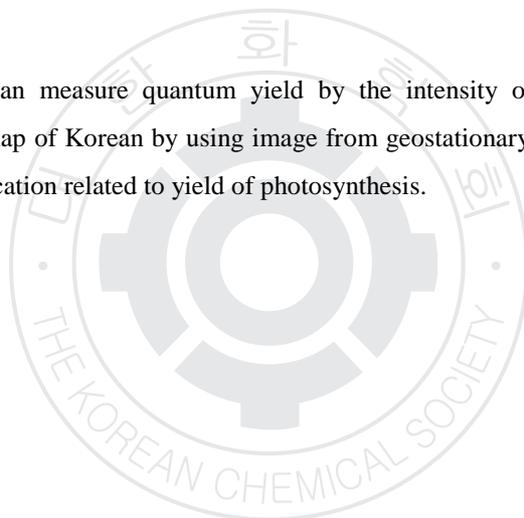
발표종류: 포스터, 발표일시: 수 16:00~19:00

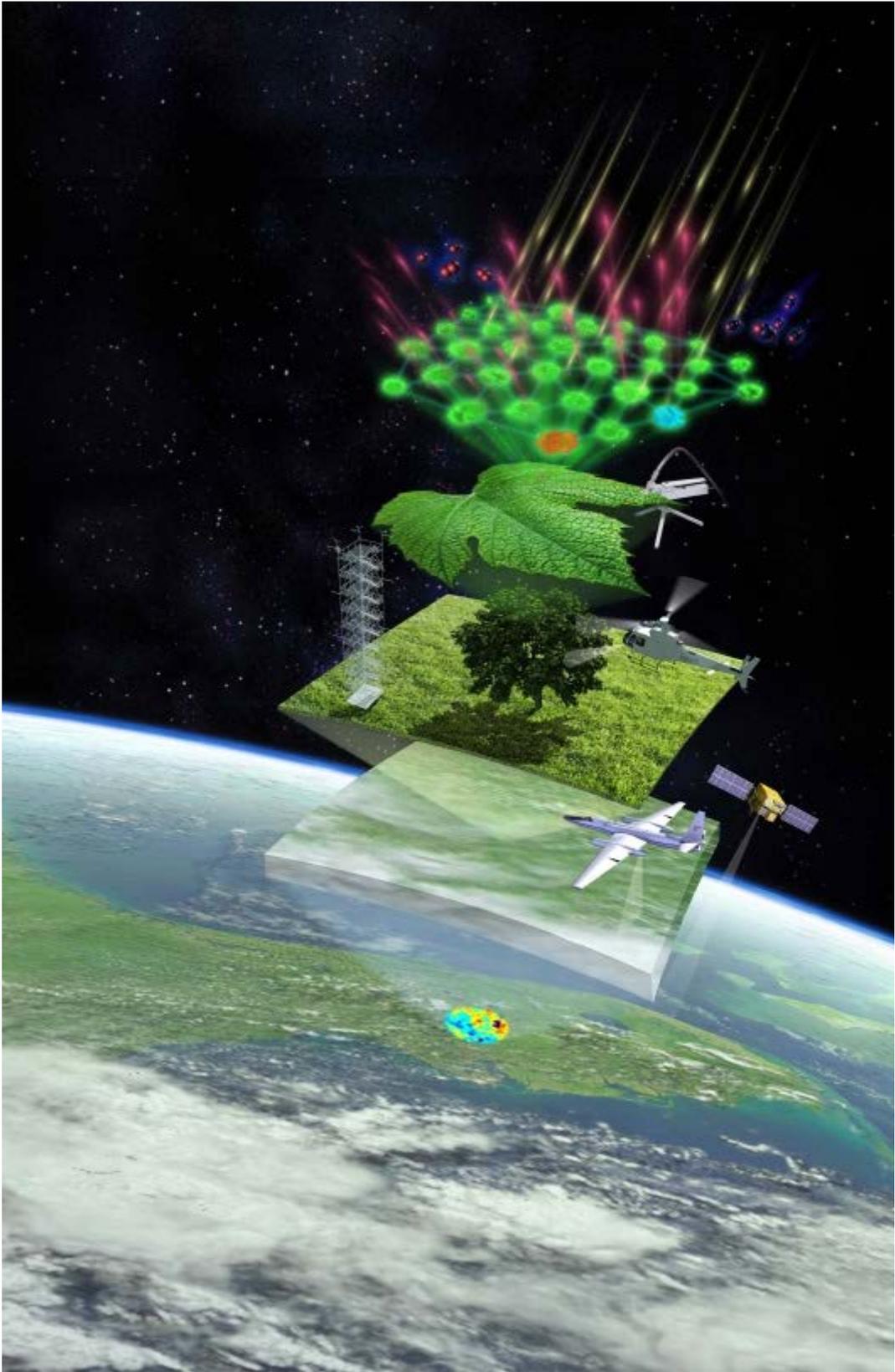
New mapping of photosynthetic efficiency from geostationary satellite

정종운 안태규^{1,*}

성균관대학교 화학과 ¹성균관대학교 에너지과학과

Photosynthesis of plants can measure quantum yield by the intensity of fluorescence. We made a photosynthetic efficiency map of Korean by using image from geostationary satellite. In addition, we had been studying a lot of application related to yield of photosynthesis.





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장소: 창원CECO

발표코드: **PHYS.P-411**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Supercapacitive properties of ruthenium oxide electrodes deposited on 3D-arrayed nano-porous nickel current collectors

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국민대학교 생명나노화학과

Supercapacitor is one of the most important electrochemical energy conversion and storage devices because of its rapid charge-discharge rate, high power density and long cycle life. Ruthenium oxide (RuO₂) is one of the most widely studied supercapacitive electrode materials due to its great specific capacitance and good electrical conductivity. One of the recent strategies to enhance the specific capacitance of the devices is to deposit the electrode materials onto the three-dimensional (3D) array of current collector nanostructures since it can provide direct paths for efficient charge transport along the 3D network as well as the significantly increased surface area. In this work, we firstly fabricated 3D arrays of nickel (Ni) nanostructures using polystyrene nano-opal substrates. We also fabricated half-cell supercapacitors by electrodepositing RuO₂ onto these Ni current collectors and investigated their electrochemical properties.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-412**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dynamic Range of IR Probe

박광희 조민행*

고려대학교 화학과

The site-specific IR probes, which were used for studying protein dynamics, should have not only structural sensitivities but also long vibrational lifetimes. Because the transient IR signals such as IR pump-probe and 2D IR signals can be measured only when the IR probes are in a vibrationally excited state. In this regard, developments of new IR probes with long vibrational lifetimes are very important for studying structural dynamics of proteins occurring on hundreds of picoseconds or even longer timescales. we studied the method of increasing lifetime of the IR probe to use the heavy atom between the peptide and probing molecules, which studied the structural dynamics of the proteins with IR probed peptide. Using various IR probe-derivatized prolines, their lifetimes in D₂O and chloroform are measured with polarization-controlled IR pump-probe spectroscopy. The measured lifetimes of 10~15 ps for azido stretch mode is short. The measured lifetimes of SeCN are 3-4 times longer than those of SCN, because that selenium atom effectively blocks the intramolecular vibrational relaxation pathways of the CN stretch mode. This result would be significant guideline for development of new IR probe, which used to studying structural dynamics of proteins.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-413**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation of Highly Ordered Self-Assembled Monoayers of 4-Fluorobenzenethiols Guided by Displacement of Cyclohexanethiols on Au(111)

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한양대학교 나노융합과학과 ¹한양대학교 화학과

Self-assembled monolayers (SAMs) of fluorinated-aromatic thiols have drawn much attention due to their interesting electrical and optical properties that may be applicable in molecular electronics. However, to improve device performance and obtain reliable data, the ability to fabricate two-dimensional ordered SAMs of fluorinated-aromatic thiols is needed. Especially, it is known that the SAMs of 4-fluorobenzenethiol (4-FBT) have usually disordered phases. In this study, to obtain long-range ordered 4-FBT SAMs, cyclohexanethiol (CHT) SAMs can be used as transient layers because of their weaker lateral interaction and lower adsorption density compared to alkanethiolate SAMs. By scanning tunneling microscopy observation, we found that well-ordered 4-FBT SAMs can be obtained via the displacement of preadsorbed CHT SAMs on Au(111) by 4-FBT. It was found that the partially ordered 4-FBT SAMs were formed after 1 h displacement, whereas the fully covered 4-FBT SAMs were formed after 2 h displacement.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation and Structure of 3-Hexylthiophene Self-Assembled Monolayers on Au(111)

김영우 강훈구 이동진 노재근*

한양대학교 화학과

The formation of self-assembled monolayers (SAMs) of 3-hexylthiophene (3-HTP) on Au(111) prepared by vapor or solution deposition method was investigated by the cyclic voltammetry (CV), scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). STM and XPS studies revealed that the surface properties of 3-HTP SAMs prepared by vapor deposition method were markedly different from those prepared by solution deposition method. Even though both of 3-HTP SAMs prepared by vapor and solution method give rise to the formation of two-dimensional SAMs through chemisorption, 3-HTP SAMs prepared by vapor deposition contained ordered structure unlike those prepared by solution deposition. Reductive desorption data shows that reductive desorption potential for 3-HTP SAMs is higher than that for thiophene SAMs, which means that the intermolecular interaction of 3-HTP SAMs is stronger than that of thiophene due to the presence of long alkyl chains of 3-HTP molecules. We found that 2-D surface properties of thiophene derivative SAMs are strongly influenced by preparation method (vapor or solution) and intermolecular interaction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-415**

발표분야: 물리화학

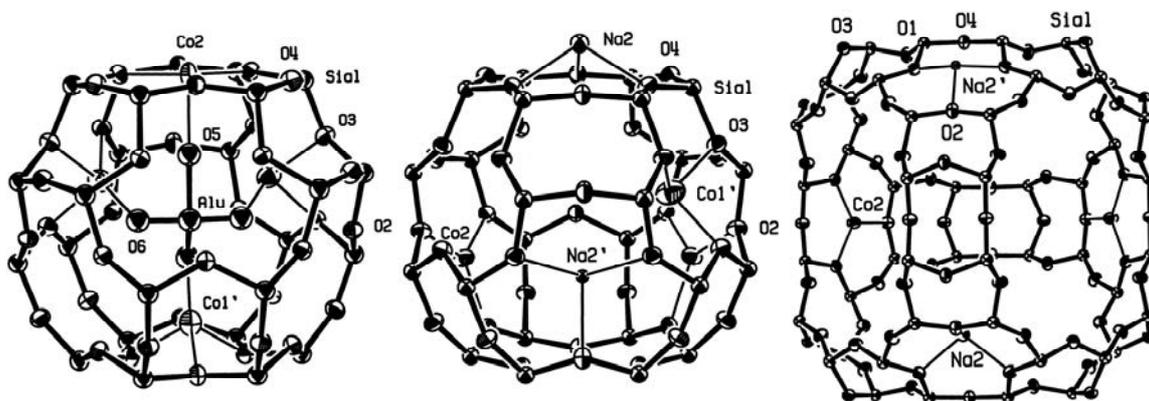
발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of Co^{2+} ion-exchange into Faujasite-type zeolites

서성만 김후식 임우택*

안동대학교 응용화학과

Three single crystals of fully dehydrated, largely Co^{2+} -exchanged zeolites X and Y were prepared by the exchange of Na_{80} -X ($[\text{Na}_{80}][\text{Si}_{112}\text{Al}_{80}\text{O}_{384}]$ -FAU, Si/Al = 1.40), Na_{75} -Y ($[\text{Na}_{75}][\text{Si}_{117}\text{Al}_{75}\text{O}_{384}]$ -FAU, Si/Al = 1.56), and Na_{71} -Y ($[\text{Na}_{71}][\text{Si}_{121}\text{Al}_{71}\text{O}_{384}]$ -FAU, Si/Al = 1.70) with aqueous streams 0.05 M in $\text{Co}(\text{NO}_3)_2$, pH = 5.1, at 294 K for 3 days. This was followed by vacuum dehydration at 673 K. Their crystal structures were determined by synchrotron X-ray diffraction techniques in the cubic space group $Fd\bar{3}m$ at 100(1) K. They were refined to the final error indices $R_1/wR_2 = 0.08/0.25$, $0.06/0.18$, and $0.07/0.24$, respectively. In all three crystals Co^{2+} ions occupy the 6-ring sites I, I', and II; Na^+ ions occupy sites II' and II. Some dealumination of the zeolite framework was seen in the first crystal (initial Si/Al = 1.40). As the Si/Al ratio of the zeolite framework increases, both the Na^+ and H^+ contents of the zeolite decrease.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-416**

발표분야: 물리화학

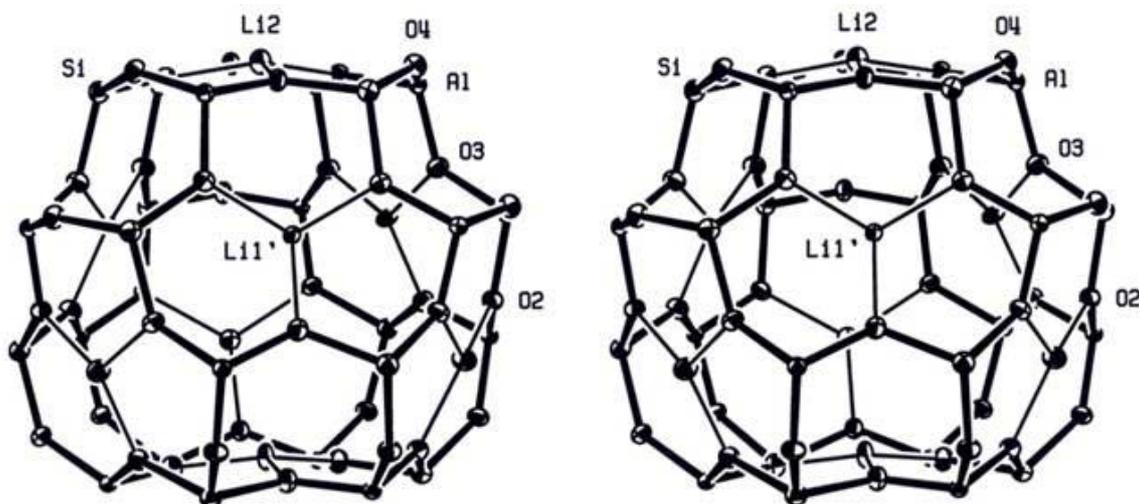
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Single-crystal Structure of Fully Dehydrated Fully Li⁺-exchanged Zeolite X

김후식 서성만 임우택*

안동대학교 응용화학과

Complete exchange of Li⁺ into zeolite Na-X, [Na₉₂[Si₁₀₀Al₉₂O₃₈₄]-FAU], was accomplished using undried methanol solvent (water concentration 0.02 M). A crystal of Na-X was treated with 0.1 M LiNO₃ in the solvent at 333 K, followed by vacuum dehydration at 673 K and 1 × 10⁻⁶ Torr for 2 days. Its structure was determined by single-crystal synchrotron X-ray diffraction techniques, in the cubic space group *Fd3*-at 100(1) K. The 92 Li⁺ ions per unit cell are found at three different crystallographic sites. The 32 Li⁺ ions occupy at site I' in the sodalite cavity: these Li⁺ ions are recessed 0.28 Å into the sodalite cavity from their 3-oxygens plane (Li-O = 1.903(5) Å and O-Li-O = 117.8(3)°). Another 32 Li⁺ ions are found at site II in the supercage, being recessed 0.26 Å into the supercage (Li-O = 1.968(5) Å and O-Li-O = 118.3(3)°). The remaining 28 Li⁺ ions are located at site III in the supercage (Li-O = 2.00(8) Å).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-417**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of novel low-bandgap molecule and its application to small-molecule organic solar cells

박다솜 이진호 임상규*

국민대학교 생명나노화학과

Small-molecule organic solar cells (SMOSCs) are attracting growing attention for their predominant advantages such as well-defined molecular structures, easy control of purification and good reproducibility of cell performances. One of the recent research trends is to develop various push-pull molecules synthesized by connecting electron donor and acceptor blocks through π -conjugated spacer (A- π -D- π -A) because of their lower LUMO level and hence reduction of band gaps which leads to a large extension of spectral photo-response. In this work, we synthesized new A- π -D- π -A compound comprising the benzodithiophene core and dicyanate terminal unit. The SMOSCs based on this new compound and fullerene (C60) were also fabricated and their cell parameters were characterized.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-418**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Computer Simulation Studies of bis-Polydiacetylene Systems

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광운대학교 화학과 ¹이화여자대학교 화학·나노과학과

Polydiacetylenes (PDAs), a family of conjugated polymers, have very unique electrical and optical properties. For example, on environmental stimulation, such as by viruses, proteins, DNAs, metal ions, and organic molecules, PDAs can undergo a colorimetric transition from blue to red which is accompanied by fluorescence enhancement. Interestingly, thermochromic assays showed that bis-PDAs have the colorimetrically reversible properties. In this study, bis-PDA membrane systems are developed in full atomistic details along with various substituents and used for molecular dynamics simulations. Various physical properties including the orientation correlation of conjugate double bonds and the tilt angle of alkyl side chains are calculated to understand the reversibility of the bis-PDA membrane systems.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-419**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Study of (-)-Epicatechin: Structural properties and Chemical Reactivity

PhamKhacDuy 이상욱¹ 정희일*

한양대학교 화학과 ¹울산대학교 화학과

Density Functional Theory (DFT) was used to study the chemical reactivity and the geometry of (-)-Epicatechin. The local reactivity sites were predicted on basis of the DFT indices. The theoretical IR spectra of (-)-Epicatechin was also clarified. In order to determine the local reactivity, which has not been well investigated so far, the frontier molecular orbital and Fukui function were plotted and the results pointed out that the carbon in para-position of benzyl ring was the most active toward electrophile attack. The Bond Dissociation Energy (BDE), proton affinity (PA), H- affinity, electron affinity (EA) and ionization potential (IP) were computed to confirm that electron density-based method was more reliable in the prediction of (-)-EC local reactivity. Moreover, these parameters gave us a global idea on the chemical activity behavior of the (-)-Epicatechin and clarified the anti-oxidizing properties. Finally, we found that the (-)-Epicatechin was an amphoteric molecule and it could participate in acid-bases reactions types as well as proton transfer chemical reactions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-420**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Prediction of the second reduction potentials of some quinones and their derivatives using density functional theory calculations

ARYALPABITRA 이상연*

경북대학교 응용화학과

The prediction of highly accurate redox potential is very useful to explain the experimental facts and to design new functional materials. The first reduction potential of organic compounds are known to be calculated with high accuracy using the density functional theory and the self-consistent reaction field method. The second reduction potentials can be calculated with the same approach but the accuracy of the calculated values are not well assessed. It is highly desirable to develop a computational protocol for the prediction of the second reduction potentials. The second reduction potentials of some quinones and their derivatives have been calculated with the Gaussian 09 program. The geometries have been optimized with the M062X/6-31+G** level, the single point energy calculations have been performed with the M062X/6-311+G** level at the optimized geometries, and the solvation energies have been calculated with the SMD/M062X/6-31+G** level. The calculated absolute redox potentials have been converted to the standard redox potentials. The calculated potentials have been compared with the corresponding experimental ones to design a protocol. The calculated results will be presented and discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-421**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Prediction of redox potentials of some iron and nickel complexes using density functional theory calculations

우동주 이상연*

경북대학교 응용화학과

The prediction of redox potential of transition metal complexes with high accuracy is very helpful for the design of electrolytes of redox flow battery. To develop a computational procedure with high accuracy and low cost, several performance tests have been made to select density functional and basis function for the geometry optimization and the computation of ionization potential, electron affinity and solvation free energy of some transition metal complexes. These test results will be presented and discussed to develop a protocol to evaluate redox potential of transition metal complexes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-422**

발표분야: 물리화학

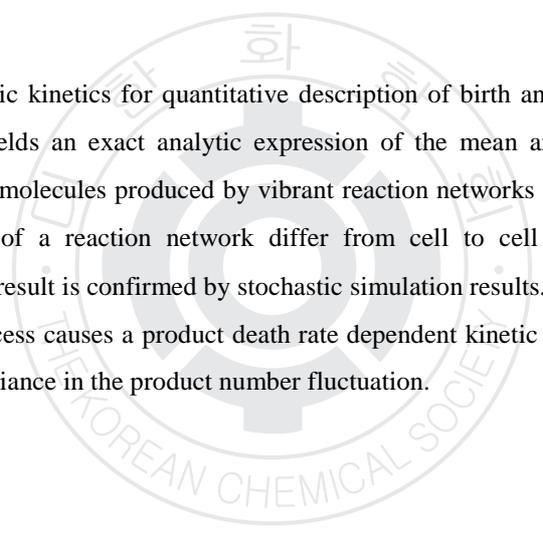
발표종류: 포스터, 발표일시: 수 16:00~19:00

New stochastic kinetics of birth and death processes in living cells

양길석 김지현* 성재영*

중앙대학교 화학과

We present a new stochastic kinetics for quantitative description of birth and death processes in living cells. Our new kinetics yields an exact analytic expression of the mean and variance in the number fluctuations of the product molecules produced by vibrant reaction networks in living cells, in which the reactivity or productivity of a reaction network differ from cell to cell and fluctuate over times. Correctness of the analytic result is confirmed by stochastic simulation results. Our analyses show that the fluctuation in the birth process causes a product death rate dependent kinetic phase transition in the time evolution of the relative variance in the product number fluctuation.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-423**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular dynamics simulation study of electrolyte system: Force field validation

이경구

군산대학교 화학과

In lithium ion secondary battery, the electrolyte system which generally consist of 1M lithium salt and carbonate-based organic solvents is a complicated system. To reveal the dynamics and kinetics of electrolyte system at atomic level, classical molecular dynamics simulation should be adopted. Force fields i.e., AMBER and COMPASS are currently available for simulating the electrolyte system. Before inspecting the interaction between molecules of electrolyte in detail, each force fields were verified. We have calculated the macroscopic thermodynamic properties such as density, diffusion coefficient and ionic conductivity from the simulation results with each force field. COMPAS force field(cff91) which is the second generation force field can better reproduce the experimental thermodynamics properties. We further investigated the reason why the second generation force field is better than the previous force fields.

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장소: 창원CECO

발표코드: **PHYS.P-424**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The DFT and HF studies on supramolecular structures of LiQ, NaQ and KQ

김소연 이대균*

(주)씨에스엘솔라 연구소

Organic Light-Emitting Diode(OLED)에서 LiQ 는 전자전달 물질이나 전자주입 물질로 널리 사용되고 있다. LiQ 같은 환상 구조의 분자들은 고체상태에서 여러개의 분자가 하나의 거대분자(super molecule)를 형성하는 형태로 존재한다. 본 연구에서는 LiQ 및 유사한 화학구조를 갖는 NaQ, KQ 의 거대분자에 대한 입체적 구조를 계산화학적 관점에서 조사하였다. LiQ 의 경우, 가능한 거대분자로는 monomer, dimer, trimer, tetramer, hexamer 가 알려져 있으며, 이러한 분자들의 가능한 입체적 구조에 대하여 양자화학적 계산을 진행하여 기저상태에서의 입체 구조, 전자의 분포상태 등에 대한 자료를 조사하였다. 분자계산 과정에서 밀도함수이론(Density Functional Theory)과 Hartree-Fock 이론을 적용하였으며 pople basis set 인 3-21G*, 6-31G(d), 6-31G(d,p)를 사용하였다. LiQ 의 경우 hexamer 가 가장 낮은 ABE(average binding energy)를 갖는 구조이며, NaQ 나 KQ 에서도 동일한 결과를 얻을 수 있었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-425**

발표분야: 물리화학

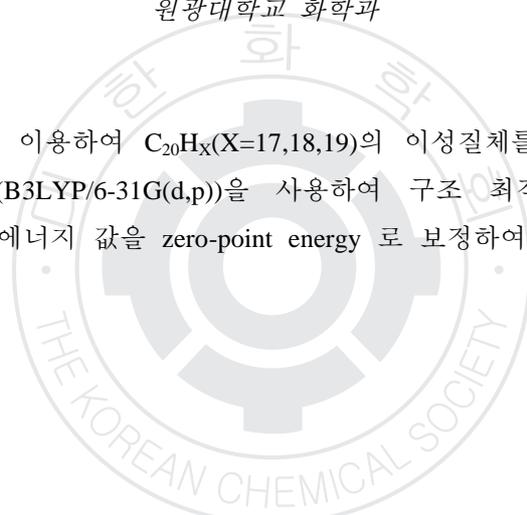
발표종류: 포스터, 발표일시: 수 16:00~19:00

Atomic Structure and Electronic Properties of $C_{20}H_X(X=17,18,19)$ by Hybrid DFT study

이설 이기학*

원광대학교 화학과

Gaussian 03 프로그램을 이용하여 $C_{20}H_X(X=17,18,19)$ 의 이성질체를 계산하였다. 각 구조를 혼성 범 밀도 함수법(B3LYP/6-31G(d,p))을 사용하여 구조 최적화를 진행하였다. 또한 Frequency 계산을 통해 에너지 값을 zero-point energy 로 보정하여 안정도와 전자적 특성을 비교하였다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-426**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

치환기 X에 따른 $C_{20}H_{20}$ 과 $C_{20}X_{20}$ 케이지 내부 부피 변화 및 전기 적 특성의 변화 비교 (X= OH, SH)

이설 이기학*

원광대학교 화학과

혼성 범밀도 함수법 B3LYP/6-31G(d,p)을 사용하여, $C_{20}H_{20}$ 에 대해서 H 를 OH 또는 SH 로 치환 할때 일어나는 케이지 내부 부피 변화 및 전기적 특성의 변화에 대하여 연구하였다. Gaussian 03 프로그램을 이용하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-427**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reduction potential of hydrated 3d transition metal ions

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Reduction potential of transition metal complexes is a fundamental research area of a battery field. It is hard to calculate reduction potential using computational quantum chemistry due to the complexity of the hydrated system. Not only the presence of a metal ion but also solvent molecules surrounding the solute atoms make the theoretical simulation more difficult. It is required to ionization potential (IP) of gas phase and solvation energy. Even though an atomic number of 3d transition metal atom is not very big, the relativistic effect for these atoms is not negligible. Coupled-cluster single, double and perturbative triple (CCSD(T)) is employed to give accurate gas phase IP with Douglas-Kroll 2nd order Hamiltonian. Very large basis sets, aug-cc-pwcv5z, is used to eliminate from the deficiency of basis sets. In this study we include solvent molecules up to the 2nd solvation shell containing 18 water molecules. The inclusion of only first solvation shell of six water molecules is not enough to consider the environmental effect. The geometry of hydrated metal ions by 18 water molecules is optimized B3LYP/6-31+G*. The solvation energy is obtained using CAM-B3LYP/6-311++G** basis sets on the geometry based on the previous calculation. It gives relatively large error of 10kcal/mol but the amount of error is similar for both ions. It is canceled out during the calculation of reduction potential. Mean absolute error of less than 0.2 is obtained.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-428**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

혼성 범밀도 함수법을 이용한 $X@C_{20}H_{20}^q$ ($X=HF, N_2$ $q=+1, 0, -1$)의 원자구조, 전자 성질, 케이지 붕괴변화 및 frequency에 대한 연구

지정민 이기학^{1,*} 이철¹

원광대학교 바이오나노화학과 ¹원광대학교 화학과

Gaussian03 package 프로그램에 있는 Hybrid DFT 인 B3LYP/6-31g(d,p) method 으로 $X@C_{20}H_{20}^q$ ($X=HF, N_2$ $q=+1, 0, -1$)에 대한 원자 구조를 최적화하고, 원자 구조와 전자 성질에 대하여 분석하였으며 frequency 를 계산하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-429**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dynamics of Br formation in the Photodissociation of Bromocyclohexane near 234nm

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부산대학교 화학과

In this work, we have studied dynamics of Br formation in the photodissociation dynamics of bromocyclohexane near 234 nm. We applied velocity map imaging technique coupled with [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme. REMPI scheme was used for state-selective detections of Br and Br* generated after photodissociation of bromocyclohexane near 234nm. Using REMPI scheme, we can monitor specific state at specific wavelength. Result of our work, we get the raw image. In case of excited state, it consists of two rings. However, ground state has just one ring. Also, we measured total translational energy distributions, recoil anisotropic parameters, and the relative quantum yields. There translational energy distribution is can fitted by two Gaussian functions of Br have been observed. The experimental result also showed that Br formation is dominant with the relative quantum yield 0.81 near 234nm.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-430**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Density functional theory reactivity studies on C₄N₂ with O

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부산대학교 화학과 ¹가톨릭대학교 화학과

Dicyanoacetylene (DCA, C₄N₂) is one of the important constituents in the interstellar medium, which is responsible for the haze around the titan's atmosphere. The reactivity of DCA with atomic oxygen (O) may provide important information about the origin of life. Hence in the present study, we have performed density functional theory reactivity studies on C₄N₂ with O. The main objective in the present study is, to explore the important aspects of potential energy surfaces of C₄N₂ reaction with singlet and triplet Oxygen. The reaction profiles of DCA isomer1 (DCA1) and isomer4 (DCA4) with O in the singlet and triplet framework have been obtained. The favorable reaction pathway has been identified. Our calculations have shown that, Intersystem crossing (ISC) is observed in DCA1 which leads singlet IMs energetically more stable than triplet IMs. Because of ISC, the barrier energy reduces, which favors singlet O reaction with DCA. In addition, Oxygen triggers C-C bond fission, in DCA1 which leads to the formation of products such as C₂NO and C₂N. However, in the case of DCA4, there is no ISC, here the singlet IMs energetically more stable than triplet IMs. The reaction through 3O+C₄N₂ => 3IM1 => ISC => 1TS1-3 => 1IM3 => 1TS3-4 => 1IM4 => 1TS4-5 => 1IM5 to product is more favorable reaction path

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **PHYS.P-431**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

CO₂ absorptions on various defects of boron nitride nanotube

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Carbon dioxide (CO₂) molecule is known to be the main source of greenhouse effect and the postprocessing of CO₂ is getting important in industrial process. In a few decades, various absorbents of CO₂ such as zeolite, carbon nanotube (CNT), and silicon carbide nanotube were developed. Recently we have proposed new possibilities of CO₂ absorbent on modified boron nanotube (BNNT). This modified BNNT makes CO₂ absorption in ambient condition. In the poster, we present further modification effects on BNNT surface from the theoretical investigation. By making various defects on BNNT, different trends of CO₂ absorption will be presented as well.

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장소: 창원CECO

발표코드: **PHYS.P-432**

발표분야: 물리화학

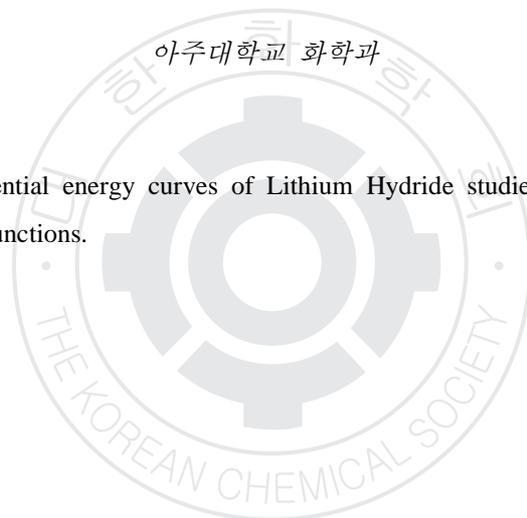
발표종류: 포스터, 발표일시: 수 16:00~19:00

**Study of highly excited states of a LiH molecule by the MRCI method
and comparison of potential energy curves obtained from experiments
by RKR and IPA and from other theoretical methods**

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아주대학교 화학과

Highly excited stated potential energy curves of Lithium Hydride studied using MRCI method and Kaufmann Rydberg basis functions.



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REMPI Spectrum of Laser-Desorbed Tryptophan

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The gas-phase spectroscopy is a very useful way to study detailed characteristics of molecules that can not be seen by liquid-phase spectroscopy and others. To do this gas-phase spectroscopy, naturally, we should make gas-phase molecules from solid or liquid-phase. Heating is a simple and stable method to vaporize a sample. For big or chemically unstable molecules, however, heating is not a good method because of thermal-decomposition. So, if we use heating to make gas-phase molecules, then we can only study very limited number of molecules, not bio-molecules. For this reason, laser-desorption technique is used to avoid this thermal-decomposition problem. In this poster, we show the REMPI spectrum of laser-desorbed tryptophan.

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Relativistic effect modified new composite method

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For obtaining the accurate thermo-chemical data while low computational cost is maintained, various types of composite methods are developed. Gn1), CBS-n2), MCCM3), Wn4), HEAT5), and ccCA6). Among them Gn theories are implemented in Gaussian program and ccCA theories for organic molecules are implemented in NWChem program. Although they covered most of molecular systems, no one covers molecular level of relativistic effect correction of molecules containing heavy elements. Using couple cluster method with relativistic effects with proper pseudo-potential and basis sets, we suggest new types of composite method. To see the relativistic effect, single point energy terms are separated to basis energy, diffusion effect, polarization effect, and method correlation effect. Using the geometry from relativistic calculation, these four single point energy are calculated in both of relativistic and non-relativistic way. Non-relativistic energy will be corrected by adding spin-orbit effect of energy difference from KRMP2 and MP2. Some test calculations were performed with hydride dimers of group 13 elements, (GaH)₂, (InH)₂, and (TlH)₂.

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한약재 추출물의 활성산소종에 대한 항산화 특성 연구

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다양한 한약재에 대한 항산화효과를 분광학적 방법으로 고찰하였다. 한약재의 종류로는 금문대황, 녹차, 연교, 황백, 지실등이고 비교시료로 비타민 C 를 측정하였다. 측정결과로 지실이 월등히 좋은 항산화 효과를 보여주었으며 나머지는 각각 황백, 비타민 C, 연교, 녹차, 금문대황의 순서로 나타났다. 가장 효과가 낮은 금문대황의 경우에는 과량의 주입에서도 전혀 항산화 경향을 나타내지 않았다. 또한 단일항 산소의 분광학적인 직접적인 증거를 고찰하였다.

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Quantitative analysis of Polyhexamethylene Guanidine (PHMG) Oligomers using MALDI-TOF Mass spectrometry

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Polyhexamethylene guanidine (PHMG) polymers are reported to cause lethal damage when used as an active ingredient in an antibacterial humidifier disinfectant. Therefore, it is important to develop a quantitative analytical method which can allow for the determination of the amount of PHMG. Recently, we have showed that MALDI-TOF is a great tool to identify PHMG and determine the average molecular mass of PHMG when used with a proper matrix. In the present study, we extended our investigation in a way that an internal standard is used to quantitatively determine the amount of PHMG in a prepared sample. As the internal standard, a small peptide with a large portion of arginine was chosen because arginine has a guanidine side chain that is also contained in PHMG. In the symposium, we will show our preliminary results towards this goal.

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Portable Rotating Disk Electrode for Heavy Metal Analysis in Korean Solar Salt Using Anodic Stripping Voltammetry

김용훈

농촌진흥청 농업공학부

Salt is one of the essential elements for human survive, because of the important biological functions in human body, such as an electrical signal transmission in nervous system and the control of water content in a body. In order to monitor the safety of Korean Solar Salt formed by the natural evaporation of seawater, the heavy metal content of the salts prepared in Honam Area of Korea are measured by Anodic Stripping Voltammetry (ASV). The manufactured portable electrode (MPE) provides the promising performance of ASV measurement to detect Pb and Cd in the aqueous media without degassing. MPE showed the favorable response with respect to the redox reaction of stripping analysis. The system demonstrated the linearity and the responsivity in the low and high concentration ranges, sufficient to apply the in-situ monitoring of heavy metals. In addition, the stripping analysis of real samples such as saturated salt solutions reflects that the system is sufficient for the application of various fields of food safety.

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Easy preparation of ground S-ketoprofen MIP particles for chiral HPLC separation of ketoprofen enantiomers

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Molecule imprinted polymer (MIP) is widely used as chromatographic media for separation of the template enantiomers when the MIP is made with one of the enantiomers as the template. Ground MIP particles from hard bulk MIP have been the prototype of such application. Tedious and time-consuming grinding and sieving of the MIP are in general required. We here demonstrate a useful approach of MIP formation where rather soft MIP is made by subtle control of formulation of the MIP reaction mixture. The soft MIP can be easily smashed with a spatula or similar thing to give particles of proper size distribution, which enables removal of sieving process. For example, to the mixture of S-ketoprofen (template), 4-vinylpyridine (functional monomer), ethylene glycol dimethacrylate (cross-linking monomer), AIBN(initiator) in acetonitrile (porogenic solvent) that had been reported for preparation of hard S-ketoprofen MIP in the literature, a certain amount of methacrylic acid was added to yield a soft MIP. The resultant MIP was soft enough to be easily smashed into small particles. After washing the particles to remove the template, the particles were packed in a microcolumn. The resultant column showed quite better chiral separation performance for ketoprofen enantiomers than the column packed with the particles obtained from the conventional hard MIP.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Capillary Electrochromatography on Clindamycin Phosphate-Zirconia Hybrid Monolith

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영남대학교 화학과

An organic-inorganic hybrid zirconia monolithic capillary column was prepared by sol-gel process in a fused-silica capillary with 3-triethoxysilylpropyl isocyanate derivative of clindamycin phosphate as the chiral selector. The column was employed for electrochromatographic enantioresolution of some basic drugs using mobile phases consisting of acetonitrile, methanol and ammonium acetate. Excellent separation was observed for enantiomers of sertraline, cetirizine, atropine, Tröger's base and indapamide. Effects of the compositions of organic solvents and electrolyte on enantioseparation were studied.

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Enantioseparation of Basic Drugs by Aqueous Ion-pair Capillary Electrophoresis using Penicillin G as a Chiral Selector

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International Conference on Harmonization (ICH) and its parties [i.e., European Federation of Pharmaceutical Industries and Associations (EFPIA) and U.S. Food and Drug Administration (FDA)] have issued a comprehensive set of guidelines for registration of new chiral pharmaceuticals which demand investigations of stereospecific fate of drugs in the body and enantiomeric purity determination of chiral drugs before their introduction into the market. Therefore, development of efficient analytical methods for enantioseparation has become an essential part of the drug development process. Ion-pair capillary electrophoresis (CE) using non-aqueous mode is an established technique for enantioseparation [1, 2]; however, only one publication was found that describes enantioseparation using aqueous mode [3]. The present work describes enantioresolution of five basic chiral drugs (namely, darifenacin, citalopram, sertraline, metoprolol and propranolol) by ion-pair CE using penicillin G (PenG) as a chiral selector (CS) in aqueous mode. Systematic experiments were performed to investigate the effects of concentration of CS, composition of background electrolyte (BGE), applied voltage and capillary temperature on chiral separation. A CS concentration of 10.6 mM was found to give the best resolution for enantiomers of darifenacin, citalopram, sertraline and propranolol; while 15.9 mM was found to be the best for metoprolol. Baseline resolutions for all the analytes were obtained in BGE composed of water: methanol (10:90, v/v) at 20°C with an applied voltage of 5 kV. CE was established as an efficient and versatile technique for its several advantages, such as, high efficiency, rapidity and simple instrumentation. The present study indicates that aqueous ion-pair CE can be further explored to develop methods for enantioseparation.

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Detection and Characterization of Inorganic Nanomaterials in Nanoproducts

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한국표준과학연구원(KRISS) 미래융합기술부/나노바이오융합센터

The engineered nanomaterials have been increasingly used in various fields such as scientific, industrial and medical applications, owing to their unique properties. However, the lack of physicochemical data addresses the issues for the NanoSafety. We are currently developing the standard operating protocols (SOPs) for detecting inorganic nanomaterials and characterizing their physical properties in nanoproducts. The Au and TiO₂ nanoparticles in shampoo matrix were detected in a spiking test. It was carried out that an organic and an inorganic matrix were first removed in the washing process using DI water that was verified in the change of UV-Vis spectrum. Then the centrifuged pellet, washed at least twice, was investigated to characterize the size, the shape and the composition of extracted nanoparticles by using SEM and SEM-EDX analyses. The SOP developed by the spiking test was applicable to the detection of nanomaterials in nanoproducts such as a shampoo containing gold nanoparticles.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical study of silicon doped LiFePO_4 as a cathode material for Li rechargeable battery

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울산대학교 화학과

Olivine type lithium iron phosphate (LiFePO_4) has been one of the most promising cathode materials for the second generation of lithium rechargeable battery due to its improved safety, low environmental cost, and high theoretical current capacity (170 mAh/g). However, the poor electronic conductivity of LiFePO_4 due to the low lithium-ion diffusion rate makes difficulties of its commercial applications. Appropriate element doping could be a potential approach to enhance the electronic conductivity of LiFePO_4 . Herein, silicon doping in olivine LiFePO_4 has been applied to improve the electrochemical performances including the rate capability and cycling life. The silicon doped LiFePO_4 samples have been also characterized by X-ray diffraction (XRD) and transmission electron microscope (TEM).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Profiling of Oxidized Phospholipids in Different Lipoprotein Classes from Patients with Coronary Artery Disease by Asymmetrical Flow-Field Flow Fractionation and nanoflowUPLC-ESI-MS-MS

이주용 문명희*

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Lipoproteins are macromolecular particles consisted of phospholipids, apolipoproteins, cholesterol, and triglycerides and their function is to transport fats and cholesterol around the body via blood. In clinical laboratory, these lipoproteins are common markers in diagnosing coronary artery disease (CAD) by comparing the amount of low density lipoprotein (LDL) and high density lipoprotein (HDL). Recent studies have revealed that normal lipoproteins are oxidized by metalloprotein hemoglobins (Met-hemoglobin), and they accumulate at the vascular wall and create foam cells and plaque, which are the major factors of promoting CAD. Thus, profiling of phospholipids and apolipoproteins that are produced by the oxidation process of lipoprotein is important in understanding of biochemical processes of CAD. In our laboratory, three major classes of lipoproteins of human plasma including HDL, LDL and VLDL (very low density lipoprotein) were fractionated by using AF4 without any pre-treatment of the samples. A group of ten patient plasma samples and another group of ten healthy control plasma samples were pooled to examine the composition of various phospholipids in each lipoprotein class. Followed by extracting lipids from each lipoprotein subclass fractionated by AF4, oxidized and intact phospholipids in each sample were analyzed by nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nanoflowLC-ESI-MS-MS).

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Influence of the Concentration of Sodium Chloride on the Structure of Sodium Hyaluronate using Asymmetrical Flow Field-flow Fractionation and Multi-angle Light Scattering (AF4-MALS)

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Hyaluronic acid (HA), a water-soluble polymer with high molecular weight, is easily found in nature and human body such as placenta and skins. Due to the highly viscous and elastic properties of HA, it is used in a wide range of fields from cosmetics to cataract surgery and lubrication of the knee joints. Since HA has a few million Daltons in molecular weight, it is difficult to determine the accurate size or MW distribution. A size exclusion chromatography (SEC) is one of the most conventional methods to determine the MW of water-soluble polymer, but there are limits in determining exact MWD due to the lack of appropriate calibration standards. Flow Field-flow Fractionation (FFF), an elution method based on size, makes up for the drawbacks of SEC by using an empty channel to separate polymers. In addition, an absolute molecular weight of HA can be calculated by connecting the FFF channel to MALS detector. In this study, the influence of the concentration of NaCl on the structure of HA was examined. Depending on the repeated processes of ultrafiltration of HA dissolved in NaCl with deionized water, changes in Mw and distribution of HA can be analyzed.

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Fractionation of subcellular organelles by Asymmetrical flow field-flow fractionation

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Subcellular organelles have their own specific roles in cells. When organelles become malfunctioning in cells, activities of proteins or phospholipids in cells can be affected, causing organelle related diseases. Therefore, research on discovering biomarkers of disease by separating subcellular organelles has attracted increased attention in biological and biochemical research fields. Usually, separation of subcellular organelles is conducted by centrifugal methods. Centrifugal method has an advantage for its relatively simple use, however, it is difficult to well fractionate different organelles with ultracentrifugation and it is time-consuming. Furthermore, pure organelle fractions are difficult to obtain by the centrifugal methods. Besides centrifugal methods, fractionation of subcellular organelles can be conducted by flow cytometry or affinity purification methods. However, these methods usually require relatively complex preprocessing steps. Therefore, in this study, use of flow field-flow fractionation separate subcellular organelles in a high speed without any complex preprocessing steps. Asymmetrical flow field-flow fractionation (AFI-FFF) is an elution method based on size-separation and is applied for the separation of lysed cell mixtures in a steric mode. Human embryonic kidney 293 T cell line was gently lysed first and resulting mixtures containing nucleus, cell debris, and subcellular organelles were separated by AF4 in 5 minutes. After separating cell mixture, the size distribution of collected fraction was observed by Scanning Electron Microscopy (SEM).?

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Lipid analysis of Gaucher disease using nLC-ESI-MS/MS

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Lipids have been important analytes for the past decades for their crucial role in cell signaling, structure, and energy storage. Served for therapeutic purpose, lipid biomarkers can be used as early diagnostic test for their ability to detect and monitor a presence of biological process linked to the clinical manifestations and possible development of disease at an early-onset. Gaucher disease is a rare genetic disorder, in which mono-hexosylceramide (MHC) accumulates in lysosome due to a deficiency of an enzyme called β -glucocerebrosidase. When undigested MHC are stored inside the lysosomes in macrophages abnormally high, these enlarged macrophages become Gaucher cells, accumulating in various parts of organs such as liver, spleen, lymphatic system, and possibly central nervous system. As various kinds of manifestations by Gaucher disease overlap with other types of metabolic or neurological diseases, studying a rare Gaucher disease can elucidate and provide a unique insight on how these diseases are related. A comprehensive lipid analysis of plasma and urine samples from healthy control and Gaucher patients before and after enzyme replacement therapy were performed using nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS/MS). A total of 125 and 102 lipid species from plasma and urine, respectively, were detected and analyzed quantitatively. Among these, 18 and 9 species from plasma and urine, respectively, exhibited a distinct difference between patient and control group while all four species of MHC showed greater than two-fold increase among patients in both plasma and urine.

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Simple Isotope-coded Carbamidomethylation for Quantitation of Lectin-specific N-Glycoproteins of Liver Cancer Using Online mHFER-nLC-ESI-MS-MS

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In mass spectrometry (MS)-based proteomics study, quantitative approaches for proteome, which are related to diseases or important biological processes, are carried out using various quantitative MS strategies. The shotgun proteomic method can be a promising tool for relative quantitation of targeted proteome with various methods such as O18 labeling, N15 labeling, or stable isotope labeling by amino acids in cell culture (SILAC). Among these methods, carbamidomethylation-based method is an alternative labeling technique using a typical side chain modification of cysteine residue after proteolysis. Although carbamidomethylation-based method has a critical limitation, in which targeted peptides are essentially required to have at least one cysteine residue, it is still an effective technique for quantitative analysis of peptides due to its high efficiency of stable labeling. Prior to this study, we developed a microbore hollow fiber enzyme reactor (mHFER), which is a simple, highly reproducible, inexpensive to assemble, and user friendly device, that can be on-line coupled to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS-MS) for on-line digestion method for global shotgun proteomics. In this study, we applied the on-line mHFER-nLC-ESI-MS-MS to the carbamidomethylation-based method to quantificate lectin-specific N-linked glycopeptides from human sera of healthy controls and patients diagnosed with liver cancer system. Aleuria Aurantia Lectin (AAL, α -1,6 linked fucose specific) was used to enrich highly core-fucosylated glycopeptides from blood serum and 64 core-fucosylated glycoproteins from controls and patients were quantified in MRM mode.

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Top-Down approach for Quantitative Analysis of Phospholipids by On-line Chip-type AF4-ESI-MS-MS Using Selected Reaction Monitoring

양이슬 문명희*

연세대학교 화학과

In this study a chip-type asymmetrical flow field-flow fractionation coupled with electrospray ionization tandem mass spectrometry (cAF4-ESI-MS/MS) has been applied for the direct lipidomic analysis of lipoproteins in human blood plasma. Flow FFF has been utilized for the size fractionation of lipoproteins from human plasma with coronary artery disease (CAD), a common heart disease which is caused by plaque stacking up material such as low density lipoprotein(LDL) in blood vessel walls. Plasma samples were prepared by depleting albumin and immunoglobulin using a protein depletion kit to reduce ionization suppression by high abundant proteins. Lipoproteins in depleted plasma sample were separated by cAF4 by sizes, and phospholipids in lipoproteins were directly analyzed by ESI-MS-MS. Carbonic anhydrase (CA, 29 kDa) was added to plasma sample as an internal standard so as to calculate relative peak area ratio of each phospholipid for quantitative analysis of lipids. Then, we evaluated both reproducibility and ionization efficiency of lipoprotein lipids because CA added in plasma may interfere with lipid ionization. For the direct feeding of cAF4 outflow to ESI-MS-MS, the flow stream was splitted with adjusting flow rates to keep a stable spray efficiency and in-source fragmentation for minimizing multimeric form of lipoprotein was applied during ESI. Studies were focused on the quantitative analysis of a number of phosphatidylcholine (PC), phosphatidylehanolamine (PE), phosphatidylglycerol (PG), phosphatidylinositol (PI), sphingomyelin (SM) species which were in lipoprotein by utilizing selected reaction monitoring (SRM) in positive and negative mode.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-449

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of ground organic monolith particles and their application as separation media in HPLC

이진욱 정원조*

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The molecule imprinted polymer (MIP) technique was incorporated to make organic monolith that can be easily smashed into particles of proper size and porosity. A mixture of methacrylic acid, crosslinker EDMA, and initiator AIBN dissolved in a mixed solvent composed of toluene and iso-octane was prepared. Then a special MIP template polyethylene glycol (PEG) was added to the reaction mixture. By subtle control of the composition of the reaction mixture, the resultant polymer monolith had proper softness/hardness to be easily smashed into particles of proper properties such as particle size distribution and porosity. These particles were well washed in 2-propanol/water for formation of meso-pores by removal of template molecules, dried, and packed in a glass-lined stainless steel column (1mm I.D., 300 mm length) for examination of their separation performance in HPLC. By optimization of amount and molecular weight of the template, good separation efficiency was reproducibly obtained ($N \sim$ over 10,000) for a 30cm packed column.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-450

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Immobilization of styrene-acrylamide co-polymer on partially sub-2 μ m silica monolith particles and inner surface of fused silica capillary by RAFT polymerization to give stationary phases for the separation of D-glucose anomers

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인하대학교 화학과

Styrene-acrylamide co-polymer was immobilized on porous partially sub-2 μ m silica monolith particles and inner surface of fused silica capillary (50 μ m ID and 28 cm length) to result in μ LC and CEC stationary phases, respectively, for separation of D-glucose anomers. Reversed addition-fragmentation transfer (RAFT) polymerization was incorporated to induce surface polymerization. The spacer ligand (4-chloromethylphenylisocyanate) was bonded to silica via isocyanate-hydroxyl reaction with dibutyl tin dichloride (DBTDC) as catalyst, and the attached ligand was reacted with sodium diethyl dithiocarbamate (RAFT initiator entity). Acrylamide was employed to incorporate amide-functionality in the stationary phase. The resultant μ LC and CEC stationary phases were able to separate isomers of D-glucose well. The CEC stationary phase also gave good separation of other saccharides such as maltotriose and Dextran 1500 (MW~1500) with reasonable separation efficiency (number of theoretical plates around 300,000/m).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-451

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasensitive Detection and Quantification of PSA as a Biomarker for Diagnosis of Breast Cancer

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건국대학교 생명공학과

Prostate specific antigen (PSA), a single chain 33 kDa glycoprotein protease, is an abundant protein secreted from human prostate epithelium. PSA is widely used as a biomarker of prostate cancer for diagnostics and prognostics after treatment, because the high level of PSA is always observed in prostate cancer patients. Recently, it has been known that PSA also can be a useful biomarker for the diagnosis of breast cancer. The level of PSA in patients of breast cancer is much lower than that in patients of prostate cancer, and therefore, the method for ultrasensitive detection and quantification of PSA is required for breast cancer diagnosis. In this poster, we introduce an efficient method for selective detection and quantification of PSA using gold nanoparticles (AuNPs) and biochips. The PSA in a sample was captured by two antibodies on AuNPs and on a biochip through a sandwich assay format. The presence of PSA was then verified by subsequent Laser Desorption/Ionization Time of Flight Mass Spectrometry (LDI-TOF MS) analysis. AuNPs carried huge number of reporter molecules, called Am-tag. In this manner, MS analysis afford amplified mass signal of Am-tag which enabled ultrasensitive detection of PSA. In addition, PSA in the sample was quantitated by using an internal standard (IS) which was prepared with AuNPs and isotope-labeled Am-tag. The IS has the same structure as Am-tag but heavier molecular weight, and therefore, comparing the mass intensities between the Am-tag and the isotope-labeled Am-tag allowed absolute quantification of PSA. We believe our method to identify PSA quantitatively and highly sensitively will be applied to patients' serum for the diagnosis of breast cancer.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-452

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Use of Maleimide-Terminated Gold Nanoparticles and MALDI-TOF MS for Selective Extraction and Quantification of Glutathione

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건국대학교 생명공학과

Glutathione (GSH), a thiol-containing tripeptide, is the most abundant non-protein thiol in living organisms. GSH plays important roles in various cellular activities including redox activities, xenobiotic metabolism, signaling processes, and antioxidant activities. Particularly, GSH modulates the oxidative stress which is associated with various diseases with regard to cellular redox homeostasis. Therefore, the detection and quantification of GSH has been studied intensively, mostly by using high performance liquid chromatography, capillary electrophoresis, and gas chromatography. In this poster, we describe a new method for selective extraction and absolute quantification of GSH using matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF MS) and maleimide-terminated gold nanoparticles (AuNPs). Our strategy utilized the Michael addition of thiol to maleimide, which allows the selective extraction of GSH in samples to AuNPs having maleimide functionality (Mal-AuNPs). After the extraction step, the GSH bound on Mal-AuNPs was analyzed directly by MALDI-TOF MS. In addition, the extracted GSH was quantitated with internal standard (IS) which was prepared with Mal-AuNPs and isotope-labeled GSH. The IS has the same structure of the GSH but heavier molecular weight, and therefore, is able to allow absolute quantification of GSH by comparing the mass intensities between the GSH and the isotope-labeled GSH. We believe this strategy for absolute quantification of GSH would be useful by providing the quantitative information for diagnostic purposes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-453

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Survey of Matrix Assisted Laser Desorption/Ionization Mass Spectrometry Methods for Ganglioside Analysis

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A ganglioside is a glycosphingolipid with one or more sialic acids, and gangliosides play important roles in many biological processes such as immune response, cell-to-cell communication, and tissue differentiation. MALDI MS analysis of gangliosides is challenging because they are not easily ionized in the positive ion mode, and also because they are fragile and therefore significant in-source fragmented ions are produced. In this study, we performed analyses of gangliosides with several known or novel MALDI methods and evaluated their performances systematically. Matrix systems tested include conventional organic MALDI matrices with or without additives, carbon-based nano-materials such as graphene oxide, metal-based nanoparticles such as gold nanoparticles. Performance evaluation criteria are as follows; sensitivity in the positive and the negative ion mode, degree of in-source fragmented peaks, spectrum simplicity, and quality of tandem mass spectra.

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장소: 창원CECO

발표코드: ANAL.P-454

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Control of Crystallinity and Oxidation States of Copper Oxide Nanofibers by Calcination Process

박주연 강용철*

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The Cu oxide/polyvinyl alcohol (PVA) nanofibers were synthesized by sol-gel and electrospinning technique. The obtained Cu oxide/PVA nanofibers were heated to remove the PVA compound at 673 and 873K. The ultrafine Cu oxide nanofibers were characterized with scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The SEM images showed that the Cu oxide nanofibers were successfully prepared by electrospinning and calcination and the average diameters of the electrospun Cu/PVA nanofibers were 268.9 ± 97.2 nm. After the nanofibers were calcined at higher temperature than rt, the morphologies of the nanofibers were changed. XRD results indicated that the crystalline structure was changed from amorphous phase to monoclinic CuO through cubic Cu_2O . TEM images also verified the crystal phase of Cu oxide nanofibers. XPS spectra revealed that the thermal oxidation of Cu proceeded during calcination.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-455

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Characterization of Tin Nitride Thin Films by Reactive RF Magnetron Sputtering at Various Nitrogen Gas Ratios

최수진 박주연 강용철*

부경대학교 화학과

The tin nitride thin films were deposited on Si (100) substrate by reactive rf magnetron sputtering method at various nitrogen gas ratios. The surface morphology of the tin nitride thin films was investigated by the scanning electron microscopy. The thickness and roughness were measured by means of surface profiler. The thickness and surface roughness of tin nitride films were decreased with increasing the nitrogen gas ratios. The crystallinity of the films was verified with X-ray diffraction and the peaks of tin nitride with amorphous structure at high nitrogen ratio were observed. The chemical environment of the thin films was investigated with X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy. The formation of bonding between tin and nitrogen was confirmed by XPS. And the electrical properties were measured by means of the four point probe method. And work function of tin nitride thin films was measured with Kelvin probe.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-456

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimization of dynamic reaction in ICP-MS to determine metal contaminants in BOE

최혜원 박지현 김영현 임홍빈*

단국대학교 화학과

Buffered oxide etchant (BOE) is one of the most important etching solutions used in semiconductor manufacturing process. Therefore, accurate and sensitive determination of ultra trace metal contaminants has become the biggest issue in the process control. The current BOE analysis has various difficulties because it was vulnerable to contamination and loss in sample treatment and suffered from matrix interference in ICP-MS measurement. In this presentation, we studied a measurement technique to eliminate spectral interference in ICP-MS by gas dynamic reaction. Dynamic reaction cell (DRC) adopted by PE (perkinelmer) can remove the interference through the transfer reactions of charge, proton and hydrogen atom. Generally the system used gases like NH₃, CH₄, O₂ and controlled the parameters of RPq and RPa in Q-MS, which resulted in significant sensitivity enhancement for certain elements, such as nickel, potassium, sodium, calcium and iron. We optimized the dynamic reactions for more than 25 elements spiked in BOE and obtained the detection limits in the range of 0.002 to 0.2 ng/ml from the calibration curve. Clean room facility can raise the analytical performance for practical applications.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL.P-457**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An electrochemical immunosensor for immunoglobulin G (IgG) based on multiwall carbon nanotubes (MWCNTs) and chitosan coating

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A highly sensitive electrochemical immunosensor was developed for the detection of immunoglobulin G antigen (IgG) using the IgG immobilized chitosan coated multiwall carbon nanotube (Ch/MWCNT/IgG) as an immunosensor probe and anti-IgG antibody (anti-IgG)-gold nanoparticles (AuNPs)-methylene blue (MB) (anti-IgG-AuNPs-MB) bioconjugate as a signalling label. The immunosensor probe and the bioconjugate were characterized using scanning electron microscopy (SEM), ultraviolet visible (UV-vis) spectroscopy, x-ray photoelectron spectroscopy (XPS), and electro-analytical experiments. The immunosensor probe was first treated with the anti-IgG-AuNPs-MB followed by the displacement of the bioconjugate by the addition of free IgG in a phosphate buffer solution. The low level detection of IgG was achieved by monitoring the MB reduction peak before and after displacement of the bioconjugate.

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장소: 창원CECO

발표코드: ANAL.P-458

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A stable and sensitive voltammetric immunosensor based on a new non-enzymatic label

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A stable and sensitive electrochemical carcinoembryonic antigen immunosensor based on a new non-enzymatic label (3, 3', 5, 5'-tetramethylbenzidine (TMB)) was fabricated using gold nanoparticles-deposited polydopamine film (PD/AuNPs) as an anti-CEA antibody immobilizing platform. TMB was conjugated with CEA and utilized as an electrochemical label. The PD/AuNPs platform provides enhanced conductivity, thus the redox reaction of TMB label was observed at the immunosensor probe. The immunosensor probe was characterized using scanning electron microscopy and electrochemical impedance spectroscopy. The CEA detection was based on the competitive binding of free- and TMB-conjugated-CEA to the anti-CEA antibody. Using differential pulse voltammetry, CEA can be selectively detected as low as 10 ± 0.6 pg/mL. The present immunosensor method was applied to CEA-spiked human serum samples and the recovery results were satisfactory.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-459

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Increased Electrocatalyzed Performance through Dendrimer-Encapsulated Gold Nanoparticles and Carbon Nanotube-Assisted Multiple Bienzymatic Labels: High Sensitive Electrochemical Immunosensor for a Protein Detection

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과학기술과

A high sensitive electrochemical carcinoembryonic antigen (CEA) immunosensor was fabricated by covalently immobilizing a monoclonal CEA antibody (Ab1) and a mediator, thionine (Th) on gold nanoparticles (AuNPs)-encapsulated dendrimer (Den/AuNPs). Multiwall carbon nanotubes (MWCNT)-supported secondary antibody (Ab2)-conjugated multiple bienzymes, glucose oxidase (GOx) and horseradish peroxidase (HRP) (Ab2/MWCNT/GOX/HRP) was used as electrochemical labels. The high sensitive detection was achieved by the increased HRP electrocatalyzed reduction of hydrogen peroxide, which was locally generated by the enzyme, GOx. Square wave voltammetry (SWV) technique was used to monitor the increased electrocatalyzed reduction of hydrogen peroxide by horseradish peroxidase (HRP). The linear dynamic range and the detection limit were determined to be 10.0 pg/mL to 50.0 ng/mL and 4.4 ± 0.1 pg/mL, respectively. The validity of the immunosensor response was tested in various CEA spiked human serum samples and the results were compared to an enzyme-linked immunosorbent assay (ELISA) method.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL.P-460**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Plasma treated parylene-N film for biosensor application

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A parylene film without functional group ("parylene-N") will be presented for the effective immobilization of proteins by physical adsorption. Parylene-N was modified by using plasma treatment for the protein immobilization, and the efficiency of immobilization was compared with the conventional polystyrene and parylene-N film by using proteins with different surface charges (isoelectric point) as model analytes. The surface morphology and the surface charge were analyzed by using AFM and contact angle after plasma modification of polystyrene, and parylene-N film. The plasma treated parylene-N film was applied to SPR biosensor for immunoassays.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-461

발표분야: 분석화학

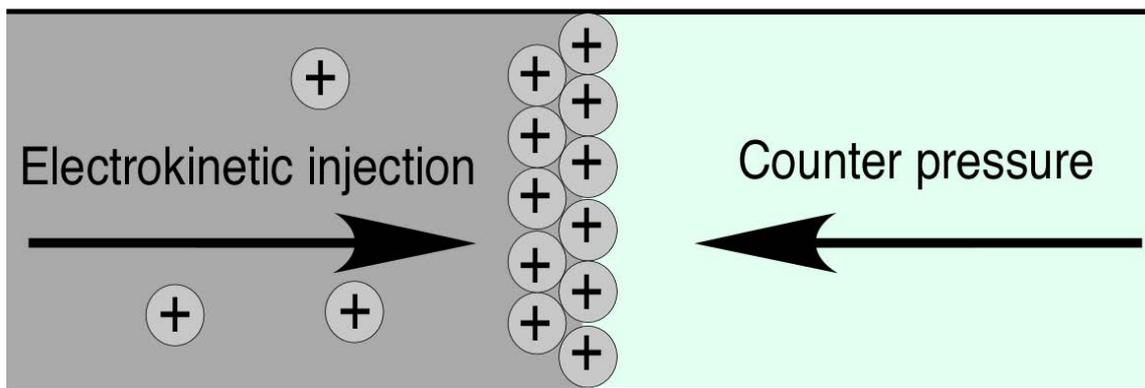
발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of low concentration catecholamines by counter flow electrokinetic supercharging

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Electrokinetic supercharging is one of the most powerful sample stacking methods that combines field amplified sample injection and transient isotachopheresis. In counter flow electrokinetic supercharging, a constant counter pressure is applied during sample injection in order to counterbalance the movement of the injected sample zone. As a result, there will be a pronounced increase in the amount of sample injected and the portion of the capillary available for electrophoresis. In this report, counter flow electrokinetic supercharging optimization factors such as the electric field application in the constant voltage and constant current modes, the effect of counter pressure, the length of injection time, and the terminating electrolyte concentrations were investigated. The enrichments obtained with a 30 min injection of 10 nM catecholamines in 5 mM terminating electrolyte solution in the 30 kV constant voltage mode applying a counter pressure of 1.3 psi were 25,000-fold for dopamine, 20,000-fold for norepinephrine, and 29,000-fold for epinephrine, yielding detection limits of 1.9, 1.2, and 1.4 nM, respectively with absorbance detection at 200 nm. [1]Reference.1. Joon Yub Kwon, Seo Bong Chang, Yong Oh Jang, Mohamed Dawod, and Doo Soo Chung. *J. Sep. Sci.*, accepted for publication (2013).



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장소: 창원CECO

발표코드: ANAL.P-462

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

항체와 압타머를 이용한 저분자량, 도파민의 샌드위치 분석법

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서울여자대학교 화학과

샌드위치 분석법은 샌드위치가 의미하는 것처럼 분석대상물질과 결합할 수 있는 두 개의 결합단백질이 필요하다. 그러나, 저분자량인 도파민은 항원결정기 (epitope)가 두 개 이상 존재하지 않으므로 샌드위치분석법이 갖는 많은 장점에도 불구하고 하나의 항체만으로는 샌드위치 면역분석법을 적용할 수 없다. 이에, 항체 외에 다른 결합체로서 항체를 능가하여 많은 장점을 가지는 압타머를 통해 샌드위치 분석법을 시도하고자 한다. SELEX 를 통해 얻은 RNA 압타머의 염기서열에 상응하는 DNA 압타머는, 도파민과의 친화력은 유지하면서 Rnase 에 의한 영향을 받지 않으므로 안정하다는 점을 착안하여 57mer DNA 압타머를 이용한 경쟁적인 면역분석법을 시도하였으며 그 결과 도파민의 검출한계를 3.2×10^{-12} M 까지 낮추는 좋은 결과를 얻었다. 본 연구에서는 두 개의 결합체인 도파민의 항체와 57mer DNA 압타머를 각각 capture protein 과 detector protein 으로 (또는, 역으로) 사용한 샌드위치 분석법을 시도하였다. 두 개의 결합체 중에 크기가 작은 압타머를 capture 로 사용한 경우, 표적물질인 도파민과 결합하게 되면, 그 뒤에 오는 항체는 입체 장애를 받지 않고 결합이 가능하리라고 본다. 역으로, 크기가 큰 항체를 capture 로 사용하면, 도파민과 결합 후 압타머가 detector 로 첨가되었을 때, 입체적 방해에 의한 결과를 예상할 수 있다. 이에 대한 비교 실험은 실험조건의 최적화를 통해 연구한다.

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발표코드: ANAL.P-463

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

도파민 압타머의 혼성화에 따른 두 자리 면역분석법

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서울여자대학교 화학과

도파민은 중추신경계의 중요한 신경전달물질 중의 하나로 카테콜아민에 속한다. 도파민의 생체 내 존재량은 $10^{-8}M \sim 10^{-6}M$ 으로 부족할 경우 파킨슨 병, 치매 그리고 주의력결핍 행동장애와 같은 질병을 일으킨다. 압타머란 SELEX 과정을 통하여 얻어진 한 가닥의 올리고뉴클레오티드이다. 항체가 가진 단점을 보완할 수 있다는 점으로 인해 면역분석에서 분석물질을 인식하는 새로운 인자로 대두되고 있다. 앞선 연구에서, 본 연구실에서는 압타머를 이용한 경쟁적인 효소-결합 압타머 분석법을 발표했으며, 이에 본 연구에서는 두 가지 압타머(57,67 mer DNA)를 이용하여 두 자리 면역분석법을 개발하고자 한다. 하지만 일반적인 두 자리 면역분석법과는 상반되는 결과를 얻었으며 이러한 결과들을 통하여 두 가지의 압타머가 쌍을 이루는 염기서열을 통하여 혼성화를 예상하였다. 두 압타머는 같은 RNA pool 의 SELEX 과정으로부터 얻어낸 염기서열을 갖고 있기 때문에 같거나 비슷한 도파민 인식자리를 가질 것이다. 이로부터 하나의 압타머가 도파민과 결합하면 뒤에 들어오는 압타머는 상대적으로 결합할 자리를 잃게 된다. 이 후 자유롭게 존재하는 압타머간의 염기서열의 혼성화가 이루어질 것이다. 이 가정을 검증하기 위해 염기서열이 다른 올리고뉴클레오티드를 이용하였다. 혼성화 가능성을 확인한 후 실험의 조건을 최적화하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-464

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantitative detection of ultrasensitive cardiac troponin I by chemical deposition method

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한국전자통신연구원(ETRI) 반사형표시소자연구실

Cardiac troponin I (cTnI) is a biochemical bio-marker for heart disease. The normal concentration range of cTnI is 30 pg/ml or less; therefore, an ultrasensitive detection technology is required. Troponin is a kind of protein that controls calcium-dependent interaction of myosin on actin when muscle contracts. Troponin exists in skeletal muscle and cardiac muscle. Cardiac troponin gives great helps in the evaluation of patients with chest pain because cTnI has high specificity on cardiac muscle cell damage. Troponin has been analyzed by monoclonal antibody immunoassay or enzyme-linked immunosorbent assay (ELISA). Recently, monoclonal “sandwich” antibody qualitative test method have been also used for the analysis of troponin. The first two analysis methods require approximately 2 hours. They are expensive and require highly skilled specialists. The “sandwich” method can be performed within 20 minutes next to the bed of patients; however, it has limitation in detecting low concentration troponin. This presentation describes a new quantitative cTnI detection method that can analyze troponin in short analysis time (within one hour) and at high sensitivity (~10 pg/ml). It exploits nanoparticles and chemical deposition of nanoparticles on well-type plastic substrate. It is possible to induce nanoparticles to plastic substrates by specific binding among biomolecules. By deposition solution containing silver ions, the growth of nanoparticles and the amplification of optical signal could easily be achieved. The cTnI concentrations in the range from 0.01 ng/ml (10 pg/ml) to 100 ng/ml are analyzed and the coefficient of variation (cv) of 10% or less is observed.

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장소: 창원CECO

발표코드: ANAL.P-465

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Liquid chromatographic resolution of fendiline and its analogues on a crown ether-based chiral stationary phase

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부산대학교 화학과

Fendiline is clinically effective agent used in the treat of coronary heart disease. It is also sub-sorted lipophilic calcium antagonist group. It combines with the calcium channel and reacts as calmodulin like smooth muscle relaxation, inhibition of the trance membrane calcium current. Some of fendiline analogues were found to increase the concentration of cytoplasmic Ca^{2+} in borine parathyroid cells and inhibited parathyroid hormone(PTH) secretion. Fendiline is a chiral medical substance. So it occurs different biological activity in chiral condition like human body. All of these influences were found to the stereoselective, the (R)-enantiomer being 10-to 100-fold more potent them the (S)-enantiomer. Thus, resolution of fendiline and its analogues is very important. In this study, we synthesized fendiline and its analogues and resolved them on chiral stationary phases(CSP) based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid. The chiral resolution method we report here will be very valuable to the study related to the stereoselective outcomes of fendiline and its analogues.

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장소: 창원CECO

발표코드: ANAL.P-466

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantiomeric separation of methamphetamine related drugs on a chiral stationary phase based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid

탁경미 현명호*

부산대학교 화학과

The separation of chiral drugs consisting of two enantiomers has been considered as very important research, because each enantiomer often shows different pharmaceutical effects in living system. HPCL (High Performance Liquid Chromatography) chiral stationary phase (CSP) method has been regarded as one of the most effective means for the exact determination of the enantiomeric purity of chiral compounds. In this study, we synthesized several methamphetamine analogues such as methoxyphenamine and 2-fluoromethamphetamine. Methamphetamine is a central nervous system stimulant drug and has two enantiomers. The effect of d-methamphetamine as a psychostimulant is found to be stronger and longer than those of l-methamphetamine. Methoxyphenamine and 2-fluoromethamphetamine are similar in structure to methamphetamine. Methoxyphenamine is a β -adrenergic receptor agonist used as a bronchodilator and 2-fluoromethamphetamine is a stimulant drug which increase energy, insomnia and blood pressure. As an effort to determine enantiomers of analogues, we synthesized several analogues of methamphetamine and try to resolve them on a CSP based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid under various mobile phase conditions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-467

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In-line coupling of headspace-no drop microextraction with capillary electrophoresis using a commercial instrument

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서울대학교 화학부

Headspace (HS) extraction is a 3-phase extraction technique from a sample donor phase to a HS above the donor then from the HS to an acceptor phase. HS extraction is fit for volatile/semi-volatile compounds in a complex matrix. Recently, HS single drop microextraction (SDME) has been demonstrated using a drop of an acceptor phase hanging at the inlet tip of a capillary for subsequent capillary electrophoresis (CE). The large surface-to-volume ratio of the drop enabled high enrichment factors to be obtained in a short extraction time. However, it is difficult to hang a drop of very small volume in the HS of high temperature stably for a long extraction, and we introduce a new scheme of HS extraction, HS-no drop microextraction (NDME). Without hanging a drop, the liquid inside a separation capillary for CE is used as an acceptor phase. Using a basic run buffer as an acceptor for chlorophenols in an acidic donor solution, a capillary filled with the run buffer is just placed in the HS. Owing to the robust nature of the acceptor phase, the temperature and time ranges of HS-NDME can be extended significantly, compared to HS-SDME. As a demonstration of the sample cleanup and enrichment powers, HS-NDME was applied to red wine samples spiked with chlorophenols. Due to the complex matrix of red wine, the buffer capacity of the acceptor was increased.

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장소: 창원CECO

발표코드: ANAL.P-468

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A pair of Light Emitting Diodes for Absorbance Measurement

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Light emitting diodes(LEDs) have been widely used in analytical chemistry as a light source because LEDs are small, cost-effective, monochromatic and stable. Furthermore, LEDs are possible to measure photocurrent for certain range of wavelengths. A LED-based spectrophotometer was fabricated and evaluated: two red LEDs($\lambda_{\text{max}}(\text{emission}) = 655\text{nm}$) were used as a light source and a detector, respectively. The red LED can sense the wavelength range of 550 ~ 660nm centered at 615nm. This system was evaluated by measuring absorbance of bromothymol blue(BTB) in NaOH because this dye's maximum absorption wavelength is near to the 620nm. The calibration curve($r^2\text{-value} = 0.9945$) shows the linear range in two orders(0.1?M ~ 10?M). Absolute noise level was found to be 0.0002Abs and the limit of detection(LOD, S/N = 3, based on peak-to-peak noise) of BTB was 0.03?M. Note that this two LED-based photometer is designed to use a conventional sample cuvet so measured absorbance errors caused by a measurement by a measurement is the dominating factors: 0.001Abs of noise level was found in this case. In the future, building a spectrophotometer(equipped with two LEDs) is quite interesting both in scientifically and pedagogically(i.e. undergraduate lab course).

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장소: 창원CECO

발표코드: ANAL.P-469

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

혈청 내 글루코스 정량분석의 최적화

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뇌, 신경, 폐 조직에 있어서 glucose 는 에너지원으로 필수적이며 혈중 glucose 농도에 민감하게 반응하여 결핍이 되면 즉각 경련을 일으키게 된다. 최근에 서구화된 식생활, 운동부족, 고령화 등으로 인하여 당뇨병 발병률이 급속히 증가하고 있다. 당뇨병 여부를 판단하고 이를 효과적으로 관리하기 위해서는 혈당 수치를 결정하는 혈액 속의 glucose 농도를 주기적으로 점검해야 한다. 하지만 다양한 형태로 존재하는 생체 물질의 특성상 분석 오차가 발생하고 있다. 본 연구에서는 이러한 오차를 최소화 하기 위해서, 혈청 내 글루코스 정량분석의 최적화를 수행하고자 한다. 그 방법으로는 혈청 시료에 동위원소표시물질을 첨가한 후 혈청 내 glucose 와 동위원소물질이 평형에 도달하는 시간의 따른 최적화 방법이다. glucose 와 동위원소 물질이 평형에 도달하는 시간을 0 시간에서 12 시간까지 변화시켜 glucose 의 농도를 ID-LC/MS/MS 로 정량분석 하였다.

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발표코드: ANAL.P-470

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification of Currency Counterfeits manufactured in Korea

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Numerous counterfeits of bills, bank checks and gift certificates are in circulation in Korea, those fake ones are being manufactured using everyday office sophisticated equipment or not. The flood of forgery has made new security features be embedded on Korean bills (or bank checks/gift certificates), and these security features have let peoples identify fake ones with naked eyes in most of cases. Some of counterfeits, however, have remained difficult to detect, and several different types of detectors have been used to monitor counterfeits. But these are not perfect since each detector cannot monitor all specific security features. In this paper, we proposed a spectroscopic method to identify counterfeit bills, bank checks and gift certificates using micro-attenuated total reflectance (ATR) FTIR spectroscopy, and it was found that ATR FTIR is a suitable method for establishing the connection between genuine and counterfeit printed in office printer, and it appears to be a valuable nondestructive tool to verify the authenticity of those bills, bank checks and gift certificates. Keywords: Forensic Science, Micro-ATR FTIR, Counterfeit bill, Counterfeit bank check, Counterfeit gift certificate, IR Database

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장소: 창원CECO

발표코드: ANAL.P-471

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification of available QSAR tools for the human health and environmental endpoints for K-REACH

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(사)분자설계연구소 소재설계팀 ¹연세대학교 생명공학과

In 2013, The K-REACH Act was legislated to prescribe the matters for chemical registration, evaluation of hazard and risks of chemical substance and to protect human health and environment by producing and utilizing the information of chemical substance. The use of in silico toxicity prediction methods, such a QSAR model, is a good alternative to reduce the time and costs of experiments for existing chemical substances and new chemicals. For this purpose, the effort to build prediction system for analysis of QSAR models published in the literature, commonly used software tools, and available databases suitable for QSAR models before utilizing those predictions was being performed. However, it had to be prepared in advance that the selection of candidate models among commonly used software tools predicting human health and environmental endpoints of high-priority registration chemical substances for K-REACH requirements by comparing the performance of those models with quantitative manners. Firstly, we evaluate the scores of QSAR models following published criteria for comparing the credibility and ease-of-use among QSAR models. And the evaluation and comparison of applicability domain of each model based on the chemical structural similarity was also performed for comparing the degree of reliability of predicted results. Finally, the reflection and validation of those compared results into our toxicity prediction & management system is in progress. This subject is supported by Korea Ministry of Environment (MOE) as "Eco-Innovation Program (Project No. 412-111-009)".

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장소: 창원CECO

발표코드: ANAL.P-472

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification of cellular biomarkers of gamma-radiation exposure using UPLC/Q-TOF mass spectrometry

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Radiation exposure is a threat to public health issue because it causes many diseases such as cancers and birth defects due to the genetic modifications of cells. Compared to the past, people are more frequently exposed to the radioactivity due to increased usage of diagnostic and therapeutic radiation devices. In this study, we applied UPLC-MS-based metabolite profiling to analyze metabolites in the methanolic extracts of human diploid fibroblasts (HDF), which are exposed to gamma-radiation from cesium 137 (2.73 Gy/min). This study carried out time (24, 48 and 72 h) and dose (0, 1, and 5 Gray dose of cesium 137 γ -ray ionization radiation) dependent experiments. A total of 3269 features in positive mode and 1644 features in negative mode were detected, and each feature was normalized by the corresponding relative protein concentration of cells. The partial least squares-discriminant analysis (PLS-DA) score plots showed moderate separations among different dose and different time models, and the levels of some metabolites such as amino acids, lipids and nucleosides were significantly different depending on radiation and time dose. These results suggest that UPLCMS-based metabolite profiling of human diploid fibroblasts, which are Gamma-radiation exposure, could provide biomarkers for radiation exposure.

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발표코드: ANAL.P-473

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Application of Prolinol Derived New Chiral Stationary Phase

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본 연구실에서는 과거 alaninol, leucinol, phenylglycinol 등을 기반으로 하는 β -산성 키랄 정지상을 개발하여 다양한 키랄 화합물의 분리에 적용하였다 1, 2. 이들 중 leucinol 과 phenylglycinol 유도체의 정지상은 다양한 키랄 물질에 대해서 성공적인 분리효능을 보였다. 3 본 연구에서는 amino alcohol 중 2 차 amine 작용기를 지닌 prolinol 을 선택하여 키랄 정지상을 합성하였다. Prolinol 은 다른 amino alcohol 과 달리 키랄 중심 탄소가 고리 구조로 고정되어 있는 특징이 있으므로 free-rotation 이 가능한 다른 amino alcohol 과 특성을 달리할 것으로 예상된다. 따라서 prolinol 유도체 키랄 정지상의 합성과 키랄 분리에의 적용을 실시하였으며, 앞서 보고된 leucinol 과 phenylglycinol 유도체 정지상 또한 본 연구의 합성 방법을 그대로 적용하여 새로 제조하여 3 종의 키랄 정지상의 키랄 분리 정도를 비교하였다. 1. J.J.Ryoo et.al. *chirality* 14, 329, 2002. J.J.Ryoo et.al. *Microchemical J.* 63, 128, 1993. J.J.Ryoo et.al. *J. Chromatogr. A*, 987, 429, 2003.

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장소: 창원CECO

발표코드: **ANAL.P-474**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

카레로부터 향산화물질인 커큐민의 새로운 추출법 개발

김어진 김태훈 표동진*

강원대학교 화학과

평소에 자주 접할 수 있는 음식 중 카레는 몸에 좋은 효능에 대해서 알려진 바가 많다. 카레는 항산화효과와 항염증효과, 치매예방효과와 함께 최근에는 항암효과가 있다는 것도 발표되고 있다. 이러한 좋은 효능을 나타내는 카레의 대표적인 성분은 커큐민이다. 강황에 많이 들어있는 이 커큐민은 노란색을 띄고 있어서 카레도 노란색으로 보이는 것이다. 본 과제에서는 카레로부터 커큐민을 추출하는데 있어서 좋은 효율을 가지고 있는 초임계유체 추출법을 개발하였다. 몇 가지 유기용매를 이용하여 유기용매 추출한 커큐민과 초임계유체 이산화탄소를 이용하여 추출한 커큐민의 함량을 비교하였다. 초임계유체 추출 시 온도와 압력 등을 변화시켜서 최적의 추출조건을 확립하였다. 추출한 커큐민의 양은 HPLC 를 이용하여 정성 및 정량분석하였다. Column 은 Waters spherisorb@ ODS column(4.6 x 250mm, 5 μ m)을 사용하였고 이동상은 methanol 과 물을 적절히 섞어서 사용하였다. Detector 는 Jasco 사의 UV-2075 plus detector(424nm)를 사용하였다.

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발표코드: ANAL.P-475

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

수중 남조류독소 측정을 위한 스트립 분석법과 HPCL 분석법의 비 교

김태훈 김어진 표동진*

강원대학교 화학과

지구 온난화에 따라서 국내도 여름이 길어지고 비가 많이 내리는 아열대성 기후로 변하고 있다. 이런 현상은 주요 상수원과 부영양화된 호수나 유속이 느린 하천에서 녹조류, 남조류, 등의 조류가 과다 번식하는 녹조현상으로 이어지고 있다. 남조류 중 마이크로시스티스에서 발생하는 마이크로시스틴 - LR 은 간장독소 물질로 강한 독성을 나타낸다. 현재까지는 국내에서 이런 독소에 의한 피해 사례가 보고된 바 없으나, 세계적으로 남조류 중독에 따른 가축의 폐사나 인체에 유입되어 사망한 사례들이 보고되었다. 이에 세계 보건 기구(WHO)에서도 상수원에 1ug/L 이상 농도의 마이크로시스틴 ? LR 이 포함되어 있을 경우 취수 중단을 권고하고 있다. 이에 따라서 마이크로시스틴을 좀 더 빠르고 간편하게 검출 할 수 있는 방법과 검출장비에 대한 관심이 증가하고 있다. 현재 가장 보편적으로 사용되는 검출 방법은 HPLC, GC 등을 이용한 방법들이 있다. 하지만 측정을 하기 위한 전처리 과정과 측정 자체에 걸리는 시간이 길기 때문에 면역 분석법이 이런 문제를 해결할 수 있는 대안으로 제시되고 있다. 이런 면역 분석법 중 스트립을 이용한 스트립 분석법이 기존의 분석 방법보다 훨씬 간편하고, 고감도로 측정하기 좋기 때문에 기존의 분석법인 HPLC 와 비교해 보고자 하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-476

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

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

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Human transmembrane proteins (hTMP) are known to play an essential role in a variety of biological function. These proteins are closely related to human disease and are the main target of recent medicinal drugs. In order to study the structure and function of these hTMP, it is important to prepare reasonable amounts of proteins. However their preparation is seriously difficult and time-consuming. We are interested in membrane proteins related with dementia and obesity. Amyloid- β (hA β) was strongly associated with dementia. The hA β transmembrane protein shows membrane-bound oligomeric state, and the Ca²⁺-permeable ion channel formation of non-fibrillar state in the cell membrane. Human melanocortin-4 receptor (hMC4R) has a critical role in the regulation of food intake and energy homeostasis. Heterozygous mutations in second transmembrane domain of hMC4R relate in genetic cause of severe human obesity. We tried to produce large amounts of these membrane proteins and succeed to obtain sufficient quantity of the hA β -TM, the second trans-membrane domain from the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). Circular Dichroism and MALDI-TOF MS spectroscopy were used to identify the initial secondary structures and purity. Structural characterizations of these proteins in the membrane-like environments were obtained by solution and solid-state NMR spectroscopy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-477

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoparticle-integrated Surface Sandwich Assays for Chronic Heart Failure Biomarkers in Serum Samples

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경북대학교 화학과

In this poster, a new surface sandwich assay platform for an important biomarker named brain natriuretic peptide (BNP) in chronic heart failure is demonstrated. In order for creating sandwich assay, we have first investigated two bioreceptors which can interact with different moieties of BNP. Binding constants of each chosen receptors to BNP were measured using surface plasmon resonance biosensors. A surface sandwich was then formed via the interaction of BNP onto receptor 1 (BNP aptamer) immobilized on SPR chip surface followed by the specific interaction of receptor 2 (anti-BNP conjugated gold nanocubes). The sandwich formation reaction was monitored using real-time SPR. The novel sandwich platform was finally employed to the detection of BNP concentration in human serum samples.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-478

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aptamer Coated Nanoparticle-Enhanced Biosensors for Proteins

백승희 이혜진*

경북대학교 화학과

본 포스터 발표에서는 특정한 단백질에 높은 결합력을 갖는 앵타머를 공유결합을 통해 금 나노입자에 고정화한 후 목표 단백질을 검출할 때에 얻어지는 광학적 신호를 증폭하는 방법에 대해 나타냈다. 이를 위해 먼저 검출하고자 하는 단백질과 특이적으로 결합하는 앵타머를 고안하였다. 고안된 앵타머는 다양한 모양과 크기의 금 나노입자에 이중 기능기를 갖는 링커를 이용하여 고정되었으며 이들 앵타머-나노입자의 안정성, 재현성 등의 성능을 조사하였다. 그 중 앵타머 활성을 지니며 상온에서 적어도 일주일 이상 안정한 금 나노입자를 선정하여 이를 최종적으로 표면 플라즈몬 공명(Surface plasmon resonance, SPR) 바이오센서에 도입함으로써 단백질을 검출하는 데에 적용한 결과를 나타내었다.

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장소: 창원CECO

발표코드: ANAL.P-479

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Microscopic Monitoring Method for Biofunctionalized Nanoparticles

김혜림 이혜진*

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본 포스터 발표에서는 바이오품질로 기능성을 도입한 나노 파티클들을 실시간으로 모니터링할 수 있는 광학적 방법을 개발하고자 하였다. 먼저 암시야 현미경을 이용하여 ITO 유리 기판과 Au(III) 이온 용액이 접촉한 상태에서 간단한 환원방법에 의해 기판위에 금 나노입자가 성장되는 것을 실시간으로 관찰하였다. 이러한 금 나노입자에 바이오품질 (예: 단백질)을 도입하는 표면고정화학을 진행하였을 때 나타나는 금 나노입자의 국부적인 변화를 실시간으로 모니터링한 예비 데이터를 보여주고자 한다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-480

발표분야: 분석화학

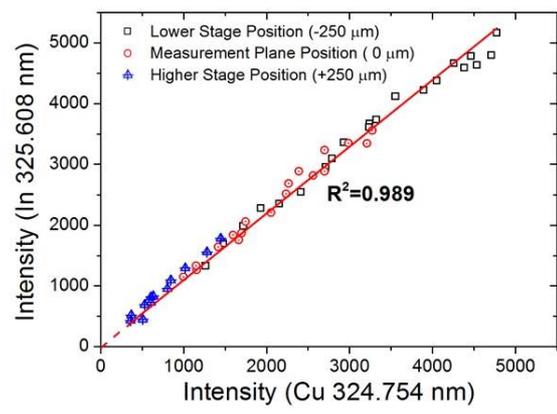
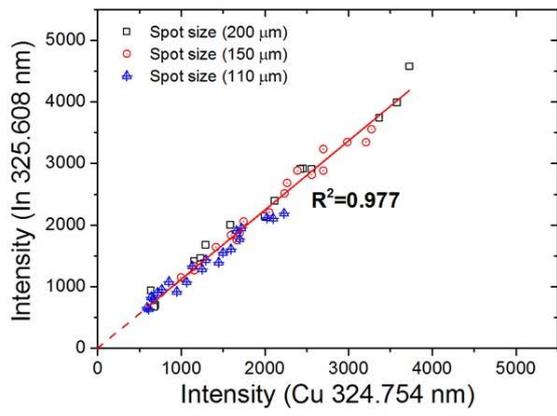
발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantitative analysis of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ thin film with fluctuation of operational parameters using laser-induced breakdown spectroscopy

인정환 김찬규 이석희 정성호*

광주과학기술원(GIST) 기전공학부

To enable a quantitative analysis of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ (CIGS) thin solar cell films using laser-induced breakdown spectroscopy (LIBS), a new method based on internal standard principle is proposed to identify the spectral line pairs immune to the fluctuations of measurement conditions. Due to nonlinear calibration curves caused by the high concentration of constituent elements of CIGS, the standard deviation of measured line intensity ratios divided by the slope of calibration curve was introduced as a new figure of merit to determine the precision of LIBS analysis along with the linearity of data points in the correlation plots. From the analyses of 39 Cu, 10 In, and 5 Ga emission lines, Cu 324.754 nm-In 325.608 nm, Cu 219.975 nm-Ga 287.424 nm, and In 303.935 nm-Ga 287.424 nm line pairs were identified as the spectral lines of which intensity ratios were least influenced by the fluctuations of spot size, position of collection optics, and/or laser energy. The selected line pairs, except the Cu 219.975 nm line, had similar upper level energy and consisted of strong resonance lines. It was found that the use of these strong lines has advantages of better reproducibility and precision for the analysis of elements with high concentration for which the calibration curve may become nonlinear due to self-absorption.



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장소: 창원CECO

발표코드: ANAL.P-481

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of organophosphorous pesticides on apple peel using liquid extraction surface analysis coupled with capillary electrophoresis

성인혜 정두수*

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A surface-sampling technique called liquid extraction surface analysis (LESA) was coupled with capillary electrophoresis (CE) to determine organophosphorus pesticides, including glufosinate-ammonium, aminomethylphosphonic acid, and glyphosate on the external surface of a fruit such as an apple. A solution containing the pesticides was sprayed onto a solid surface. Without any sample pretreatment, the dried analytes on the surface were directly extracted to a hanging drop of extractant at the inlet tip of a capillary. This extraction was made possible by a liquid microjunction that is formed between the sample surface and the extractant drop. The extraction efficiency was enhanced by repeating steps of dispensing and aspirating the extractant drop. After extraction, the analytes were derivatized on-capillary with a fluorophore 4-flouro-7-nitro-2,1,3-benzoxadiazole and analyzed by CE-laser induced fluorescence detection. The limits of detection of the glufosinate-ammonium and glyphosate with LESA-CE were 20-fold lower than the EPA tolerance levels.

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장소: 창원CECO

발표코드: ANAL.P-482

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of Pb isotope ratios in bronze with multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS)

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Lead has four stable isotopes and their natural variations have been widely used to unravel the provenance samples or geochemical processes of them. Isotope-dilution mass spectrometry used for certification of lead concentration in reference material, which is widely accepted as a primary measurement method, has also based on the accurate measurement of lead isotope ratios. However, since variations of isotope composition have shown very small differences in figures of parts per thousand (0/00) or even less, it is not easy to figure out whether the measured results are comparable or not. To obtain high precision at this level, multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS) has been used for the analysis of lead isotopes. In this study, isotopic composition of lead in a bronze sample was studied using MC-ICP-MS. The dominant elements of copper (Cu) and tin (Sn) in bronze matrix were reduced by anion exchange chromatography with AG1-X8 resin and hydrobromic acid. Method validation during the matrix separation procedures was carried out with NIST SRM 981 lead isotope standard solution dissolved in synthetic matrix containing Cu, Sn, Tl, and Hg. Little difference in lead isotope ratios from the reported values of NIST SRM 981 was observed. The instrumental mass bias effects were corrected by external bracketing methods and mass bias correction by Tl spike was also conducted for comparison. This study can be a starting point for the long journey to obtain reliable measurement results with traceability and comparability and to develop reference material for the isotope composition of elements in KRISS.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-483

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of ochratoxin A based on immunoassay using magnetic nanoparticles and a lab-built DCL

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Ochratoxin A (OTA) is one of the mycotoxins produced by *Aspergillus ochraceus*, *Aspergillus carbonarius* and *Penicillium verrucosum* which can be contaminated food products such as crops, coffee, wine grapes and dried grapes. OTA has shown toxicity such as carcinogenic and neurotoxic to humans. Also, OTA is immune suppressant and teratogen to animals. The European Commission has established the concentration limit of OTA in several goods (e.g., 2 μ g/kg in wine, 5 μ g/kg in unprocessed cereals, 10 μ g/kg in dried vine fruits). The current techniques to measure the OTA, such as liquid chromatography(LC), gas chromatography(GC) and high-pressure liquid chromatography(HPLC), have some drawbacks like long analysis time, high cost and the difficulty of operation. Enzyme-catalyzed chemiluminescence (CL) relies on the use of an enzyme as a label, usually horseradish peroxidase (HRP) which can be detected by the addition of a suitable CL substrate. This approach has been widely demonstrated to provide superior analytical performance, yielding high detectability, short assay times and low sample and reagents consumption. A novel and sensitive lab-built drop-type chemiluminescence (DCL) immunosensor was fabricated for the detection of ultra trace levels of OTA based on immunoreaction and enrichment using magnetic nanoparticles as the capture probes.

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장소: 창원CECO

발표코드: ANAL.P-484

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enrichment and determination of arsenic speciation in tap water by carrier-mediated electromembrane extraction and capillary electrophoresis

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Arsenic is an element widely distributed in the crust of the earth, causing a worldwide problem of groundwater contamination. Four arsenic compounds arsenite [As(III)], dimethylarsinic acid (DMA), monomethylarsonic acid (MMA), and arsenate [As(V)] in an unbuffered water sample were enriched by carrier-mediated electromembrane extraction (EME) and then analyzed by off-line coupled capillary electrophoresis (CE). Under an electrical potential, anionic arsenic analytes such as DMA, MMA, and As(V) were transferred from the sample solution to an aqueous acceptor phase, mediated by a carrier CH₃(C₈H₁₇)₃N+Cl⁻ (Aliquat 336) in the supported liquid membrane (SLM). Neutral As(III) was oxidized to As(V) by potassium permanganate and then enriched by EME for indirect determination. Several EME parameters such as the composition of SLM, pH of donor and acceptor phases, extraction temperature, stirring rate, applied voltage, and extraction time were optimized. Under the optimal conditions, enrichment factors of 110 to 290 for the 4 arsenic species were obtained. The relative standard deviations for the migration times and peak areas ranged 2.1-2.6% and 7.6-9.2%, respectively. Good linear relationships were observed in the ranges of 130-4000 nM for DMA, 67-2000 nM for As(III), 67-2000 nM for MMA, and 67-2670 nM for As(V). The limits of detections obtained with a tap water sample 10-fold diluted with deionized water were 3.0 ppb for DMA, 1.6 ppb for MMA, 1.5 ppb for As(V), and 1.7 ppb for As(III), all of which were below the WHO drinking water guideline of 10 ppb total arsenic.

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발표코드: ANAL.P-485

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An Investigation on the four (or five) arsenic species in a seaweed

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Arsenic is a highly toxic substance and exists in our environment universally, the determination of arsenic is significant. The toxicity and biological effects of the arsenic depend on its species while the inorganic arsenic (As^{3+} and As^{5+}) are more toxic than organic arsenic. The route of human ingestion of arsenic primarily is through foods, especially aquatic foods containing high level of arsenic. In this study, we focused on the matrix interference for the quantitative analysis of arsenic species in seaweed by ion chromatography (IC) combined with inductively coupled plasma - atomic emission spectroscopy (ICP-AES). The matrix interference gave a significant impact that the oxidation states of As^{5+} and the retention times of the organic arsenic species (MMA and DMA). Thus, various pretreated methods were investigated to eliminate the matrix interference. The determination of the four (and five) arsenic species in seaweed was carried out successfully.

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장소: 창원CECO

발표코드: ANAL.P-486

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Effect of Protein-Solvent interaction on Protein Fibrillation: Denaturation and Hydrophobic interaction

최태수 이종화 김준곤*

포항공과대학교 화학과

Several senile disorders such as Alzheimer's disease, Parkinson's disease, and spongiform encephalopathy are associated with self-assembly process of misfolded proteins called amyloidosis. Generally, hydrophobic regions of the amyloidogenic proteins are placed inside the protein to avoid contact with water. When hydrophobic region is exposed outside by a misfolding event, protein fibrillation is initiated to minimize the contact area between the region and water. We investigate insulin fibrillation under the condition of formamide and its methyl derivatives in the presence and absence of water. Thioflavin T assay reveals that the binary solvent mixtures of the formamide derivatives and water enhance β -sheet abundance at the plateau while the lag time is shortened compared to the incubation in water. On the other hand, the absence of water suppresses the formation of insulin fibril with much longer lag time than the presence of water. Using solution small angle X-ray scattering (SAXS) combined with molecular dynamics simulation, it is suggested that α -helical structure of B11-B17, which is the core sequence of amyloid fibril, undergoes denaturation into random coil. Additionally, differential scanning calorimetry (DSC) shows that formamide derivatives, whose functional group resembles the peptide backbone, reduce the activation barrier of the fibrillation process by exposing the hydrophobic residues outside. This study emphasizes that the role of water is different in both denaturation of the protein and hydrophobic interaction of the denatured proteins.

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장소: 창원CECO

발표코드: ANAL.P-487

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Glucose biosensor using the new organic film that polymer-modified electrode which nickel nanoparticles are attached

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Electrode/organic layer/nanoparticles (NPs) assemblies have recently attracted significant attention due to their fascinating optical, electronic and catalytic properties. The surprising aspects of these electrode/organic layer/NP assemblies are the ability to restore the electrochemistry of passivated surfaces upon addition of the nanoparticles and the fact that distance-independent electron-transfer behaviour. The surface studies of the immobilized polymer/NiNPs on the electrode was investigated by scanning electron microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). The catalytical currents were amplified by GOx which are electrically mediated by $\text{Fe}(\text{CN})_6$ redox films, converting the films into an electrocatalysts for the electrooxidation of glucose. The resulting catalytical currents were linearly related with the low concentrations of glucose.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-488

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Characterization of Pyridin-liganded Ferrate Complexes Mediator

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단국대학교 화학과

A series of novel, electro-active complexes of ferrate were prepared and then characterized using electrochemical techniques. The ferrate complexes contain the four kind of pyridin ligands. The redox mediators presented here are described in shorthand as $[\text{Fe}(\text{CN})_5(\text{X})]$ which were immobilized with mixture onto the screen printed carbon electrodes (SPEs). The electrical signals were measured by voltammetry techniques. Also, catalytical currents were amplified by GOx which is electrically mediated by new ferrate redox complex, conversion the complex into an electrocatalysts for the two-electron reduction of oxidation of glucose. The two resulting catalytical currents were linearly related with the concentration of glucose. X : py, py-COOH, py-NH₂, dmo-bpy

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-489

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of home-built solid-state NMR probes for the in-situ analysis

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한국의국어대학교 화학과

The solid-state NMR has been widely used for various insoluble materials like industrial polymers and biological samples. Analysis of membrane protein using solid-state NMR on lipid bilayer or bicelle for membrane-like environments, is valuable especially for a predominantly their helical secondary structure. But, most of biological lipid samples caused a loss of probe efficiency by high dielectric property due to containing large amounts of lipids, water, and salts. This electrical property causes a loss of probe efficiency. For these reasons, a specific probe with high efficiency is required to study biological samples by using solid-state NMR. Development of solid-state NMR methodologies for the study of orientational information are used for the in-situ analysis of membrane protein in lipid bilayers and liquid crystalline materials in LCD panels as well as Li materials in Li ion batteries. But, these cannot be analyzed using conventional MAS equipment. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) $1\text{H}-15\text{N}$ solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore (NB) $1\text{H}-15\text{N}$ solid-state NMR probe with strip-shield coil to prevent heating by high RF power for the study of biological sample. $1\text{H}-15\text{N}$ 2D SAMPI4 spectra from a single crystal and membrane proteins in oriented bicelles was successfully obtained by using these solid-state NMR probe. Also, we present a home-built 500 MHz NB $19\text{F}-13\text{C}$ double resonance solid-state NMR probe with a flat-square coil. It was the first application for the in-situ analysis of LCD panel samples. These probes provide short pulses, high power capability, and good RF homogeneity.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-490

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Immersion No Drop Microextraction Using Commercial Capillary Electrophoresis Instrument

고영진 정두수^{1,*}

서울대학교 화학과 ¹서울대학교 화학부

Single drop microextraction (SDME) has been demonstrated using a drop of an acceptor phase hanging at the inlet tip of a capillary for subsequent capillary electrophoresis (CE). One practical issue in SDME was how to keep the drop attached to the capillary stably. Here we present novel but quite simple no drop microextraction (NDME) to solve this as well as other issues in SDME. The NDME is a new method that doesn't form a drop at the capillary tip. Our present study, NDME, is application in many liquid phases, either 2- or 3-phase, immersion microextraction using commercial CE instruments. For immersion microextraction, the acceptor phase was injected into a separation capillary which had been filled with the run buffer. the analytes in acidic donor are extracted into acceptor phase (organic or basic) in the capillary. During extraction, the analytes from an acidic donor phase were concentrated into an organic acceptor or a basic acceptor phase. For 3-phase immersion microextraction, A thin layer of an organic liquid was used to separate the aqueous acceptor phase in inlet of a capillary from the aqueous donor phase. For high sensitivity, 2-phase immersion microextraction was performed using the stacking method. After extraction, the capillary inlet was inserted in the run buffer vial and electrophoresis of the extracted analytes was carried out. Due to the lack of a hanging drop, the method of NDME, a convenient method for CE, was performed using commercial CE instrument and full automated instrumental control. The NDME is simple, robust extraction method than SDME.

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장소: 창원CECO

발표코드: ANAL.P-491

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SERS-Based Optofluidic Sensor for Rapid Detection of Bacteria

고주희 주재범^{1,*}

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The time required for identification of pathogenic bacteria is a key factor in the diagnosis of infectious disease; therefore the interest in rapid bacteria detection is increasing. Conventional culture-based biochemical and serological assays are effective but suffer from disadvantages of being time consuming, costly and labor intensive procedure. This study presents highly sensitive pathogenic bacteria detection with surface-enhanced Raman scattering (SERS) in a microfluidic chip. Here competitive assay format has been used to detect poly-D-glutamic acid (PGA) capsule. Bacillus anthracis is surrounded by the anti-phagocytic capsule that is composed of PGA. Thus, PGA could be an effective immunoassay marker for early, specific, rapid and inexpensive diagnosis of anthracis. In this work, high affinity monoclonal antibodies (mAbs) reactive with PGA were used to construct an immunoassay platform for PGA. The assay has an extraordinarily high sensitivity, with a lower limit near sub-ng/mL. The result in this work provides a new immunoassay prototype for fast and sensitive detection of anthracis using a PGA marker.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ANAL.P-492**

발표분야: 분석화학

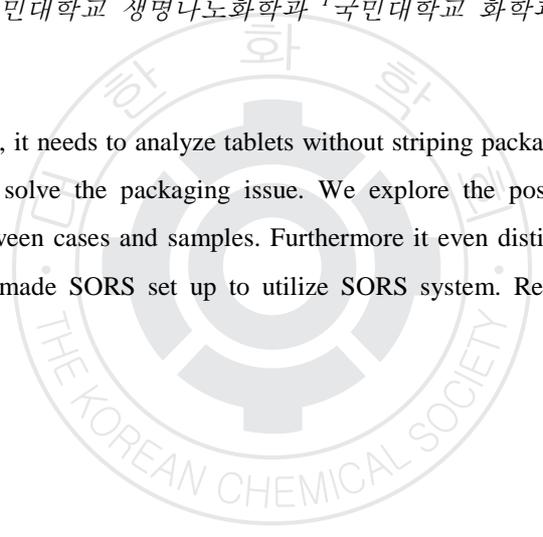
발표종류: 포스터, 발표일시: 수 16:00~19:00

Noninvasive detection of drug materials through Packaging Using Spatially Offset Raman Spectroscopy

조영호 김형민* 박찬량^{1,*}

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In a pharmaceutical factory, it needs to analyze tablets without stripping packages. Spatially offset Raman spectroscopy (SORS) can solve the packaging issue. We explore the possibility of using SORS to distinguish the signals between cases and samples. Furthermore it even distinguishes the other types of shells. We designed homemade SORS set up to utilize SORS system. Results show that SORS can remove shell signal.



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장소: 창원CECO

발표코드: ANAL.P-493

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Investigation of Sample Rotation Effects for Suppression of Convective Flows in PGSE Diffusion Experiments

김민경 민지은 이소정 진경수 장석규 안상두*

중앙대학교 화학과

The relation between convective flow and sample rotation was investigated using PGSE NMR diffusion experiments to find out the possibility of controlling the convection in an NMR tube by sample rotation itself. The viscosity effect on suppressing the convective flow by sample spinning was also examined using four solvents with different viscosity, acetone-*d*6, n-hexane-*d*14 and pyridine-*d*5, D₂O. The sample rotation showed apparent convection suppressing effect at 308K for the low viscosity solvents, acetone-*d*6, n-hexane-*d*14, even at the spinning rate of 5Hz, and it seemed that the effect continued in the controlled spinning rate of 0~30 Hz. The same pattern was also observed for pyridine-*d*5 and D₂O which have high viscosity, however, the convection suppressing effect of sample rotation was observed at higher temperature of 318K and 328K, respectively. From those results, it is thought that the convective flow in 5mm NMR tube might be quite restrained by simple sample rotation. This phenomenon might be explained by the Coriolis effect which generates downward flow in rotating fluid.

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장소: 창원CECO

발표코드: ANAL.P-494

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of the Restricted Rotational Dynamics around Metal Coordinated Amide Bond

진경수 민지은 김민경 이소정 배지희 곽경원 장석규 안상두*

중앙대학교 화학과

The rotational barrier about the C-N bonds in the complex of 1,4,7,10-Tetraazacyclododecane-1,4,7-triacetic acid, 10-[2-(diethylamino)-2-oxoethyl]-,1,4,7-tris(1,1-dimethylethyl) ester with metal ion was investigated by variable temperature (VT) NMR spectroscopy and computational calculations with the GAUSSIAN 09W. From the VT-NMR data, rotational barriers about C-N bond have been determined with Gibbs energy by the line-shape and coalescence temperature (TC) analyses. On the other hand, from the computational calculations, as the condition of 6-311G(d) basis set with the charge of metal ion and doublet spin, the Gibbs energy was calculated by using the density functional theory(DFT)-B3LYP method. When analyte forms the metal complex, the electrons of nitrogens in cyclododecane ring, ester oxygens and amide oxygen make coordinate bonds with metal ion. As a result, we could observe the changes in the chemical shift of N-CH₂-CH₃ groups in ¹H NMR spectra before and after the complexation with metal ion. It seems that if the electrons in the amide oxygen participate in the coordination of metal ion, the electrons of amide nitrogen is more donated to C-N bond, which means that double bond character of the C-N bond becomes stronger. This can be verified from the NMR experiments and computational calculations.

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장소: 창원CECO

발표코드: ANAL.P-495

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metabolite profiling of Arisaema species grown in Korea using ^1H NMR spectroscopy and multivariate analysis

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Leaves and roots of Arisaema have poison, so it was used as toxic substance in the past. Recently, tuber of Arisaema, however, is used for remedy of stroke and hemiplegic. Various Arisaema species grown in Korea have similar appearances, but they have different metabolic patterns. In this study, four species of Arisaema such as Arisaema peninsulae, Arisaema ringens, Arisaema heterophyllum and Arisaema amurense grown in Yokiido and Jejudo of Korea were used. They were characterized using ^1H nuclear magnetic resonance (NMR) spectroscopy followed by multivariate data analysis. Principal component analysis (PCA) score plot derived from ^1H NMR spectra showed a clear distinction between different four species. The major metabolites contributed to the discrimination factor include various sugars (glucose, fructose and sucrose), amino acids (isoleucine, leucine, valine, threonine, arginine, glutamine, glutamate, asparagine, glycine, tyrosine, histidine and phenylalanine) and other organic compounds (caprate, lactate, 4-aminobutyrate, malate, succinate, citrate, fumarate). The results demonstrate that ^1H NMR based metabolic profiling coupled with multivariate analysis can be used to find the similarities and differences between four species of Arisaema.

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장소: 창원CECO

발표코드: ANAL.P-496

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of CdS Quantum Dot (QD) using field-flow fractionation (FFF)

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한남대학교 화학과

Quantum Dot (QD) is a semiconducting nano-crystal that emits light of characteristic wavelength. Their optical property is attracting attention as a next-generation display material and show great potential in many areas of applications such as fluorescent labeling agent, disease-diagnostic reagents, optical technologies, media industries and solar cells. The color of the emitting light usually depends on the size of the QD, and thus the quality control of QD requires accurate determination of its size distribution. Field-flow fractionation (FFF) is a separation technique that is useful for physical characterization of various types of in sizes ranging from a few nm up to about 100 μm . FFF provides separation of components based on their hydrodynamic diameter (d_H), thus allowing direct measurement of d_H from their retention times. In this study, CdS-QD complex was synthesized by a simple γ -ray irradiation, and then were analyzed using dynamic light scattering (DLS), transmission electron microscopy (TEM), X-ray diffraction (XRD), sedimentation FFF (SdFFF), and asymmetrical FIFFF (AsFIFFF). From XRD analysis, the primary single crystallite size of 3.92 nm was estimated, which was confirmed by UV/VIS absorption spectrum ($\lambda_{\text{max}}=3.38$ nm) and HR-TEM (4 nm). TEM images indicate that the primary particles were aggregated to form secondary particles. Results from AsFIFFF and SdFFF were compared with those obtained from TEM (110 nm) and DLS (146 nm). Effects of various FFF parameters including the type of surfactant, ionic strength of the carrier liquid, the flow rates and external field were investigated to optimize AsFIFFF and SdFFF for analysis of CdS-QDs.

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장소: 창원CECO

발표코드: **ANAL.P-497**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of PAMAM-DNA complex using AsFIFFF-UV/VIS-MALS

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한남대학교 화학과

The unique properties of dendrimers have spawned a whole range of new research areas ranging from drug and gene delivery applications to processing and nano-engineering. The interior regions of polyamidoamine (PAMAM) dendrimers are assembled by dense tertiary amines to construct nanovessels for cluster nucleation, and the outer shells can maintain the stability of nanodots and be conjugated with biomolecules for further applications. Field-flow fractionation (FFF) is a family of separation techniques, where a carrier liquid is transported through a channel forming a parabolic flow profile with layers of different velocities. In this study, asymmetrical flow field-flow fractionation (AsFIFFF) was combined online with UV/VIS, multiangle light scattering (MALS), and a fluorescence detector (AsFIFFF-UV/VIS-MALS) to characterize PAMAM-DNA complexes, which were prepared by mixing PAMAM and DNA. AsFIFFF provided good separation of dendrimers and DNA, and MALS yielded absolute size, molecular weight and conformation of DNA and PAMAM-DNA complexes. It was also found that treatment of PAMAM-DNA complex with fluorescent ammonium persulfate yielded enhanced detector sensitivity and gene transfection.

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장소: 창원CECO

발표코드: ANAL.P-498

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Electropolymerization of 2,4-Diaminobenzenesulfonic acid and Its Application As Silver Ion Selective Electrode

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경상대학교 화학과

A new potentiometric sensor for the determination of silver based on poly(2,4-diaminobenzenesulfonic acid) electrode was constructed. Poly(2,4-diaminobenzenesulfonic acid) films were synthesized electrochemically on platinum electrode by cyclic voltammetry. The optimized analytical performance (E6) was evaluated Nernstian response with slope of 56.1mV decade⁻¹ in the concentration range of 10⁻⁶ to 10⁻² M silver ion. And in solution of pH 5.0 - 8.0. The limit of detection was found to be 10^{-6.50} M. The response time of the sensor was 20 s and its life time is about one week. To check the selectivity of the E6 for silver ion, potential interferences various cations were tested. The E6 was also suitable as an indicator electrode in the potentiometric titration of silver ion with chloride.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-499

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of Gold Nanoflower Tags for SERS-based Ultrasensitive Immunoassay

이혜영 주재범^{1,*}

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We report a facile synthetic method of flower-like gold nanoparticles for highly sensitive surface-enhanced Raman scattering (SERS) detection. The size of gold nanoflower can be controlled by changing the ratio between HEPES and HAuCl₄ solution. Gold nanoflowers show a strong enhancement effect caused by the tips on the particle surface, which generate potential hot spots. In addition, surface plasmon band of gold nanoflower is close to the excitation wavelength (633 nm) of helium-neon laser. It makes stronger enhancement effects by the resonance effects between its electronic excited state and the laser wavelength. Thus, these advantages in gold nanoflowers allow them to be used as SERS nano tags for highly sensitive biological or environmental detection. In this study, we investigated the enhancement effects of gold nanoflowers in accordance with their size and surface morphology. In addition, a cardiac marker (troponin I) assay has been performed to validate the function applicability of gold nanoflowers as SERS nano tags.

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장소: 창원CECO

발표코드: ANAL.P-500

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functional polythiophene-appended dithioamide : Electropolymerization and ion-selective response for mercury

김정환 김동완 김재상*

경상대학교 화학과

A composite Platinum (Pt) electrode modified with poly(Dithioamidodithiophene) (PDTADT) was used as solid state-ion selective electrode for determination of mercury. The electrooxidation of monomer Dithioamidodithiophene(DTADT) onto Pt was accomplished from the 10⁻²M DTADT in 0.1M TBAP. The electrode displayed Nernstian response with slope of 29.1 mV decade⁻¹ in concentration range of 1×10^{-6.5} to 1×10^{-2.5}M and in solution of pH 3.5. The limit of detection for electrode was 3×10^{-6.9} M with response time of 20 s. The electrode was also suitable as an indicator electrode in the potentiometric titration of Hg²⁺ with EDTA.

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장소: 창원CECO

발표코드: ANAL.P-501

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Separation and characterization of wheat and barley using asymmetrical flow field-flow fractionation: Application in antidiabetic activity

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한남대학교 화학과

The capacity of asymmetrical flow field-flow fractionation (AF4) coupled online with multiangle light scattering (MALS) and refractive index detector (RI) (AF4-MALS-RI) in monitoring of the change in molecular conformation of wheat and barley during germination process was evaluated. AF4 provides separation of macromolecules based on their hydrodynamic size, and MALS provides the molar mass and molecular size (radius of gyration). The effects on AF4 analysis of starch by dissolution procedure and the sample storage were investigated. In vitro and in vivo anti-hyperglycemic effect of germinated wheat and barley was also studied. The relationship between antidiabetic activity and molecular conformation was, for the first time, investigated. The ratio of the radius of gyration (R_g) to the hydrodynamic radius (R_h), together with the apparent density were proven to be important parameters as they offer an insight into conformational properties of the macromolecules. Results showed that, when it was germinated, the apparent density and the antidiabetic activity of barley were significantly increased, suggesting germination makes the macromolecules more compact which could contribute to enhance antidiabetic activity. It seems that germination is a promising technique for improving the yield of plant "secondary metabolism" and the nutraceutical and nutritional potential of low processed food. The information obtained by AF4-MALS-RI in this study is valuable for understanding of germination mechanism, and thus for developing functional foods. This study also indicates germination may reduce the risk by diabetic agents.

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장소: 창원CECO

발표코드: ANAL.P-502

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Speciation of trace arsenic compounds in drinking water with transient isotachopheresis

이영우 이호균 조성민 남우영 정두수*

서울대학교 화학부

Arsenic (As), the 33rd element, is a kind of metalloid that is well known for its high toxicity. The arsenic contamination of drinking water is a worldwide problem. Although the toxicity varies very significantly depending on the arsenic species, most official guidelines for arsenic in drinking water such as the WHO's 10 ppb limit are in terms of the total arsenic concentration. We report a highly sensitive but simple way of arsenic speciation using a commercial capillary electrophoresis (CE) instrument equipped with a UV absorbance detector. We used an on-line sample preconcentration method, transient isotachopheresis which combines isotachopheresis and CE in a single capillary. The phosphate ion and N-cyclohexyl-2-aminoethanesulfonic acid were used as a leading electrolyte and a terminating electrolyte, respectively.

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장소: 창원CECO

발표코드: ANAL.P-503

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inhibition of Amyloid Fibrillation by Cucurbit[7]uril

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포항공과대학교 화학과

Amyloid proteins form insoluble self-aggregates composed by β -sheet structure. The aggregation is observed as fibril-like structure, therefore, the aggregation process is called as amyloid fibrillation. This phenomenon is related to many severe diseases, such as Alzheimer's disease, type II diabetes, Parkinson's disease, and spongiform encephalopathy. We introduce a new inhibition strategy with host-guest chemistry using cucurbit[7]urils (CB[7]). Insulin and amyloid β are chosen as examples of structured and unstructured amyloid proteins. CB[7] specifically interact with Phe residues. Once they are bound, their size and rigidity cause structural change of proteins, preventing self-aggregation by increasing kinetic barriers with a thermodynamic advantage. By controlling ratio and the time of CB[7] conduction during the aggregation process, amyloid aggregation is effectively blocked. With residue specific targeting, CB[7] modulates amyloid proteins from the monomeric state to multimeric states. In consequence, the study suggests potential applications for therapeutic strategy for amyloidosis.

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장소: 창원CECO

발표코드: ANAL.P-504

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metabolomic profiling of blood plasma from X-irradiated rats model using ^1H NMR spectroscopy

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Radiation exposure is a form of damage to organ tissue caused by excessive exposure to ionizing radiation. Radiation exposure can also increase the probability of developing some other diseases, mainly cancer, tumor, and genetic damage. In this study, we applied ^1H NMR-based metabolite profiling to analyze changes at metabolite levels in the rat plasma. Rats were irradiated with 0(control), 2, and 6 Gray of X-ray irradiation dose and plasma samples were collected at day 1, 2 and 3 post irradiation. Rat plasma were analyzed by proton NMR (^1H NMR) spectroscopy, and metabolite profiling coupled with multivariate analysis was applied to characterize the differences between control and irradiated groups. The multivariate data were analyzed by Principal components analysis (PCA). PCA score plots showed both dose- and time- dependent clustering of irradiate groups and metabolic changes in irradiated rat plasma were significantly different from control groups. Rats treated with higher dose (6 Gray) showed symptoms at day 3 post irradiation and could easily be separated from controls through PCA score plot. Prominent changes in plasma metabolites, which are Creatine, Glycine, Glutamine, Citrate, Succinate, were observed in all irradiated groups compared to controls. After exposure to X-rays, Creatine, Glycine and Glutamine showed a marked increase as a result of dose- and time- dependent. However, Citrate and Succinate showed a decrease level regarding dose-dependent. Radiation induced changes could be reflected as biochemical perturbations in plasma and relevant metabolic pathways. These results will be helpful in projecting metabolomic fingerprinting in humans exposed to radiation.

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발표코드: ANAL.P-505

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Large scale splitter-less FFD-SPLITT fractionation efficiency : Effect of flow rate and channel thickness

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부

SPLITT fractionation (SF) allows continuous (and thus a preparative scale) separation of micron-sized particles into two size fractions ('fraction-a' and 'fraction-b'). SF is usually carried out in a thin rectangular channel with two inlets and two outlets, which is equipped with flow stream splitters at the inlet and the outlet of the channel, respectively. A large scale splitter-less gravitational SF (GSF) system had been assembled, which was designed to avoid the flow stream splitters and thus is operated by the full feed depletion (FFD) mode (FFD-GSF). There is only one inlet through which the sample is fed. In the FFD mode, there is no carrier liquid fed into the channel, and thus prevents the sample dilution. The effects of the sample-feeding flow rate, the channel thickness and particle density on the fractionation efficiency of FFD-GSF (*FE*, number % of particles that have the size predicted by theory) was investigated using industrial polyurethane (PU) latex beads. The carrier liquid was water containing 0.1% FL-70 (particle dispersing agent) and 0.02% sodium azide (used as bactericide). The sample loading rate was 4.2~7.2 L/hr with the sample concentration fixed at 0.01%. The GSF channel thickness was varied from 900 to 1300 μm . Particles exiting the GSF channel were collected and monitored by optical microscopy (OM). Sample recovery was monitored by collecting the fractionated particles on a 0.45 μm membrane filter. It seems the new splitter-less FFD GSF system could become a useful tool for large scale separations of various micron-sized particulates including industrial and environmental particles.

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장소: 창원CECO

발표코드: ANAL.P-506

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid Synthesis of Silver Nanoparticles and Its Application to Trace Analysis of Herbicide in a Microdroplet Channel

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Surface-enhanced Raman scattering (SERS)-based microdroplet platform, which is a microfluidic channel combined with highly sensitive SERS detection, has been applied for the highly sensitive trace analysis of herbicide. In the conventional bench-top synthesis of novel metal nanoparticles, the SERS signal intensity was decreased with time by the degradation of nanoparticles. To resolve this problem, a merging microdroplet chip has been designed and fabricated. This chip was composed of two compartments. One is the compartment for the on-chip synthesis of silver nanoparticles, and the other is the SERS detection compartment for trace analysis. As shown in Figure 1, silver nanoparticles were synthesized in the upstream channel (red droplets). Then the synthesized particles were directly merged with another droplet including analytes in the downstream channel (blue droplets). By the on-chip synthesis of silver nanoparticles, the drastic decrease of SERS signal intensity could be avoided, and the highly sensitive trace analysis of herbicide could be achieved using this SERS-based on-chip detection. This platform is considered to be a powerful multi-functional SERS detection platform for the rapid and sensitive trace analysis of various pesticides.

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Metabolite profiling of genus *Polygonatum* (Liliaceae) from different species Using ^1H NMR spectroscopy

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Genus *Polygonatum* (Liliaceae) is traditional medical herbs in Korea. It is used to treat sugar diabetes and hypertension, and have an effect on anti-aging and fatigue recovery. In this study, four samples belong to liliaceous genus *Polygonatum* (*Polygonatum involucreatum* Max, *Polygonatum lasianthum* Max, *Polygonatum odoratum* var. *pluriflorum* ohwi, *Polygonatum odoratum* var. *pluriflorum* for. *Variegatum* Y. N. Lee) were used to discriminate species. Methanolic extracts were analyzed by ^1H nuclear magnetic resonance(NMR) spectroscopy, and metabolite profiling coupled with multivariate analysis was applied to characterize the differences among species. Principal component analysis(PCA) and partial least-square-discriminant analysis(PLS-DA) showed distinction among genus *Polygonatum* from different species. A one-way ANOVA was performed to statistically certify the metabolite differences. The metabolites that showed significant difference were 4-aminobutylate, alanine, asparagines, betaine, citrate, formate, glucose, glutamine, isoleucine, malate, O-phosphocholine, succinate, sucrose, threonine, tyrosine, valine .The concentration of most metabolites except for formate, glucose, tyrosine in *Polygonatum odoratum* var. *pluriflorum* ohwi and *Polygonatum odoratum* var. *pluriflorum* for. *Variegatum* Y. N. Lee were relatively higher than *Polygonatum involucreatum* Max, *Polygonatum lasianthum* Max. This study demonstrates that NMR-based metabolomics is an efficient method for fingerprinting and determining differences among species of liliaceous genus *Polygonatum*.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on degradation of butadiene rubber using size exclusion chromatography, HPLC and thermal field-flow fractionation

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Butadiene rubber (BR) a homopolymeric rubber, and usually shows good mechanical and dynamic properties. Butadiene rubber (BR) is widely used in various products such as tires and electric wires. BR also shows good aging stability when it is mixed, and thus protected by additives such as stabilizers, antioxidant, and slip agents. The measurement of molecular weight (MW) and molecular weight distribution (MWD) of BR is necessary to evaluate and control the performance of the end products. Applicability of BR can be markedly increased by using additives such as stabilizers, antioxidant, and slip agents, etc. SEC is a separation-based sizing technique, where molecules are separated based on their sizes. SEC yields the size distribution as well as the average size, and allows monitoring of change in molecular weight of BR. Thermal field-flow fractionation (ThFFF) is also an elution-based separation technique that is useful for separation and characterization of high MW macromolecules. It has been reported that ThFFF provides higher resolution than SEC for high MW polymers. Online coupling of SEC or ThFFF with light scattering (LS) and UV/VIS detector allows determination of MW, MWD, and molecular size without the need for system calibration, thus yielding 'absolute' measurements. In this study, five different types of antioxidant (Irgafos 168 (I168), a phosphate-type antioxidant, Irganox 1010 (I1010), Irganox 1076 (I1076), Irganox 1520 (I1520) and BHT, a phenol-type antioxidant) were selected, and mixed with the same BR. Then the changes in physical properties (e.g., MW and MWD) of BR were analyzed using various techniques including SEC, HPLC, ThFFF, and TGA. For HPLC, water/acetonitrile was used for the mobile phase, and VP- ODS column with a UV/VIS detector were employed. With TGA, the change in the weight of BR with time was measured during oxidation process. Results of this study allow comparison of antioxidants in their capabilities against oxidation of BR.

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발표분야: 분석화학

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Synthesis and characteristics of carbon nanofibers and Si/CNFs composites prepared by Chemical Vapor Deposition

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계명대학교 화학과

The carbon nanofibers and Si/CNFs composites were prepared by a facile chemical vapor deposition(CVD) technique with iron and copper nitrate as the catalyst source and ethylene as the carbon source. The fiber thickness and surface area have been studied from the influence of catalysts concentration. The carbon nanofibers and Si/CNFs composites were prepared by dissolving the calculated amounts of metal catalysts and silicon powder in water. The precipitate of catalysts obtained through filtering after drying at 110 °C. The CVD process in a high-temperature furnace by the following steps: 1) heating up to 700 °C at a rate of 10 °C/min in a N₂ for 1h and 10min to reduce the Fe³⁺ to Fe; 2) stabilized at 700 °C under the flow of H₂/N₂ for 30min; 3) CVD process in mixture of 20% ethylene and H₂/N₂ at 700 °C for 1h. Finally the resultant samples were analysed via SEM, BSE, XRD, XPS and BET. The CNFs have an average diameter of 50 nm and a specific surface area of 269 m²/g. And the Si/CNFs have an average diameter of 16-42 nm and a specific surface area of 284 m²/g. 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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Electrophoretic deposition of iron catalyst on C-fiber textiles for the growth of carbon nanofibers

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계명대학교 화학과

Carbon nanofibers mean the ones with the shape of fibers less than $1\mu\text{m}$ but containing more than 90% carbon. Such carbon nanofibers have high strength, excellent electrical conductivity and thermal conductivity, and their application fields depend on the shapes and microstructure. This research was conducted to electrophoretic deposition of iron catalyst on C-fiber textiles for the growth of carbon nanofibers. Prior to iron deposition, the C-fiber substrate was oxidized by refluxing in concentrated nitric acid for 30 mins. The oxidation creates hydroxyl group containing surface groups on C-fiber which acts as anchoring sites on which the Iron precursor can nucleate and anchor. For the deposition of iron, we varied the concentration of Iron solution before electricity flows and then experiments were conducted by the various deposition time and voltages. In reduction process, H_2/N_2 gas mixture was used. In the last step, CNFs were grown on C-fiber textiles by flowing ethylene gas. The resultant samples were characterized by Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), X-Ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS) and N_2 -sorption (BET). 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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Synthesis of Si-CNFs composite as an effective anodic material for lithium-ion batteries

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This study synthesized carbon nanofibers(CNFs) on Co and Cu catalysts by Chemical Vapor Deposition (CVD). We prepared this CNFs to Si-CNFs composite as an effective anodic material for lithium-ion batteries by combining with Si. The CNFs on the surface of Si particle can provide flexible space to relieve volumetric expansion during charge. The CNFs composite on Si particles was prepared on the basis of following 2 samples ; Sample 1: CNFs were grown on the simple mechanical mixing of Si particle and catalysts. Sample 2: CNFs were grown on the surface of pyrolytic carbon coated Si particles. The morphology and compositions of Si-CNFs composite were analyzed by SEM and EDS measurements. Physical properties were investigated using XRD, Raman and XPS analyses. The suggested Si-CNFs composites can be a solution to provide higher discharge capacity and cycle-ability facilitating the 1st cycle coulombic efficiency of cheap metallic Si particles as an appropriate anodic material for Li-ion battery.

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발표코드: ANAL.P-512

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Copper(II) ion Selective PVC Membrane Electrodes Based on m-Xylenyl Salphene Complex as an Ionophore

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The m-Xylenyl Salphene have been synthesized and used as a copper(II) ion selective PVC membrane electrodes of ionophore. The membrane electrode showed a linear Nernstian response over the range 10⁻⁶ M to 10^{-2.5} M with slop of 27.26 mV per decade and its detection limit was 10^{-6.2} M of the pH range 5-6. The introduced electrode showed high selectivity and response for copper(II) ion.

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Analysis of Silica nanoparticles by Asymmetrical flow field-flow fractionation (AsFIFFF)

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Silica nanoparticles were synthesized by a traditional emulsion polymerization by mixing ethanol with ammonium hydroxide, water and tetra ethyl orthosilicate (TEOS) at room temperature, which yielded particles of 100-200 nm in diameter. Effects of reaction temperature, stirring rate (in RPM), and TEOS-dropping rate on particle size distribution was investigated. Particle size of silica nanoparticles were characterized using various sizing techniques such as asymmetrical flow field-flow fractionation (AsFIFFF), sedimentation FFF (SdFFF), dynamic light scattering (DLS) and electron microscopy (EM). For AsFIFFF analysis, aqueous carrier composition and the cross and channel flow rates were optimized. For SdFFF analysis, the field strength (channel rotation rate), carrier composition, and flow rate were optimized. It was found that, as the reaction temperature increases, the size of silica particles tended to decrease. And, as the stirring rate increases, the size of silica particles also tended to decrease. It was also found that FFF could be a useful tool for monitoring of change in particle size during synthesis of various types of nanoparticles.

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Detection of Explosive Materials using THz Spectroscopic Analysis

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연구부

Terrorist activities using improvised explosive device (IED) have been one of the major concerns of modern societies. IED could be used not only in regular warfare but also in any cities over the world. One of the approaches to the solution of this problem is trace detection of explosives. There are many technologies under research to achieve this goal. THz spectroscopy is one of the emerging methods for this purpose, since its spectrum can provide characteristic information for the identification of unknown materials, and can differentiate explosives and harmful materials from others. For his purpose, we tried to analyze military explosive materials used to be utilized to make IEDs including TNT, RDX, and HMX using THz spectroscopic methods. As an initial step, 0 ~ 3 THz wave was used to prove and analyze the interaction between explosive molecules and THz wave. Both of transmission and reflection method were tested for optimal analysis. In this presentation, the experimental procedure and the result of experiment will be reported.

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Growth and Characterization of CNFs on electroplated Ni-Cu catalyst/C-fiber textiles

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계명대학교 화학과

It is necessary to find an optimal nano-materials as a catalysts support with a high surface area and high electric conductivity, which can be applied to electrode. Carbon nanofibers(CNFs) are well-known candidates for cathodic material, because it has high physical and chemical stability of large electrical and thermal conductivity, high surface area. Accordingly, CNFs can have potential application in fields such as composite materials, hydrogen storage, electrodes, catalyst supports, field emission devices, etc. In this study, CNFs were grown by CVD(Chemical vapor deposition) method. Catalysts for the growth of CNFs were deposited on C-fiber textiles by electroplating in Hull-cell. Ni was plated on C-fiber textiles in nickel acetate solution and Ni-Cu were plated on C-fiber textiles in Ni-Cu mixed solution. As a second way, Ni was plated on Cu pre-plated substrate, after Cu was plated on C-fiber textiles in Cu solution. Each electroplated substrates were dried at 80 °C for 12 hours and reduced at 700 °C for 2 hours in N₂-H₂ mixed gas. Then CNF was grown on C-fiber textiles using ethylene gas at 700 °C for 2 hours. The grown CNFs were characterized by SEM(Scanning Electron Microscopy), EDS(Energy Dispersive X-ray Spectroscopy), XRD(X-ray Diffraction) and N₂ sorption(BET). Acknowledgment : This research was financially supported by the Ministry of Education (MOE) and national Research Foundation of Korea(NRF) through the Human Resource Training Project fo Regional Innovation (No. 2012026209)

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Comparison of chemical compositions according to the different methods and locations of gilsonite, oil shale extracts, and heavy crude oil by 2D GC-MS

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Despite the growing interest in using energy sources other than petroleum, it will be decades before our energy and transportation infrastructure can be adapted to new energy sources. Therefore, more research has to be done to develop unconventional hydrocarbon sources, like oil shale and gilsonite. Characterization of shale oil and gilsonite is one of the important research areas that help utilizing the unconventional energy source. Therefore, wide range of analytical techniques including gas chromatography (GC) and Fourier transform ion cyclotron mass spectrometry (FT-ICR MS) has been used to characterize shale oils and gilsonite. However, there has only a few studies applying 2D GC to compare and understand the gilsonite and shale oils. In this study, saturate and aromatic fractions of gilsonite, oil shale extracts, and heavy crude were analyzed and compared by 2D GC-MS.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

SEPARATION OF UNCONVENTIONAL CRUDE OILS BY REVERSE PHASE HIGH PERFORMANCE LIQUID CHROMATOGRAPHY AND IDENTIFICATION OF THE FRACTIONS BY HIGH RESOLUTION MASS SPECTROMETRY

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Crude oil is a complex mixture composed of numerous compounds and hence the complexity poses a difficulty in understanding the material at the molecular level. High resolution mass spectrometry has been successfully applied to understand the detailed chemical compositions of crude oil but it has been shown that it is necessary to combine separation with high resolution mass spectrometry for more complete understanding of crude oil. Conventionally, saturates, aromatics, resins, and asphaltenes (SARA) separation technique has been widely used to separate crude oil into fractions. However, the conventional SARA fractionation procedure includes many manual steps and hence reproducibility of the method is critically dependent on the skill of the operator. In this study, fractionation of crude oils has been performed by reverse phase high performance liquid chromatography (HPLC) connected with an automated fraction collector. The optimum conditions for the separation were investigated and the obtained fractions were characterized by use of high resolution mass spectrometry.

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Analysis of 6 arsenic speciation in seaweed using IC-ICP-MS

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비소는 독성을 가진 유해 중금속 원소로서 자연적 또는 인위적인 원인에 의해 여러 형태의 비소 화학종으로 존재한다. 1 급 발암물질로 분류되어 있는 비소는 무기비소와 유기비소의 형태가 있다. 사람은 특히 해양식품을 섭취함으로써 과량의 비소를 흡수하게 되는데, 해양식품 중 비소는 주로 유기비소 상태로 많이 존재하고 있다. 그 중에서도 해초에는 AsC와 AsB의 형태로 주로 존재한다. 현재까지 비소의 오염도에 대한 평가는 총 비소 함량을 기준으로 평가되고 있어 해양식품 중 비소 분석은 정확한 판단이 이루어지지 않고 있으며, 최근 비소 중 분리 분석법은 유기비소인 AsB와 무기비소인 As(III)의 피크가 잘 분리되지 않아 정량이 힘들다. 또한 완충용액을 이동상으로 사용하기 때문에 질량분석기에 손상을 줄 수 있다. 본 연구에서는 질산을 이동상으로 이용하여 질량분석기의 손상을 최소화하고 0.999 이상의 직선성을 얻었다. 또한 물을 추출용매로 이용한 초음파 추출방법을 사용하여 80~110%의 좋은 회수율과 ppb 단위의 낮은 LOD와 LOQ를 얻음으로서 비소 중 분리에 적합한 분석법을 확립하였다.

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Development of Syringe Pump Assisted Headspace Sampling Techniques for Needle Trap Device (NTD)

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Headspace analysis is a technique to separate, collect, and analyze volatile compounds from different sample matrixes such as water, solids, and fruits. Headspace analysis has divided in two techniques: dynamic and static. Dynamic headspace utilizes “purge and trap” to enrich the volatiles on a sorbent more efficiently while Static headspace is simple and provides a cost effective way to collect VOCs. This headspace analysis is widely used with GC in the analyses of alcohols in blood, analyses of monomers in polymers and plastics, flavors in food, beverages and perfumes. A needle trap device (NTD), like solid-phase microextraction (SPME) fibers, is another approach for one-step solventless sample preparation and injection technique for GC. The major advantages of NTD, as a sorbent trap technique, are simplicity and convenience for sampling and injection. We utilized a stand type, step motored syringe pump to develop headspace sampling technique for analyzing VOCs in liquid samples especially for NTDs. In this report, mainly static headspace sampling technique will be introduced but dynamic headspace sampling technique reported several years ago will be presented also.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Enantioseparation on Carboxymethyl- β -Cyclodextrin Modified Zirconia Magnetic Nanoparticles

김종화 AVVARU PRAVEEN KUMAR 이용일*

창원대학교 화학과

Separation of enantiomers of a chiral compound is one of the most interesting and challenging tasks because of their identical physical and chemical properties. Magnetic materials possessing chiral functionality on their surface can not only exhibit magnetic properties but also recognize chirality. The present work explores the synthesis of carboxymethyl- β -cyclodextrin modified zirconia magnetic nanoparticles (Fe₃O₄@ZrO₂@CMCD) and their application in selective enantioseparation of amino acids. The Fe₃O₄@ZrO₂@CMCD magnetic nanoparticles (CMCDZMNPs) are characterized by transmission electron microscopy (TEM), X-ray Diffraction (XRD), Fourier transform infra red (FT-IR) spectroscopy, thermogravimetry (TGA), elemental analysis (EA), X-ray photoelectron spectroscopy (XPS) and vibrating Sample magnetometer (VSM). As-synthesized CMCDZMNPs are applied for separation of amino acids and it was proposed that the functional groups at chiral center of the amino acid molecules might interact with hydroxyl group of CMCD and makes hydrogen bond formation resulted in selective adsorption of enantiomer. Most importantly the synthesized CMCDZMNPs have shown an excellent magnetic property that reflects in their easy separation from solution.

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장소: 창원CECO

발표코드: ANAL.P-521

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Impact of L-Cysteine on fluorescent Properties of CdTe QDs and its reactivation of degenerate fluorescence

김잔디 B.T.Huy 이용일*

창원대학교 화학과

In this research, we synthesized L-Cysteine capped with CdTe quantum dots (CdTe@Cys) in aqueous solution and achieved what we were expected. The first one is stability. The second one is functionalized surface with bio-materials. The interactions between CdTe@Cys were characterized by fourier transform infrared (FT-IR), photoluminescence (PL), transmission electron microscopy (TEM), confocal microscopy and antibacterial test. We found the optimized condition for preparing CdTe@Cys. The intensity of PL results were affected by under the influence of ratio of Cd:Te:L-Cysteine, pH value, chemical stability of CdTe@Cys. Moreover, the CdTe@Cys can be reactivated by easy technique through addition of L-Cysteine. The PL intensity and lifetime of L-Cysteine capped with CdTe QDs increased noticeably when the cysteine solution was added to original samples. So, we tried to conjugate QDs with the E.coli cell and observed an image of fluorescense microscope of the attached cell. In addition to this, addition of L-Cysteine result on the reduced toxicity of CdTe.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Novel Homogeneous Assay for Simultaneous Determination of Fluoroquinolones in Water based on Upconversion Fluorescence Resonance Energy Transfer

GerelkhuuZayakhuu 강지훈 이용일* Zhen Zhang¹

창원대학교 화학과 ¹school of the environment, Jiangsu University

A novel homogeneous method for simultaneous sensing of trace fluoroquinolones (FQs) in water using upconversion fluorescence resonance energy transfer (FRET) was developed. Lanthanide-based upconversion nanophosphors(UCPs) have attracted much attention because of wide application in biological labeling, sensing, and imaging. It was attributed to its unique characteristics of low toxicity, nearly-zero background auto-fluorescence, narrow emission band, high photoluminescence intensity, and photostability. Although the surface functionalization of UCPs with good hydrophilic and strong luminescence in aqueous solution has been performed, the application in biological assays is still few, especially for organic pollutants in foodstuffs and environmental waters. We present the facile synthesis of monodisperse, size-tunable, and highly efficient UCPs(β -NaLuF₄:Gd,Yb,Er³⁺) linked with -COOH groups which can be used as a donor after conjugation with our produced FQs monoclonal antibody. The corresponding antigens labeled gold nanoparticles (AuNPs) was treated as an acceptor. In competitive reaction, dissolved FQs and labeled AuNPs competed each other to combine with FQs antibodies labeled UCPs. The original green light was quenched by the acceptor when excited by near-infrared light (980 nm) to donor, and the intensity shows the linear relationship with the concentration of FQs in water. Keywords: Upconversion nanoparticles, fluoroquinolones, fluorescence resonance energy transfer (FRET), near-infrared light

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발표코드: ANAL.P-523

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Up-conversion luminescence enhancement of NaGdF₄:Yb³⁺, Er³⁺, Tm³⁺ nanoparticle by solvothermal method

정종원 GerelkhuuZayakhuu 이용일*

창원대학교 화학과

Nanoparticle materials have been the subject of increased scientific interest, both for fundamental research and for a wide area of application. This interest has arisen for various reasons. The large surface-to-volume ratio in nanoparticles can have a significant impact and influence on their physical properties compared to their bulk counterparts. The tendency for ever-smaller electronic devices opens the possibility for the use of nanoparticles. In addition, small particles are increasingly used in various medical applications, such as drug targeting, magnetic fluid hyperthermia, magnetic resonance imaging and other. Recently, in this area has greatly intensified due to the recent development of lanthanide-doped oxide nanoparticles that exhibit NIR-to-visible up-conversion emission. Nanoparticle up-conversion phosphors can be incorporated into a broad range of materials and devices and are suitable for sensing at the molecular scale. Although, the optical properties of Ln³⁺ ions are widely studied in several fluoride matrices in the bulk, studies on their corresponding dispersible nanoparticles are mostly restricted to NaGdF₄:Er³⁺, Tm³⁺ and Yb³⁺ doped NaGdF₄ phosphors were prepared by solvothermal reaction method. The preparation ReCl₃ solution (Re = Gd, Er, Tm and Yb). This rare earth solution (1 mol/L) added 8ml oleic acid (OA) and 18 ml 1-octadecene (ODE). The solution was heated to 160 °C for 30 min and then cooled down to room temperature. Thereafter, 10 ml methanol solution of NH₄F (4 mmol) and NaOH (10 mmol) was added dropwise under stirring for 30 min. After methanol evaporated the solution was heated to 300 °C under nitrogen atmosphere and the temperature should be maintained for 0.5 hr to 1.0 hr, during this procedure the condenser pipe was needed and the stirring speed was about 1,000 rpm. The resulting nanoparticles were precipitated by the addition of ethanol, collected by centrifugation washed with ethanol several times. Their crystalline structures, surface morphologies and phase

transitions were investigated according to annealing process by using X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and photoluminescence (PL).



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Magnetically Recoverable Ruthenium nanoparticles: Synthesis, characterization and catalytic performance in hydrogenation reactions

백민욱 이용일* AVVARU PRAVEEN KUMAR

창원대학교 화학과

Catalysis is becoming a strategic field of science because it represents a new way to meet the challenges of energy and sustainability. The present work explores synthesis and catalytic activity of new magnetically recoverable ruthenium ($\text{Fe}_3\text{O}_4@\text{Ru}$) nanocatalysts by co-precipitation method in a single step. The synthesized magnetic Ru nanocatalysts are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray powder diffraction (XRD), vibrating sample magnetometry (VSM), X-ray photoelectron spectroscopy (XPS) and atomic absorption spectrophotometry (AAS). As-prepared $\text{Fe}_3\text{O}_4@\text{Ru}$ nanocatalysts have been applied for olefin hydrogenation reactions. The results indicate that the supported Ru catalysts can be conveniently recovered by applying an external magnetic field and the activity of the supported Ru catalyst for hydrogenation of olefins can still reach up to over 90% after being reused at least five times. Keywords: $\text{Fe}_3\text{O}_4@\text{Ru}$ nanocatalysts, co-precipitation method, Characterization, Hydrogenation of olefins.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of artificial sweeteners by CE with LED-induced in multiple capillary molecular imprinted polymer/solid phase extraction

안지용 강지훈 AVVARU PRAVEEN KUMAR 이용일*

창원대학교 화학과

A novel capillary electrophoresis (CE) and monolithic molecular imprinted polymer (MIP) based in-column and open-tube molecularly imprinted solid phase extraction (MISPE) concentrator method was developed for selective and sensitive determination of sweeteners by using light emitting diode (LED) induced polymerization system. With multiple capillaries that coated a short layer of MIP material (about 3 mm long) under irradiation of LED is connected to end of separation column. Compared with MISPE fiber that takes center stage in separation chemistry, the MISPE concentrator provides better selectivity extraction without significant loss of separation efficiency. In this work, LED-induced in multiple capillaries MISPE was used for extraction of artificial sweeteners that sucralose and aspartame is typical artificial from food samples. The majority of ingested sweeteners had not broken down by the body therefore it is non-caloric. Further, the artificial sweetener are approximately hundreds times as sweet as sucrose. The in-column MISPE-CE system is also suitable for on-line renewing or fabrication MISPE concentrator conveniently. The in-multiple capillaries MISPE gives high affinity, selectivity, analysis to various samples at one swoop and high recoveries to MISPE-CE analysis.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Catalytic Applications of Ru Nanoparticles Supported on Silica Coated Magnetic Microspheres

백민욱 이용일* AVVARU PRAVEEN KUMAR

창원대학교 화학과

Green chemistry, also called sustainable chemistry, is a philosophy of chemical research and engineering that encourages the design of products and processes that minimize the use and generation of hazardous substances. Green catalysis is a subchapter of green chemistry and probably the most important one. We here report the synthesis, characterization and catalytic performance of recoverable ruthenium (Ru) supported on silica coated magnetic microspheres ($\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{Ru}$). The immobilized Ru nanoparticles catalyst ($\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{Ru}$) was obtained after reduction of Ru^{3+} on the amine-modified core-shell magnetic $\text{Fe}_3\text{O}_4@\text{SiO}_2$ microspheres. As-prepared Ru catalysts were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), powder X-ray diffraction (XRD) and Fourier Transform Infra Red (FT-IR) spectroscopy. The synthesized Ru catalyst was successfully applied for organic catalytic reactions. The central Fe_3O_4 cores are superparamagnetic at room temperature with strong magnetic response to externally applied magnetic field, thus providing a convenient means for separating the catalyst from solution. Keywords: Green synthesis, $\text{Fe}_3\text{O}_4@\text{SiO}_2$ microspheres, Ru nanoparticles, Catalytic applications.

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발표코드: **ANAL.P-527**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, characterization and magnetic properties of biocompatible FeCo nanoparticles

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창원대학교 화학과

The study on colloidal nanoparticles has attracted intensive interests owing to their unique magnetic, optical or chemical features and their promising applications in biology, especially the diagnosis and therapy of critical diseases. Magnetic nanoparticles with tailored surface modifications have been widely used experimentally for numerous in applications. For example, iron oxide nanoparticles exhibit superparamagnetic property and have been intensively investigated on the application of analytical chemistry, targeted drug delivery, hyperthermia treatment and magnetic resonance imaging (MRI). In this study, the biocompatible FeCo magnetic nanoparticles have been prepared FeCo, chitosan, polyethylene glycol and zirconium oxide by simple and effective approaches. The prepared magnetic nanoparticles are composed of cubic-like with an average size of 12-15 nm. The saturation magnetization (Ms), coercive field (Hc), and remanence magnetization (Mr) of functionalized FeCo were estimated. The results from FT-IR spectra, magnetic properties open up the wide applicability of FeCo.

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발표분야: 분석화학

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Novel Dithiol Capped CdSe Quantum Dots for Solar Cell Applications

AVVARU PRAVEEN KUMAR B.T.Huy B.Prem kumar 이용일*

창원대학교 화학과

The quantum dots (QDs) are the fluorescent semiconductor nanocrystals which have the potential for many diverse applications in solar cells, optical and electronic devices, biological, biochemical, biomedical and drug delivery so on through their unique properties. The most recent researches on semiconductor QDs are the employment for solar energy conversion and have led to the development of high-efficiency solar cells. We report dithols as new capping ligands to synthesize dithiol capped CdSe QDs for solar cell application. The work investigates systematically the influence of the nature of dithiol-type capping ligand on the optical properties of highly luminescent CdSe QDs which are synthesized in organic media. The growth rate, size distribution and quantum yield of CdSe QDs are strongly depends on the type of dithiol ligand used. The process and mechanism of solar cell application of dithiol-capped CdSe quantum dots (QDs) are experimentally studied. Keywords: CdSe QDs, Dithiols, Optical properties, Solar cell applications.

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발표분야: 분석화학

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Quantitative Separation of D/L-amino acid modified derivative by applying Kinetic method

TSOGOO ARIUNZAYA 김잔디 이용일*

창원대학교 화학과

Chiral analysis is an important task of analytical chemistry. One mass spectrometric approach is based on Cook's kinetic method. We can separate D/L-amino acid modified by N,N-Dimethylformamide dimethylacetal (DMF-DMA) derivative reagent using on-line LCQ-MS by applying single ratio kinetic method. Singly changed copper(II)-amino acid cluster ions $[\text{CuII}(\text{A})(\text{ref}^*)_2\text{-H}]^+$ (A=amino acid such as D/L-Try and D/L-Phe; ref^* =chiral reference ligand, selected in L-Pro) undergo competitive collision-induced dissociation (CID) in a quadrupole ion trap to form the dimeric complexes $[\text{CuII}(\text{A})(\text{ref}^*)\text{-H}]^+$ and $[\text{CuII}(\text{ref}^*)_2\text{-H}]^+$. Chiral discrimination is calculated from the fragment ion abundance ratios using the kinetic method. The ratio of the individual branching ratios R_{iso} is found strongly dependent on the references and the metal ions.

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발표코드: ANAL.P-530

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Microchip Magnetophoresis for Separation of Native Single Super-paramagnetic Nanoparticles

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경희대학교 대학원 화학과 ¹경희대학교 응용화학과

Real-time dynamics of different sizes native super-paramagnetic nanoparticles (SPMNPs) were observed in a microchip at single-particle level. By using differential interference contrast detection, the magnetophoretic performances of individual SPMNPs were directly detected without any fluorescent-labeling. The SPMNPs with 160 nm and 500 nm-diameters were separated using a Neodymium-iron-boron permanent magnet as a magnetic field source. The differences of magnetophoretic velocities between individual native single-SPMNPs in the microchip showed the possibility of separation the different sizes SPMNPs from polydispers mixture. Based on the optimized magnetic field condition obtained at the single-nanoparticle study, the two SPMNPs were successfully separated within 15 s from the model polydispers mixture. Taking advantage of successive real-time images of the native single-SPMNPs under magnetophoresis, the dynamics of SPMNPs during the separation processes indicated the more violent random Brownian motion and diffusion of small (160 nm) SPMNPs, and explained the peak broadening

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of Short-Chain Chlorinated Paraffins by Two-dimensional Gas Chromatography Mass Spectrometry

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경북대학교 화학과

Chlorinated paraffins (CPs) are complex chemical substances that persist in the environment and cause adverse effects to human health in persistent organic pollutants (POPs). Therefore, many studies have been carried out for better understanding of CPs over the years. Comprehensive two-dimensional gas chromatography (GC x GC) based on quadrupole mass spectrometry (qMS) coupled to a thermal modulator is a powerful technique to separate, characterize, and classify the chemical composition for the analysis of highly complex mixtures such as CPs. Also, GC x GC with a flame ionization detector (FID) applied to study for partially quantification of CPs. Short-chain chlorinated paraffins (SCCPs, C₁₀-C₁₃) with a chlorine content of 51.5, 55.5 and 63% and chloroparaffin C₁₀ Mix were used in this study. The obtained GC x GC qMS spectra showed that classification of SCCPs were possible by interpreting fragmented ions. This interpretation could be successfully applied to study SCCP mixture. Furthermore, SCCPs with chlorine contents were quantitatively analyzed by using GC x GC FID. Therefore, the GC x GC qMS is shown to be a powerful technique to study CPs.

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발표코드: **ANAL.P-532**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal-composite nanodendrites for a SERS substrate and electro-catalyst

장결 정희일*

한양대학교 화학과

Diverse nanostructures have been extensively demonstrated in recent years. An impetus for developing these nanostructures is based on promising advantages in their use for chemical sensing as well as catalyst. Especially, a nanodendrite draws a great attention since it has a hierarchical structure with high population of edges, thereby proving a large number of active sites for SERS (Surface Enhanced Raman Scattering) and catalytic activity. Here, we have synthesized metal-composite nanodendrites which incorporated several metals optimally into a nanodendrite structure. First, we synthesized an Au-Ag bimetallic nanodendrite via simultaneous co-electrodeposition and used it as a platform for SERS-based sensing system. Second, a 3D Pt-Au-Ag trimetallic nanodendrite forest was fabricated using competitive galvanic replacement reaction (GRRs). In the structure, Ag, Pt and Au contributed for the nanodendrite frame with a high surface-to-volume ratio, active electrocatalytic function and long-term catalytic stability, respectively. Finally, the catalytic performance of the trimetallic nanodendrite was evaluated for methanol oxidation reaction (MOR).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of two explosives (RDX and HMX) using electrospray ionization in mass spectrometry

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충남대학교 화학과 ¹한국기초과학지원연구원 질량분석기개발팀 ²국방과학연구소 국방신기술
본부 융복합기술연구부 ³(주)센서테크 연구소

Detecting explosives with simplicity and high speed response is important but the commonly used method of ion mobility spectrometry is behind in accuracy. Thus, high resolution mass spectrometry is a useful and effective technology to characterize explosives with increased accuracy. In this study, two common explosives, cyclonite (RDX) and cyclotetramethylenetetranitramine (HMX), were comprehensively analyzed with an ion trap mass spectrometer (MS) and an orbitrap MS in negative ion mode using the direct infusion method with electrospray ionization. The analysis using an ion trap MS, which shows mass spectral peaks of adduct ions with a formate anion, i.e., $[M+HCOO]^-$. On the other hand, the analysis using an orbitrap MS provided peaks of an adduct ion with a chloride anion, $[M+Cl]^-$. We did not add any $HCOO^-$ or Cl^- in the sample solution. We are trying to find out the cause of the adduct ions. During the presentation, the current statuses of the investigation will be presented.

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발표분야: 분석화학

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Comparison of isotope patterns of hemin and standard peptide ions in Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry

김태희 이지현 김정권*

충남대학교 화학과

In this study, we investigated the change of isotope pattern of heme ion from myoglobin and cytochrome c upon the change of the irradiated laser power in the matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS). When the laser intensity was increased (from 1519 to 2519 with DHB matrix and from 1087 to 2187 with CHCA matrix), the ratio of isotope distributions of heme c was generally increased. The theoretical relative abundance of the second isotope compared to the first isotope of heme c was 40.96%, but experimental relative abundance was increased from 53.48% to 88.56% with DHB matrix and from 42.76% to 97.54% with CHCA matrix. However the ratio of isotope distributions of heme b was not changed. The theoretical relative abundance of the second isotope of heme b was 40.95%, and experimental relative abundance was about 75.71% with DHB matrix and was about 55.24% with CHCA matrix. In this study, we compared the isotope patterns of hemin and standard peptide ion upon the change of laser intensity in MALDI-TOF MS.

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발표분야: 분석화학

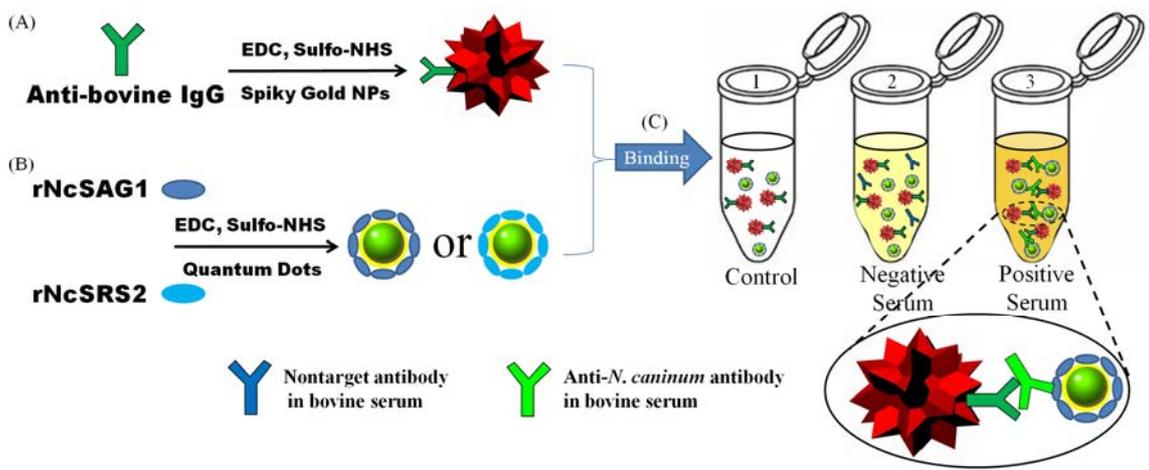
발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of Anti-Neospora Antibodies in Bovine Serum by Au-CdTe Nanocomplex

주필권 이재범^{1,*}

부산대학교 나노융합기술대학 ¹부산대학교 나노메디컬공학과

Detection of biomolecules via nanotechnology has become increasingly important in a variety of fields, including medical diagnostics, food safety, and anti-bioterrorism. Neosporosis is an infectious disease primarily of cattle, which is caused by an intracellular parasite, *Neospora caninum*, and now appears to a major cause of abortion in dairy cattle worldwide. Therefore, we report a rapid, sensitive, and inexpensive qualitative approach for neosporosis detection based on the photoluminescence (PL) enhancement between quantum dots (CdTe nanoparticles) and a unique shape of Au nanoparticles, called Au nanoparticles (UNPs) conjugated by antibody-antigen. Anti-bovine IgG functionalized-UNPs were then bound to complementary target, anti-*Neospora* antibodies (ANABs) in bovine serum. The binding of analyte to the molecular probe was monitored by the PL enhancement of CdTe nanoparticles in the PL spectrum resulting from a combination with surface roughness of Au nanoparticles by the immunological reaction. The fluorescence intensity was compared in the samples of infected and healthy cattle, resulting in significant intensity difference. The Au-QDs sandwich nanocomplex remains in solution and its optical properties allow it to be easily quantified using fluorescence absorption spectroscopy. More than 55% emission enhancement on the surface of the urchin-like NPs compared with those of CdTe NPs was observed, and the results exhibit good reproducibility. Further, the biosensor was suited for qualitative analysis of ANABs in the actual media of blood serum. The ease of operation, high sensitivity, and its generality offer specific advantages over other immunoassay methods.



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발표분야: 분석화학

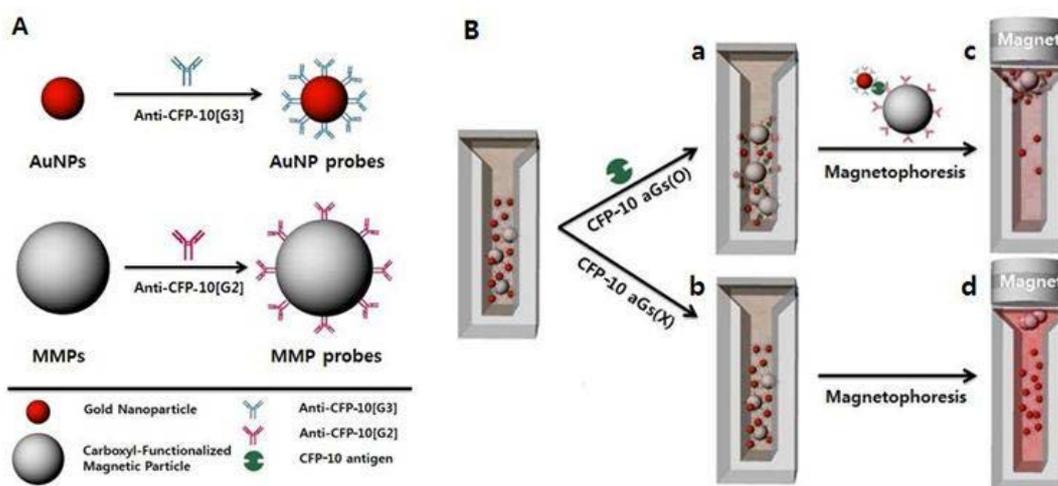
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid monitoring of CFP-10 of *Mycobacterium tuberculosis* by nanoparticles

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부산대학교 인지메카트로닉스 공학과 ¹부산대학교 나노메디컬공학과

A sandwich-type colorimetric magnetophoretic immunoassay (MPI) is introduced to monitor tuberculosis (TB) antigen, CFP-10, in cultures of *Mycobacterium tuberculosis* (Mtb) using nanoparticle complexes of Au nanoparticles (NPs), magnetic microparticle (MMPs), and TB immuno-moieties. The MPI can monitor the target antigen quantitatively and qualitatively within 10 min in the detection range of $10^1 \sim 10^4$ pg/mL. Furthermore, the quantitative analysis of the MPI in Mtb culture showed that there was linear relationship between the concentration of the secreted CFP-10 from 10^6 CFU/ml of Mtb and culture time. From these data, it is suggested that the MPI analysis can carry out TB diagnosis within 3~7 days, based on antigen secretion from Mtb. These data suggest that our MPI kit is able to be applied in early TB diagnosis through detection of TB specific antigen during culture.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ANAL.P-537

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of New pH and electroresponsive chitosan based semi-interpenetrated polymer network gels

김민경 A.Gopalan¹ 이광필^{2,*}

경북대학교 화학과 ¹경북대학교 차세대에너지기술연구소 ²경북대학교 화학교육과

We prepared the new semi-interpenetrated polymer network (semi-IPN) gels from chitosan (CS), carbon nanotube (CNT), Polyaniline (PANI) and poly (acrylic acid) (designated as CNT-CS-PAA semi-IPN gel) and characterized by fourier transform infrared, X-ray diffraction , field emission scanning electron microscopy and differential scanning calorimetry measurements. For comparison, we also prepared the CS-PAA and CS-PAA-PANI gels CNT-CS-PAA semi-IPN gels were prepared through the two step processes. In the first step, CNT-CS-PAA semi-IPN gel was prepared by the free radical grafting and cross-linking reactions among CNT, CS and PAA. In the second step, PANI was distributed into the IPN gel via impregnation of aniline monomer and oxidative polymerization. Since CS is both a biocompatible polymer with natural origin and PAA is a pH responsive polymer and PANI is an electroactive polymer, the electric field responsive polymer as CNT-CS-PAA-PANI semi IPN gels exhibited multi responsive properties. The effect of crosslinked PAA content on the swelling, thermal and electrical properties. The effect of crosslinked PAA content on the swelling, thermal and electrical properties of CNT-CS-PAA-PANI semi IPN gels has been explained by comparing the properties CS-PAA and CS-PAA-PANI gels.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: ANAL.P-538

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of graphene encapsulated new composite nanofibers

이현규 A.Gopalan¹ 이광필^{2,*} 강신원³

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과 ³경북대학교 IT대학 전자공학부

Recently, graphene-based hybrid photocatalysts have been prepared by sol-gel, hydrothermal or mechanical blending method. In this work, a series nanocomposite fibers comprising of titanium dioxide (TiO₂) nanofibers, graphene sheets (G) and metal nanoparticles (MNP) (designated as TiO₂@G/MNP NCF) were synthesized with a simple combination of electrospinning and hydrothermal approaches. The obtained TiO₂@G/MNP NCF are characterized by X-ray diffraction (XRD), Raman spectroscopy, transmission electron microscopy, X-ray photoelectron spectroscopy and ultraviolet-visible (UV-vis) diffuse reflectance spectroscopy. XRD patterns show that the crystal structures of all as-prepared samples contain anatase-rutile mixed phases. The as-prepared TiO₂@G/MNP NCF consists of uniform TiO₂ NF embedded with graphene and MNPs. The results of the present work demonstrated that graphene-MNP included NCFs can be very promising materials for development of high performance photocatalysts.

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발표코드: ANAL.P-539

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of new functional electrospun composite membranes for Lithium ion recovery

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경북대학교 화학교육학과 ¹경북대학교 나노과학기술학과 ²경북대학교 차세대에너지기술연구소 ³경북대학교 화학교육과

Membrane technologies have been developed to suit for a wide range of industrial applications, and the most of them could lead to realize in very large scale. However, in general, such composite membranes can also be applied in many other fields. Nevertheless, the potential of membranes for engineering of separation has by far not yet been used completely. We demonstrate a synthetic strategy toward functional, composite electrospun membrane by incorporating functional inorganic component into electrospun polymer nanofibers. Functional electrospun mats (f-ESM) could be prepared by post-modification of the surface of nanofibrous mats and application can be tailor designed accordingly. Therefore, developing a simple and versatile approach to tailor the surface properties or to introduce the desired functions into the as-fabricated electrospun nanofibrous mats is highly desirable. In this investigation, we developed new types of functional electrospun nanofibrous mats (FESNM) by introducing inorganic functional component which has high affinity for lithium ions. The changes in the surface morphology and structural characteristics were evaluated by field emission scanning electron microscopy, Fourier transform infra red spectroscopy and thermogravimetric analysis.. The nanostructures provide high surface area for effective functionalization and our results demonstrated the high potential for efficient extraction of lithium.

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발표코드: **BIO.P-540**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-level expression of a functional goldfish cytochrome P4501A in *Shewanella oneidensis* and its application to degradation of benzo[a]pyrene

곽동건 박장수*

부산대학교 화학과

Cytochrome P4501A (CYP1A) in fish has attracted increasing interest because of its important roles in the metabolic activation of certain xenobiotics such as aromatic hydrocarbons. CYPs are reported to be expressed in yeast, insect cells and *Escherichia coli* (with the modification of N-terminal sequence), but are critical for high-level expression. Besides, this study found that the purification of recombinant goldfish CYP1A would result in a loss of enzyme activity. Because large quantities of functional CYP1A are required, it is necessary to find a suitable host with high-level expression in the membrane fraction. In the present study, a novel expression system using *Shewanella oneidensis* was established successfully for the production of goldfish CYP1A. A signal peptide in the expression vector leads to expression in the periplasmic space, and the introduction a ribosome binding site sequence to the vector enables high-level expression. The recombinant goldfish CYP1A in shewanella cells reached up to 1?mol per liter of culture, and showed the typical P450 hemoprotein spectra. An ethoxyresorufin O-deethylase assay revealed the amount of functional proteins in shewanella to be almost ten times more than those in other expression systems.

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발표코드: **BIO.P-541**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functional Expression of a Cystine-rich Peptide (Paralichthys olivaceus β -defensin) in Escherichia coli periplasm

김서현 박장수*

부산대학교 화학과

In the present study, a peptide β -defensin, isolated from the teleost, *P. olivaceus*, was recombinant expressed in *E. coli* periplasm. The antimicrobial peptide contains six cysteine residues, that the terms of disulfide bridge pairing determines the activity of the peptide. To further verify the characterization of β -defensin, its functional expression is urgent. Here, we showed that the β -defensin could be functionally expressed in the periplasmic area of *E. coli* by jointing a mini-tag (YoaJ) in the N-terminal of peptide. The DNA sequences of β -defensin and YoaJ were cloned into pQE30 vector by PCR technology, together with a six-histidine tag and a TEV recognition site. Recombinant fusion protein was expressed in *E. coli* strain M15[pREP4], and purified by Ni²⁺-column. *This work was supported for two years by Pusan National University Grant.

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장소: 창원CECO

발표코드: **BIO.P-542**

발표분야: 생명화학

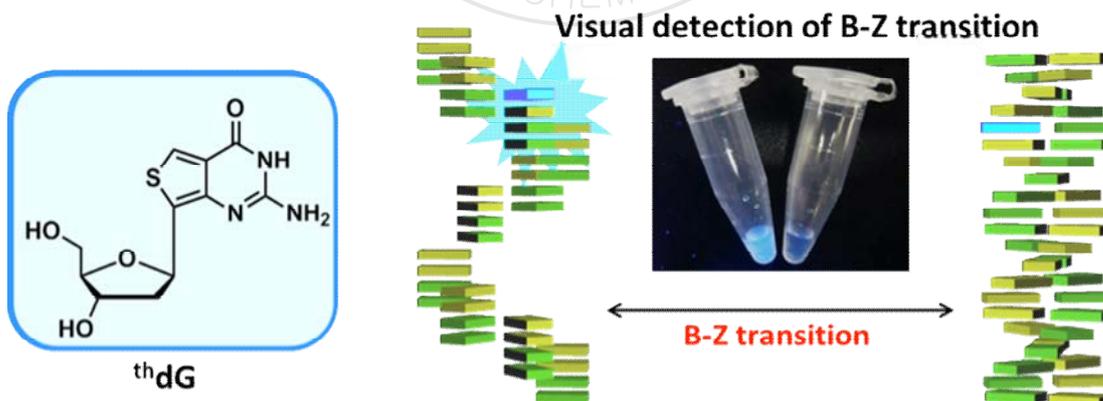
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of an Emissive Deoxyguanine Analogue and Visualization of B-Z Transition

Haruka Otomo Soyoung Park* Hiroshi Sugiyama*

Department of Chemistry, Graduate School of Science, Kyoto University, JAPAN

The development of fluorescent probes for nucleic acids is essential because nucleic acids are not fluorescent. In addition, a fluorescent base analogue has great significance for the expansion of an artificial genetic alphabet with diverse functionality. We have synthesized a novel fluorescent base analogue, 2-aminothieno[3,4-d]pyrimidine G-mimic deoxynucleoside, thdG. It has remarkable photophysical properties and can be readily incorporated in DNA. We also demonstrate that thdG could be applied successfully to the visual detection of Z-DNA based on different base stacking of B- and Z-DNA.



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장소: 창원CECO

발표코드: **BIO.P-543**

발표분야: 생명화학

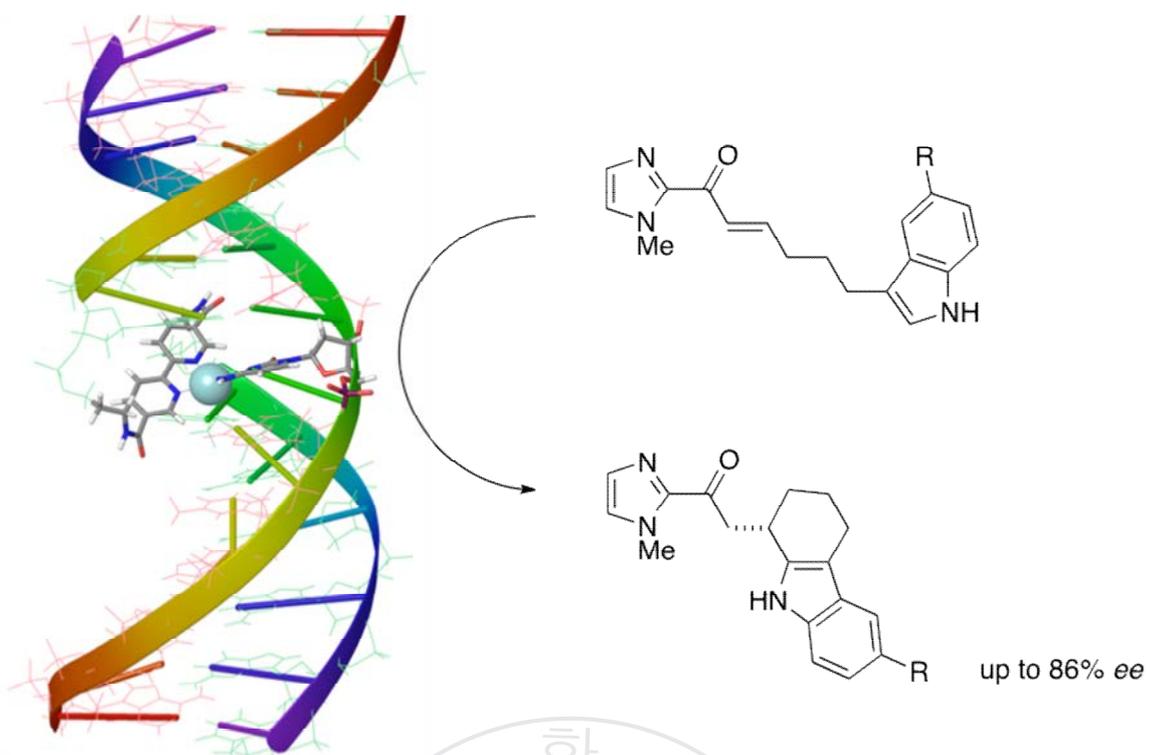
발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA-Based Hybrid Catalysts Using Covalent Anchoring Strategy

Soyoung Park Hiroshi Sugiyama*

Department of Chemistry, Graduate School of Science, Kyoto University, JAPAN

The application of DNA-based hybrid catalysts for asymmetric synthesis emerged very recently.^{1,2} DNA-based hybrid catalysts have been successfully applied to various asymmetric carbon-carbon or carbon-heteroatom bond-forming reactions. The use of DNA in Lewis acid catalyzed reactions led to high enantioselectivity, whereas the corresponding products were obtained as racemates in the absence of DNA. Therefore, it is clear that the enantioselectivity of the reactions originated from DNA; however, the stereoreinduction mechanism has been much less studied to date. In this study, we have developed DNA-based hybrid catalysts using the covalent anchoring strategy and investigated stereoreinduction mechanism of DNA-based asymmetric catalysis. [1] S. Park, H. Sugiyama, *Angew. Chem., Int. Ed.* 2010, 49, 3870-3878. [2] S. Park, K. Ikehata, R. Watabe, Y. Hidaka, A. Rajendran, H. Sugiyama. *Chem. Commun.* 2012, 48, 10398-10400.



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장소: 창원CECO

발표코드: **BIO.P-544**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functional Connection between Reactive Oxygen Species and N-terminal Cysteine Residues in the Mammalian N-end Rule Pathway

신승균 김지현 이민재*

경희대학교 응용화학과

In the mammalian N-end rule pathway, N-terminal cysteine has been recognized as an important sensor of reactive oxygen species in the cell. In sequential biochemical modifications, N-terminal cysteine becomes oxidized, arginylated, ubiquitinated, and consequently degraded by proteasome. So N-terminal Cysteine is destabilize protein in vitro. but we found the stably expressed Cys-GFP in 293 cells are long-lived in vivo. we confirm quantitative of Reactive oxygen species in the cell by Reactive oxygen species kit. We check the Cell viability by MTT experiment. Treat with Reactive oxygen species chemical there were no difference in GFP, P53, LC3 and Ub western blotting data But only RGS4 over expression have degradation change. Hereafter research we will focus this data and try to check which section is block.

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장소: 창원CECO

발표코드: **BIO.P-545**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Elongated oligonucleotide-linked immunosorbent assay for sensitive detection of a biomarker in a microwellplate-based platform

김경란 안대로^{1,*} 정민숙¹

연세대학교 화학과 ¹한국과학기술연구원(KIST) 테라그노시스연구단

The immunoassay is a representative method for detecting disease biomarkers and pathogenic biological agents. While the conventional enzyme-linked immunosorbent assay(ELISA) has been routinely used for the analysis of biological samples, methods with higher sensitivity are still in demand because the detection of low-level biomarkers is important for early diagnosis of lethal diseases. In this study, we developed a sensitive immunoassay called elongated oligonucleotide-linked immunoassay(EOLISA), employing long DNA oligonucleotides(80-mer), a fluorogenic RNA probe and RNaseH for signal amplification. The elongated DNA oligonucleotides led to a highly amplified fluorescence signal via iterative cycles of DNA?RNA duplexation and subsequent degradation of the RNA in the duplex by RNase H. The immunoassay was evaluated for sensitive detection of fatty acid binding protein(FABP) in the 0?1 ngmL-1 range. When compared with ELISA, EOLISA showed about 10-fold improved detection sensitivity. With its simple procedure and reliable detection performance in the conventional platform, the proposed immunoassay is expected to have potential applications in clinical diagnostics.

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발표코드: **BIO.P-546**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel N-end rule inhibitor, delays degradation of physiological substrates in mice brain

JiangYanxialei 최원훈 이민재*

경희대학교 응용화학과

The N-end rule pathway, as a subset of the ubiquitin-proteasome system (UPS), is a ubiquitin-dependent proteolytic system, in which destabilizing N-terminal residues of short-lived proteins function as an essential determinant of an N-terminal degradation signal. It is implicated in various essential cellular processes such as cardiovascular development, neural tube formation, spermatogenesis, and chromosomal stability. But the list of physiological functions of the N-end rule pathway is far from completed and it is becoming increasingly necessary to identify or synthesize efficient small-molecule inhibitors. Recently, we found that a neurostimulant drug efficiently inhibited the N-end rule pathway not only in vitro and in cultured cells but also in mice brains. We anticipate that the small-molecule inhibitor and its derivatives can be used as a critical tool to understand various developmental and pathophysiological process by the N-end rule pathway.

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장소: 창원CECO

발표코드: **BIO.P-547**

발표분야: 생명화학

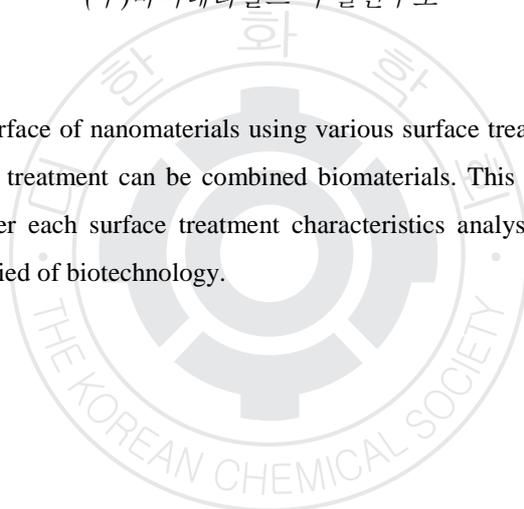
발표종류: 포스터, 발표일시: 수 16:00~19:00

Biotechnology application through of the Surface modification of nanomaterials

송미령 박수진 김준성* 정민숙

(주)바이테리얼즈 부설연구소

Silica-OH groups on the surface of nanomaterials using various surface treatment is possible. Of several surface-NH₂, -COOH, -NCS treatment can be combined biomaterials. This surface modification applied biotechnology progress after each surface treatment characteristics analysis were compared. After this surface modification is applied of biotechnology.



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발표코드: **BIO.P-548**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Spreading and Adhesion Behaviors of Mammalian Cells on Nanowires

김소연 양은경*

한국과학기술연구원(KIST) 의공학연구소

Vertical nanowires (NWs) have been extensively utilized as a universal platform for interrogating mammalian cells in vitro. Since biocompatibility of NWs is a prerequisite for their bioapplications, the present study was designed to investigate how cellular responses are affected by NWs. Using HeLa cells as a model system and different types of silicon (Si) NWs, we addressed a variety of cellular behaviors on Si NWs. First, we found the significantly reduced surface area of cells on denser and thicker Si NWs. Manipulation of membrane trafficking dynamics by either inhibition of endocytosis or addition of invasive membrane protein MT1-MMP did not affect such spreading behaviors, indicating that cells were in an inactive state of migration. For cells on long NWs, we hardly observed strong, well organized focal adhesion, possibly attributed to the reduced number of actin filament formation. On the other hand, diffusible focal complexes around the NWs were more pronounced. All of our findings suggest that cells adjust their morphology and adhesion behavior via actively organizing cytoskeletal molecules, thereby supporting cell survival. (supported by the Proteogenomic Research Program funded by MSIP)

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장소: 창원CECO

발표코드: **BIO.P-549**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Experimental considerations for assessing the cytotoxicity of nanoparticle

박수진 정민숙 송미령 김준성*

(주)바이테리얼즈 부설연구소

Currently, nanomaterials become more widely used, as a result, nanotoxicology research is now gaining attention. However, the cytotoxicity testing of nanomaterials is based on in vitro assays established for traditional hazard characterization of chemicals. Nanomaterials features may interfere with assay detection systems. We present an overview of in vitro toxicity test methods for nanomaterials and focus on limitations of application caused by nanoparticle properties.

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장소: 창원CECO

발표코드: **BIO.P-550**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparison of pH-sensitive degradability of maleic acid amide derivatives

강선영 이연*

서울대학교 화학부

Well-defined pH-sensitive chemical bonds such as acetals, orthoesters, imines, and phosphoramidates have been researched for biomedical applications. Along this line, we have explored maleic acid amide derivatives which are well known as pH dependent degradable molecules in acidic environment based on a stability of maleic anhydride ring-closing intermediates. We have demonstrated that the pH-sensitive degradability of maleic acid amide depend on a term of degree of substitution, which were investigated by ^1H NMR and HPLC respectively. This work will be contributed in field of drug delivery system that preferentially release drugs in required positions by controlling pH-sensitivity such as development of medicine for inflammatory or tumor cells with an acidic extracellular environment or endosomal escape based on the lytic activity under acidic condition.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-551**

발표분야: 생명화학

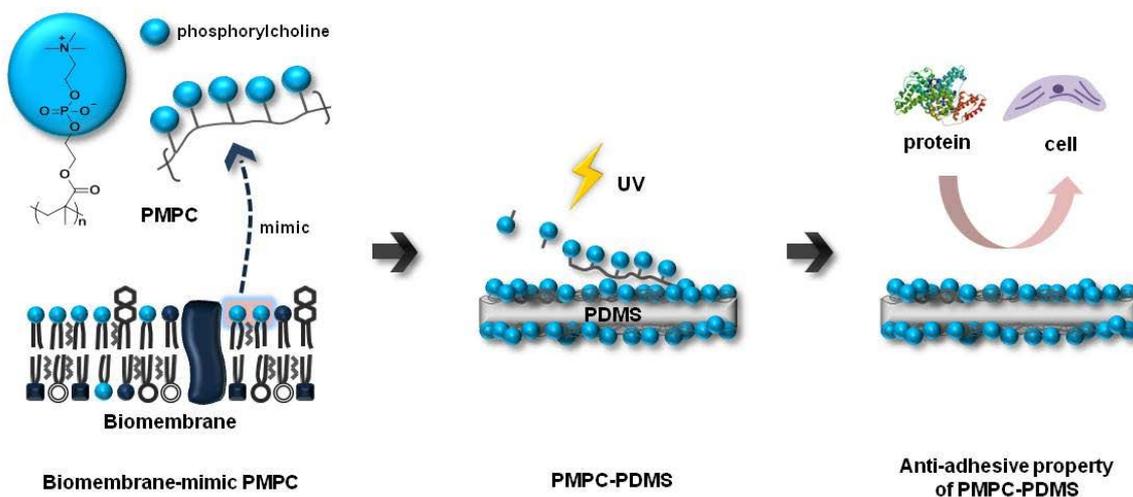
발표종류: 포스터, 발표일시: 수 16:00~19:00

Biocompatible surface coating of PDMS using a biomembrane-mimic polymer

합지연 이연^{1,*}

서울대학교 자연과학대학 화학부 ¹서울대학교 화학부

Because of transparency, high oxygen permeability and low cost, PDMS (Polydimethylsiloxane)-based materials are widely used as biomaterials such as bioimplants in plastic surgery. However, hydrophobic property of PDMS is considered to induce unwanted protein adsorption followed by harmful biochemical reactions in human body. To reduce such reactions surface coating of PDMS was performed by photo-induced radical polymerization generating a biomembrane-mimic polymer, PMPC (Poly(2-methacryloyloxyethyl phosphorylcholine)). In this experiment, the surface coating of PDMS was confirmed by the measurement of XPS(X-ray photoelectron spectroscopy) and water contact angle. In vitro biocompatibility tests showed more than 50% decrease in protein adsorption and 93% decrease in cell adhesion after coating.



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장소: 창원CECO

발표코드: **BIO.P-552**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Screening and characterization of ssDNA aptamers against *Salmonella enteritidis* and *Salmonella typhimurium*

윤문영* 이상춘 조준행¹

한양대학교 화학과 ¹한양대학교 자연과학대학

Salmonella is known as one of the most critical pathogen and causative agent of food borne disease worldwide. Among the classified more than 2,500 serotypes of Salmonella, *S. enteritidis* and *S. typhimurium* are the most primary serotypes which cause food borne disease in avian and humans. Aptamer, artificially composited oligonucleotide, is designed as the specific probe to target molecules. Aptamers can be selected by Systematic Evolution Ligands by Exponential Enrichment (SELEX). When the live cell used as target molecule, cell-SELEX is more useful and ease method than general SELEX due to no specific target molecules purification is required. In this study, we conducted SELEX technique to find out aptamer against *S. enteritidis*, and *S. typhimurium* living cell, and total 10 aptamers were obtained and analyzed for their affinity and specificity using gram negative bacteria such *E. coli* and *P. areuginosa*. To increase tight binding of aptamers, aptamers were introduced on functional polymers referred to Polyvalent Directed Aptamer Polymer (PDAP). Furthermore, various functional nanomaterials fused aptamer device in order to increase sensitivity of Salmonella detection will be discussed.

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장소: 창원CECO

발표코드: **BIO.P-553**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Screening of Aptamer-based Potent Inhibitors against *Mycobacterium tuberculosis* Acetohydroxyacid Synthase

문지영 하나름 김민서 윤문영*

한양대학교 화학과

Mycobacterium tuberculosis AHAS is a potential and promising candidate in the development of novel anti-tuberculosis drugs. Acetohydroxyacid synthase (AHAS) from *M. tuberculosis* 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). Aptamers are single-stranded nucleic acid molecules that can fold into complex three dimensional shapes, forming binding pockets and clefts for the specific recognition and tight binding of any given molecular target. In this study, an in vitro selection method, SELEX, was used to find single-stranded DNA aptamer towards *M. tuberculosis* AHAS. We found twelve ssDNA aptamers against *M. tuberculosis* AHAS through in vitro selection by SELEX. Among these, 6 aptamers of the biotinylated modified demonstrated higher binding affinity determined by aptamer-based ELISA method. These specificity of these aptamers were found to be higher in *M.tuberculosis* AHAS compared to homologous AHASs. These aptamers further showed potent inhibitory action against *M. tuberculosis* AHAS. Based on these results, we anticipate that these aptamers could further be promising candidate as novel and effective antituberculosis agents.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-554**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

siRNA library screen for human kinases and phosphatases involved in the regulation of hypoxia-inducible factor (HIF)-1 activity

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Hypoxia, a state of oxygen deficiency, is widely associated with pathogenesis of a variety of human diseases including cancer. Hypoxia-inducible factor (HIF)-1 as a main transcription factor regulates the cellular response to hypoxia. Therefore, the cellular changes induced by HIF-1 are potential therapeutic targets of cancer therapy. Previous studies have shown that the regulation of HIF-1 is involved in the activation of PI3K/AKT pathway in normoxia. However, how phosphorylation mediates the HIF1- α activation pathway in hypoxia is poorly understood. To identify signaling components that regulate the HIF-1 activity, we screened a small interference RNA (siRNA) library for kinases and phosphatases using a simple luciferase reporter assay under hypoxia. With the threshold of 50% inhibition or 150% activation, we identified 200 kinases and 33 phosphatases that likely influence the HIF-1 activity in hypoxic conditions. After categorizing such candidates by cellular signal pathways and metabolism, effects of depleting candidate kinases and phosphatases on the HIF-1 pathway are being examined. (supported by the Proteogenomic Research Program funded by MSIP)

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발표코드: **BIO.P-555**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A peptide mimetic of apolipoprotein A-I that contains 2-naphthylalanine residues enhances cholesterol efflux and inhibits oxidized LDL uptake by macrophage cells

현순실 김예원¹ 유재훈*

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Some time ago, the short peptide 4F, containing 4 phenylalanines was identified to be an apolipoprotein A-I mimetic. A library of 4F analogs, constructed using unnatural amino acid replacements, was prepared to identify peptides that have higher cholesterol efflux activities. Bis-2-Naphthylalanine containing peptide 2s has a 5-fold higher cholesterol efflux activity than 4F. Unlike previously studied peptides, 2s has high α -helicity and strongly interacts with HDL, LDL, and more selectively with oxidized LDL. As results, 2s inhibits uptake of oxidized LDL by macrophages in a manner that directly correlates with its anti-inflammatory effect. The results of animal studies using apoE null mouse and NZL rabbits show that injection of 2s in a 1 mg/Kg dose causes a 40-50% reduction in the size of lesions and macrophage infiltration in aorta. These findings suggest that 2s and related peptides could be potential drug candidates for the prevention or treatment of atherosclerosis.

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Molecular Imaging Technology for Analysis of Non-coding Cellular RNA Distribution Using AFM

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MicroRNAs (miRNAs) are known to short (19-25 nt) non-coding RNA molecules that play an important regulatory role in post-transcription. miRNAs have multiple biological functions such as cell differentiation, proliferation and secretion. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Detection and distribution of miRNAs have become an important emerging topic in biomedical fields. Therefore, spatial distribution of miRNAs is important to the single neuron, because the expression level of miRNAs is differentially associated with neuronal region such as soma, dendrite, axon, and synapse. miRNA-dependent fine-tuning has regulated various biological functions and induced diseases, but the distribution of miRNAs is not well reported. Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray and real-time RT-PCR. However, conventional tools are not easy to measure high spatial resolution of miRNAs. Therefore, a new approach for miRNA detection tool is AFM. AFM has become a powerful tool in bio-imaging field, because AFM is possible to measure simultaneously imaging and mapping of interaction forces. In this research, the spatial distribution of a specific miRNA on a sectioned brain tissue is measured by force-based AFM.

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Quantitative Analysis of Non-Coding Cellular RNA by Force-based Mapping with Atomic Force Microscopy (AFM)

구현서 박준원*

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MicroRNA (miRNA) is short (19-25 nt) noncoding single strand RNA molecule as regulator on target transcript in post-transcription. miRNAs have important roles in multiple biological functions. Additionally, the expression level of miRNAs is associated with various human diseases. Thus, miRNA detection has become an important emerging topic in biomedical fields. Many analytical approaches have been developed for detection of miRNA. However, conventional tools have several disadvantages for sensitive detection. Therefore, here we report another approach to detect miRNA at the single-molecule level using molecular recognition by force-based AFM. In this study, we generated specific force maps to visualize the detection of RNA-DNA duplex onto the substrate by AFM mapping. Likewise, we also focused on the discrimination between mature and precursor to quantify the distribution of our target molecule on the dendron-coated surface. We performed the optimization experiments for increase efficiency of hybridization during the preparation of substrate by controlling the various experimental conditions such as hybridization time, temperature and concentration of washing buffer. Force-based mapping experiments were performed in diethyl pyrocarbonate-treated PBS buffer. As a result, the non-linear force-distance curves showed specific interaction between miRNA-DNA duplex onto the surface and AFM tip. Furthermore, we examined whether the duplex-detachable molecule attached onto the dendron-coated tip would be able to discriminate between mature and precursor. Consequently, We found that force-based mapping would show the quantitative distribution of target molecule on surface and we also expect this AFM-based study will lead us to development of an ultrasensitive miRNA detection tool.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

CG7210 inhibits VSMC proliferation, as a novel and potent PDGF receptor β inhibitor

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In chemogenomics-based drug discovery, large collections of chemical products are screened for the parallel identification of biological targets and biologically active compounds. As part of a chemogenomics-based drug discovery effort, 9,939 existing chemicals were screened for PDGF-BB (25 ng/mL)-stimulated RASMCs and find out CG7210 which has the inhibitory effect of PDGF receptor β phosphorylation. We examined the effect of CG7210 on proliferation of RASMCs and the mechanism by which the compound induces cell cycle arrest. CG7210 inhibited cell proliferation in a dose-dependent manner, and decreased the phosphorylation levels of platelet-derived growth factor (PDGF) receptor β tyrosine residue 716, 751 and 1021. By contrast, CG7210 arrested cell cycle progression in the G0/G1 phase, and down-regulated cyclin D1/E and cyclin-dependent kinase (CDK) 2/4 expression. To compare the effect of AG1295 as PDGF receptor β inhibitor and CG7210 in PDGF-BB-stimulated VSMCs, PDGF receptor β phosphorylation levels were measured by western blotting. CG7210 has inhibitory effect at lower doses than AG1295. These findings verify that CG7210 mediates cell cycle arrest in PDGF-BB-treated cells during the G0/G1 phase through the inhibition of PDGF receptor β phosphorylation at lower dose than AG1295, a known PDGFR β inhibitor, and indicate that CG7210 has the capacity to a potent novel PDGF receptor β inhibitor.

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Identification of small molecule inhibitor for potent activity as polo-like kinase 1 inhibitor in human colon cancer cells

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Polo-like kinase 1 (Plk1) has an important regulator of cell cycle progression in the pathology of many cancers and DNA damage response. Drug repositioning is the application of known drugs and compounds to new indications. As the primary step for 'drug repositioning', we investigated the effect of 1619 drugs for PLK-1 inhibitor as potential therapeutic target in human colon cancer cells. We found that colchicines derivatives strongly inhibited cell proliferation. Also, cell treated with colchicine derivatives inhibited PLK-1 expression and induced mitotic arrest in cancer cells. We investigated the mechanism of colchicines derivatives for PLK-1 inhibitor. We show that colchicine derivatives induced a subsequent cell cycle arrest and inhibited PLK-1 kinase activity. We found that colchicine derivatives induced cell death by apoptosis occurs via p53-mediated prevention of caspase-independent mitotic death. These results suggest that colchicines derivatives lead to cell death in human cancer cell lines according to PLK-1 inhibition. In conclusion, we suggest that Plk1 inhibition have potential approach for cancer therapy.

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발표코드: **BIO.P-560**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new strategy against atherosclerosis; Inhibition of oxLDL formation by alpha-helical peptides

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서울대학교 화학교육학과 ¹서울대학교 화학교육과

Low density lipoprotein cholesterol complex (LDL) is known to be a major culprit for atherosclerosis and related cardiovascular diseases. Thus, LDL-lowering agents are number one selling drugs world-wide to reduce medical cardiovascular event frequency of patients. It was recently revealed, however, that oxidized form of low density lipoprotein cholesterol complex (oxLDL) makes major adverse effects of the diseases, even though its serum concentration is about three orders of magnitude lower than that of LDL. We have been designing and synthesizing various kinds of amphiphatic alpha-helical peptides that interact with cholesterol-rich surface of lipid complexes. Some of these peptides could selectively bind to LDL and inhibit formation of oxLDL in non-enzymatically and high metal ion conditions. As results of screening, peptides with aromatic amino acids in their hydrophobic face were selected as inhibitors of oxLDL formation. These peptides could be lead compounds to prevent atherosclerosis and related cardiovascular diseases as anti-oxidants.

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장소: 창원CECO

발표코드: **BIO.P-561**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

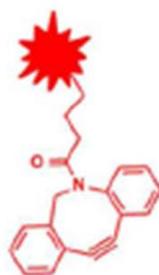
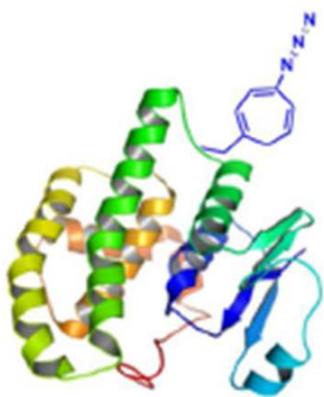
Development of a Simple Method for protein conjugation by copper-free click reaction and Its application to antibody-free western blot analysis

고우석 이현수*

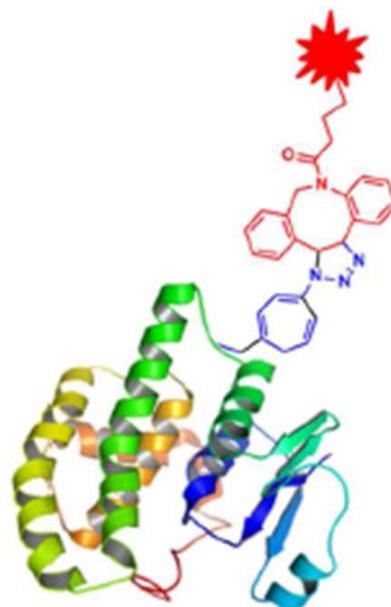
서강대학교 화학과

There are currently many methods available for labeling proteins in order to study their structure and function. However, the utility of these methods is hampered by low efficiency, slow reaction rates, nonbiocompatible reaction conditions, large-sized labeling groups, and the requirement of specific side chains such as cysteine or lysine. In this study, a simple and efficient method for protein labeling was developed, in which an azide-containing amino acid was introduced into a protein and conjugated to a labeling reagent by strain-promoted azide-alkyne cycloaddition (SPAAC). This method allowed us to label proteins by simply mixing a protein and a labeling reagent in physiological conditions with a labeling yield of approximately 80% in 120 min. In addition, the specificity of SPAAC made it possible to analyze the expression level of a protein quantitatively by simple mixing and SDS-PAGE analysis with no need for antibodies or multi-step incubations. Because the genetic incorporation of the azide-containing amino acid can be generally applied to any protein and the SPAAC reaction is highly specific, this method should prove useful for labeling and analyzing proteins.

Genetically encoded
unnatural amino acid



Biochemical probe
attached to ADIBO



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장소: 창원CECO

발표코드: **BIO.P-562**

발표분야: 생명화학

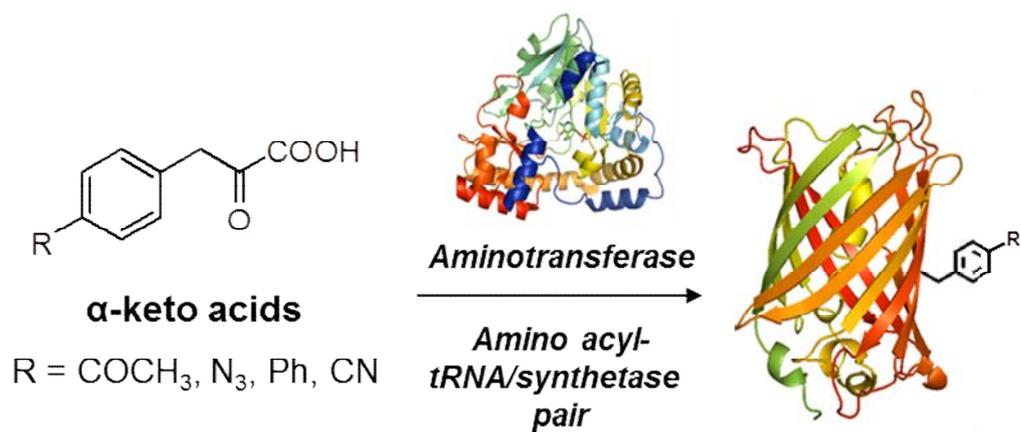
발표종류: 포스터, 발표일시: 수 16:00~19:00

Genetic incorporation of unnatural amino acids biosynthesized from α -keto acids by an aminotransferase

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Four unnatural amino acids (UAAs) were synthesized from their corresponding α -keto acids by using glutamine:phenylpyruvate aminotransferase (GlnAT) from *Thermus thermophilus* HB8. The enzyme efficiently catalyzed the conversion of the unnatural substrates, with little decrease in its activity compared to that shown toward its natural substrates. The α -keto acids were converted into the corresponding amino acids in cells and then directly incorporated into a protein with high efficiency and fidelity. Because α -keto acids have no chiral center and are synthetically readily accessible, this method will further enhance the genetic incorporation technology and may present a new approach to the preparation of optically pure UAAs. Considering the substrate promiscuity of the GlnAT observed in the study, this method can be applied to the genetic incorporation of other UAAs derived from Tyr or Phe, which constitute approximately 50% of the successfully incorporated UAAs. In addition, this study provides an impetus for the development of an autonomous unnatural organism that can synthesize and incorporate UAAs.?



Transamination and genetic incorporation



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장소: 창원CECO

발표코드: **BIO.P-563**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-throughput instant quantification of protein expression and purity based on photoactive yellow protein turn off-on label (POOL)

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Quantifying the concentration and purity of a target protein is essential for high-throughput protein expression test and rapid screening of highly soluble proteins. However, conventional methods such as PAGE and dot blot assay generally involve multiple time-consuming tasks requiring hours or do not allow instant quantification. Here, we demonstrate a new method based on the Photoactive yellow protein turn Off/On Label (POOL) system that can instantly quantify the concentration and purity of a target protein. The main idea of POOL is to use Photoactive Yellow Protein (PYP), or its miniaturized version, as a fusion partner of the target protein. The characteristic blue light absorption and the consequent yellow color of PYP is absent when initially expressed without its chromophore, but can be turned on by binding its chromophore, p-coumaric acid. The appearance of yellow color upon adding a precursor of chromophore to the coexpressed PYP can be used to check the expression amount of the target protein via visual inspection within a few seconds as well as to quantify its concentration and purity with the aid of a spectrometer within a few minutes. The concentrations measured by the POOL method, which usually takes a few minutes, show excellent agreement with those by the BCA Kit, which usually takes ~1h. We demonstrate the applicability of POOL in E. coli, insect, and mammalian cells, and for high-throughput protein expression screening

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장소: 창원CECO

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification and characterization of BAK inhibitors that prevent the formation of BAK pore which mediated apoptosis

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The pro-apoptotic BCL-2 family protein BID activates BAK, which mediate oligomeric pores in the mitochondrial outer membrane. This results in cytochrome c release into the cytoplasm, leading to cell death. Here, we utilized liposomes encapsulating sulfo-rhodamine-dextran at a controlled temperature for measuring membrane poration by BID-dependent BAK activation. We screened three inhibitors through liposome release assay system within drug library of 1,000 chemicals. We analyze the assay system using fluorescence release and screen through the NINDS drug library found three kinds of inhibitors, perphenazine, fluoxetine and benzethonium. A few chemical compounds including trifluoperazine, which was known as a mitochondrial apoptosis-induced channel (MAC) blocker, were identified to prevent the leakage of fluorescence labeled dextran from BAK pore. These inhibitors were shown to inhibit the formation of BAK-pore rather than blocking the preformed BAK pore.

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Emulation of complicated ECM architectures by a simple polymer pattern

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In nature, fibrous extracellular matrix (ECM) proteins can form its insoluble fibrous networks with existence of glycosaminoglycans (GAGs). Also, the networks consist of hybrid ECM architectures. The complicated structures play a crucial role in physical and biological functions in tissue. Limitation of current *in vitro* studies is to focus on recapitulating ECM fibers composed of a single type of ECM proteins. However, composite ECM fibers with various types of ECM proteins are necessary to fabricate specialized *in vivo* architectures and optimize unique characteristics of diverse ECM—cell or cell—cell interplay. Therefore, I suggest that GAGs mimicking polymer pattern may guide the formation of composite ECM networks spontaneously. The simple platform will become a versatile and basic substrate to fabricate complexity of ECM microenvironments, maintaining physiological and biological functions.

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Purification of a novel antimicrobial peptide from the coelenteron fluid extract of the sea anemone, *Urticina crassicornis*

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부경대학교 생물공학과

The acidified coelenteron fluid extract of the sea anemone (*Urticina crassicornis*) showed strong antimicrobial activity against *B. subtilis* and *E. coli* D31. An antimicrobial material was purified by C18 RP-HPLC. Treatment of the purified material with trypsin for 60 min at 37°C completely abolished all antibacterial activity against *B. subtilis* and *E. coli* D31. This results suggest that the purified material contains a proteinaceous antibiotic. The molecular weight of the purified material was determined to be 4,194 Da by MALDI-TOF MS. The sequence analysis of the purified peptide was analysed in processing. Our results can be used to better understand the innate immune system of the sea anemone (*Urticina crassicornis*) and to enhance research to protect it from important microbial infections. Additionally, the purified antimicrobial material can be used as alternatives to antibiotics in aquaculture.

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장소: 창원CECO

발표코드: **BIO.P-567**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Purification of a novel antimicrobial peptide from the mucus extract of the sea anemone, *Urticina crassicornis*

박남규* 고혜진 김태영

부경대학교 생물공학과

The acidified mucus extract of the sea anemone (*Urticina crassicornis*) showed strong antimicrobial activity against *B. subtilis* and *E. coli* D31. An antimicrobial material was purified by C18 RP-HPLC. To investigate the characterization of the purified peptide, the molecular weight and amino acid sequence analysis were performed by MALDI-TOF MS and Edman degradation. The molecular weight of the purified material was determined to be 5196.9 Da. The sequence analysis of the purified peptide is in processing. Our results can be used to better understand the innate immune system of the sea anemone (*Urticina crassicornis*) and to enhance research to protect it from important microbial infections.

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장소: 창원CECO

발표코드: **BIO.P-568**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inhibitory effect of laver extract on lipid accumulation of 3T3-L1 adipocytes

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인천대학교 화학과

Obesity is a global issue because it is associated with a number of diseases, such as type-2 diabetes, hypertension, dyslipidemia, and coronary heart disease. Adipocytes store excess of energy in the form of lipid and play important roles in regulating lipid metabolism and energy balance. Adipogenesis is a process by which new adipocytes are formed from mesenchymal stem cells or other precursor cells. Adipocyte differentiation is a complex process that is regulated by various transcription factors and adipogenesis-related genes. Therefore, controlling adipogenesis is a potential strategy for obesity prevention. The most important transcription factors among them are CCAAT/enhancer binding proteins (C/EBPs) and peroxisome proliferator-activated receptor (PPAR) families. During adipogenesis, C/EBP α and PPAR γ activate the expression of lipid-metabolizing enzymes, such as fatty acid synthase (FAS) and fatty acid binding protein 4 (FABP4). In this study, we examined the inhibitory effect of aqueous-methanol extract of laver (*Porphyra yezoensis*) on adipogenesis and lipid accumulation of differentiated 3T3-L1 adipocytes. The laver extract reduced proliferation of preadipocyte 3T3-L1 cells. The laver extract added to the 3T3-L1 cell cultures during differentiation significantly suppressed accumulation of lipid droplets in cells in a dose-dependent manner. And a significant reduction of adipogenic gene expression was caused by the laver extract. Our results suggest that the laver extract has antiadipogenic effect and can be useful for prevention of obesity.

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발표코드: **BIO.P-569**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Screening and Isolation of the bioactive material from the starfish (*Asterina amurensis*)

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부경대학교 생물공학과 ¹부경대학교 미생물학과

This study was screening of bioactive materials from starfish, *Asterias amurensis*'s tissue (liver, tube feet, gonad, digestive gland, muscle). Bioactive materials was extracted by 1 % acetic acid. The acidic extracts screening for antimicrobial, contractile activities and relaxing response of each animal smooth muscle. Antimicrobial activity used *E.coli* D31 and contractile activity used the dorsal muscle of each starfish. In the result of Antimicrobial activity about body extract of *Asterina amurensis* and tube feet extract of *Asterias amurensis* were high effecter than other extracts.

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장소: 창원CECO

발표코드: **BIO.P-570**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Membrane protein patterning on supported lipid bilayer

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서강대학교 화학과 ¹성균관대학교 에너지과학과 ²한국과학기술연구원(KIST) 특성분석센터 ³
서강대학교 화학과 및 바이오융합과정

In this study, we have been developed a novel method to fabricate membrane proteins incorporated lipid bilayer-patterns on solid supports. Light Harvesting Complex II (LHCII) and proteorhodopsin as membrane proteins were reconstitution into negatively charged lipid vesicles including 20 mol% DOPS. The solid supports were functionalized and patterned by micro-contact printing using 3-Aminopropyltriethoxysilane (APTES). The negatively charged proteoliposomes were only adsorbed and ruptured to transform into the membrane protein patterned lipid bilayers on the positively charged APTES patterns of solid supports. The empty areas (exposed oxide layers) were backfilled with pure lipid bilayers using neutrally charged DOPC vesicles. Finally, this method was examined with differently shaped and sized patterns and various solid supports.

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장소: 창원CECO

발표코드: **BIO.P-571**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Study of CHO Cell Membrane Glycosylation by NanoLC/MS

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Chinese hamster ovary (CHO) cells are used to produce biopharmaceutical glycoproteins because CHO cell glycosylation is very similar to that of humans. In the previous study, we found that CHO cell glycan abundances changed significantly depending on growth phase and cell line, with clear structural correlation to certain glycotransferases and glycosidases. Some specific structures, NeuGc sialylation and poly lactosamine, are known as significant difference between CHO cell and human glycosylation and were elucidated by isomer-specific nano-LC/MS/MS. Ensuring correct glycosylation on biopharmaceuticals is critical for a myriad of reasons. We examined the glycosylation of different industrially-relevant CHO cell lines under different culture conditions also glycosylation site. Since the vast majority of CHO cell glycosylation is localized at the membrane, we isolated the fraction by lysing and then ultracentrifuge the CHO cells, and enzymatically released the N-glycans. Finally, the purified N-glycans were analyzed by isomer-specific porous graphitized carbon nano-LC/MS and -LC/MS/MS. Experimental findings will be combined with known glycobiology to generate a theoretical library of all biologically possible CHO cell N-glycan compositions.

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Protective effect of laver extract against UVB-induced oxidative damage in HaCaT cells

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UVB (290-320 nm) is the most damaging component of the solar radiation that reaches surface of the Earth. UVB acts mainly on the epidermal basal cell layer of the skin and accelerates premature skin aging. Excessive amount of reactive oxygen species (ROS) generated by UVB-irradiation can induce matrix metalloproteinases (MMPs), which are responsible for breakdown of collagenous extracellular matrix proteins in skin, causing wrinkle formation and photoaging. Therefore, antioxidants have the potential to attenuate the skin cell damage and photoaging induced by UVB irradiation. It has been demonstrated recently that seaweeds contain a variety of cell-protecting bioactive components. We investigated the effects of photo-oxidative damage by UVB on human epidermal keratinocytes, HaCaT cells, and the protective effect of laver (*Porphyra yezoensis*) extract against UVB-induced cell damage. Aqueous-methanol extract of laver significantly protected keratinocytes against UVB-induced damage as assayed by cell viability. Additionally, the laver extract significantly inhibited UVB-induced increase in ROS and decreases in cellular total glutathione level and GSH/GSSG ratio. The laver extract also suppressed UVB-induced MMP-1 expression and phosphorylation of mitogen-activated protein kinases (MAPKs). Our results suggest that the laver extract can protect skin from UVB-induced damage and photoaging by stimulating antioxidant response and suppression of MMP-1 expression via modulating MAPK signaling pathways.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel method for the assay of RNA synthesis by RNA polymerase using graphene oxide

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Graphene oxide (GO) that draws huge attention due to wide variety of usage is known to interact with single-stranded nucleic acids through pi-stacking interactions and hydrogen bonds between the nucleobases and the hexagonal cells of GO, while having less affinity to the double-stranded nucleic acids. In addition, it shows fluorescence quenching when the fluorophore comes near to the GO surface. With this property of GO, we designed a novel method of RNA polymerase activity assay, where in vitro RNA synthesis using T7 RNA polymerase was monitored. We prepared double-stranded DNA template for RNA synthesis and fluorescence-tagged single-stranded peptide nucleic acid (PNA) complementary to the RNA product. Once RNAs are synthesized, PNA probe anneals to the RNA product, and the fluorescence in this RNA-PNA hybrid will not be quenched as the GO is added. However, the fluorescence-tagged PNA remaining as single stranded will be quenched when the RNA is not present. This novel RNA polymerase assay method using the GO can be applicable to screen inhibitor candidates against viral RNA polymerase.

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Orientation and Density Control of Tandem Antibody on Fluorescent Carbon Nanotubes for Detection of Cellular Cancer Biomarkers

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Recently, nanomaterials-based imaging and sensing have obtained a lot of attention due to their potential for higher selectivity and sensitivity. Controlling the orientation and density of a recognition molecule, antibody, on the surface of nanomaterials is very important for the sensitive detection of target molecules. Herein, we present a carbon nanotube (CNT) nanoprobe with a proper density and controlled orientation of tandem antibody, which showed its enhanced affinity to a cancer biomarker, HER2. The CNT/tandem antibody nanoprobe exhibited its distinct optical properties such as intense Raman signature and near-infrared fluorescence, which was used for signal transduction in biomarker detection. Finally, CNT/tandem antibody nanoprobe was successfully applied to HER2 detection in living cells.

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Efficient cellular uptake of alpha-helical peptides and its elucidation of uptake mechanism into cells

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To measure the efficiency of cellular uptake according to the structural difference, and therebyTo develop enhanced peptide carriers that could deliver biomolecules or drugs into cells, three kindsof monomer, bioreducible dimer, non-bioreducible dimer peptides were synthesized based on subunit concepts. These peptides consist of a amphiphilic(Leu/Lys) alpha-helical peptide sequence useful as efficient ligands against various RNA harpins targets. Cellular uptake of the synthesized peptides was investigated in hela cells by flow cytometry. In dose dependent manner, A monomer (Pep-F1) showed cellular uptake over 90% at 500nM for 24h and a non-bioreducible dimer (Pep-F3) showed cellular uptake over 60% at 500nM for 24h. Meanwhile, Bioreducible dimer(Pep-F2) showed even cellular uptake over 90% at 5nM for 24h. Intracellular trafficking was investigated by using confocal laser scanning microscopy (CLSM). Two pep-F1 and pep-F2 were internalized into hela cells at 4°C for 2h, but a pep-F3 was not. Meanwhile, all peptides were reached to nucleus after uptake into hela cells at 37°C for 24h. Two pep-F1 and pep-F2 were reached to nucleus after uptake into hela cells on treatment of naringenin (a endosome inhibitor), amiloride and wortmannin (macropinocytosis inhibitor) at 37°C for 24h, but a pep-F3 was entrapped into cytosol in hela cells on treatment of naringenin and also not internalized into hela cells on treatment of amiloride and wortmannin. As results of above, pep-F1 and pep-F2 were internalized into hela cells through energy-independent pathway, but pep-F3 was internalized into hela cells through energy-dependent pathway. The MTT assay demonstrated that pep-A1 and pep-A2 and pep-A3 can be safe carrier materials over 80% of cell viability.

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Detection of cell apoptosis by fluorescent dye-intercalated DNA attached to graphene oxide

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Graphene oxide (GO) has been recently used for application in cellular imaging and medical diagnostics. GO has been known for its easiness to adsorb hydrophobic molecules, single-stranded DNA and RNA via π - π stacking, electrostatic and other molecular interactions. In addition, the effective electron transfer property of GO has made it a powerful fluorescence quencher. In this study, we have designed a novel method to detect cellular apoptosis by delivering duplex DNA intercalated with fluorescent dye (SYBR green I) that is adsorbed on to GO. Cellular uptake of the GO-DNA nanocomplex is to monitor the double-stranded DNA fragments which would be released into the cytoplasm during apoptosis. Fluorescence of the SYBR green (SG) I-intercalated partial duplex DNA that are complexed with GO was initially quenched, but the fluorescence of DNA-SG/GO nanocomplex that was delivered to human cancer A549 cells would be enhanced due to the presence of nuclear DNA fragments during apoptosis. The released double-stranded DNA fragments will be complexed with fluorescent SG dyes that are delivered into the cytoplasm. We observed that treatment of apoptosis causing reagent (staurosporine) to the cells increases SG fluorescence. This result suggest that the SG delivered by DNA-SG/GO nanocomplex was transferred to nuclear dsDNA released into the cytoplasm after apoptotic disruption of nuclear membrane.

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발표분야: 생명화학

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Dependence of oil depth on protein crystallization in microbatch method using silicon oil

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Microbatch crystallization performed in the silicone oil bath is one of well-known procedures obtaining protein crystals. In this method as shown the phase diagram in Fig. 1a, we control the diffusive evaporation rate of water solvent in the precipitant solution (75 mg/ml lysozyme protein and 6.5 wt% NaCl precipitant with 0.1 M NaAc for pH 4.8) through the oil reservoir (Fig. 2b) satisfying the corresponding the path of phase condition for crystallization (the blue dashed line in Fig 1a). There are numerous factors influencing this crystallizing process, such as temperature, mechanical vibration, protein solution-precipitant ratio, salt concentration, salt type, buffer pH, so on. Although these conditions have been considered carefully, unfortunately there is still no standard guideline for the optimized conditions for a certain parameter to obtain the good protein crystals, especially regarding the oil-depth parameter. In this reason, it will be important to investigate the effect of varying oil depth, i.e., the distance from an immersed droplet to air/oil interface (Fig. 1b). If it should produce the good reproducibility, the short period and the large size of crystalizing protein with the fixed other conditions. Recently we obtained the good evidence from enzyme crystallization although the experiment was performed only for one fixed depth (ca. 1 mm), indicating that this microbatch method using oil depth variation should be a very effective way so that it can be used for the speedy protein crystallization.

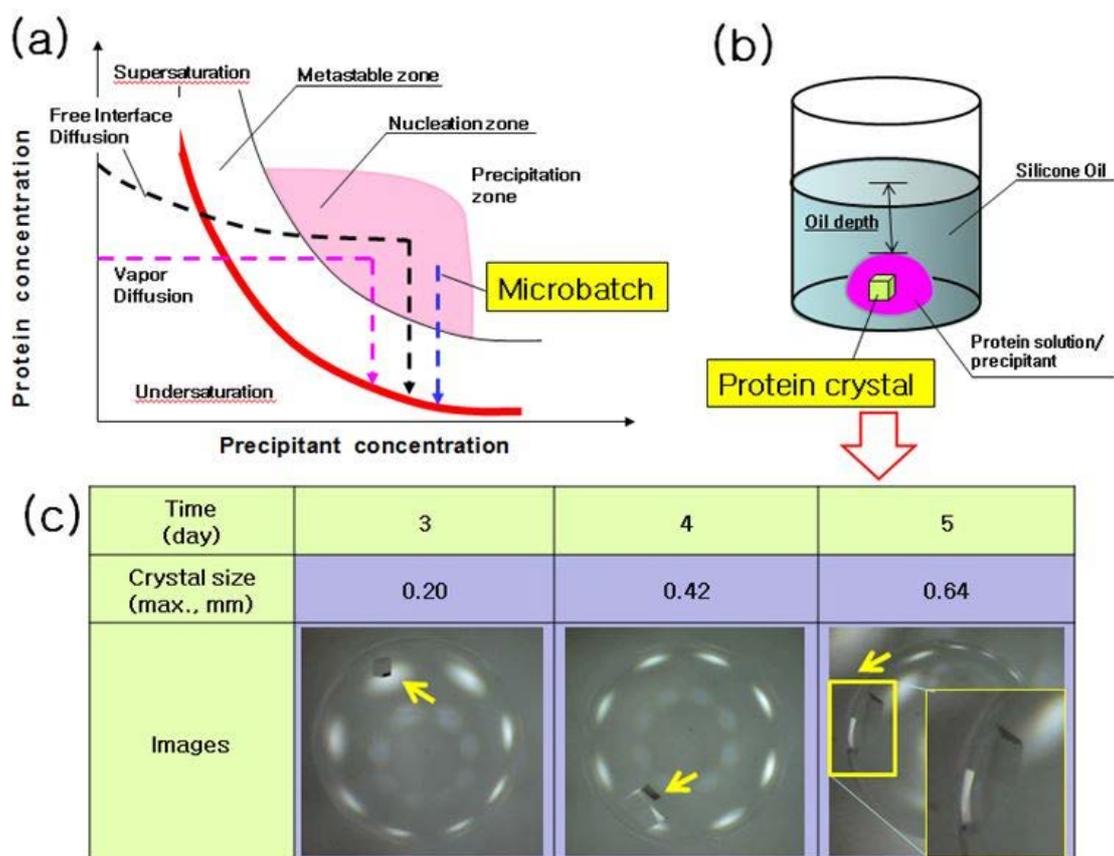


Fig. 1. Protein crystallization in microbatch method: (a) Phase diagram, (b) Experimental setup and (c) Crystallizing image of lysozyme protein. Only one crystal grows in submillimeter size.



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Behavior of drops on the paper-based open digital microfluidic devices

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Many research groups have worked towards the construction of "lab-on-a-chip (LOC)" in order to integrate chemical and biochemical analyzers on the micrometer or even nanometer scale. For the digital microfluidic devices (DMFs) among LOCs there are certain advantages such as merging, splitting, dispensing and easier access to the digitalized drops. In most of studying DMFs, the open type is preferred because of many advantages such as easily integrated into existing microchips, its fabrication ensuring high operational reproducibility and simple design. In this study, we developed a paper based open device that was successfully enabled to manipulate smoothly the digital drops. We found out the displacement of drops as a function of the gap size with respect to the different AC voltages (40 V, 70 V and 120 V) on the paper substrate coated with low viscous silicone oil to reduce the surface tension. The electrodes on these open DMFs are patterned by printing CNT ink for electrowetting control, which will be used for bio-, chemical- and medical-liquid samples. In the further work, we will analyze various bio-samples for enzyme-linked immunosorbent assay (ELISA) on our newly developed DMFs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Isomer Separation of N-Glycans on a PGC Column

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Glycosylation is one of the most common post-translational modifications of proteins and plays key roles in many biological processes. However, the isomer-specific analysis of glycans remains a major challenge because of numerous connectivity and linkage of glycans. A PGC often separates aldehyde sugars into α and β anomers increasing the complexity of isomer-specific separations, nonetheless, PGC (porous graphitized carbon) is still widely used for effective isomer-specific separation and enrichment of glycans based on polarity, size, and three-dimensional structure. Here, we aimed to optimize glycan reducing conditions to get rid of α and β anomers by reducing aldehydes to alditols using sodium borohydride. The experimental strategy was validated using three different types of glycans to determine different reductive reaction as characteristics of glycans. After releasing N-glycans using PNGase F, released glycans were purified by SPE (solid phase extraction) and reduced by sodium borohydride. Reduced glycans were purified and enriched by SPE. Reduced N-glycans were easily identified by MALDI/TOF MS due to the two Da mass increase resulting from the conversion of reducing terminal to an alditol. To obtain isomer-specific and quantitative information, glycans were analyzed before and after reduction using chip-based PGC nano-LC/MS. Indeed, we found less peaks in chromatogram after reducing N-glycans which suggest the number of glycans isomers decreased because of the removal of α and β anomers on a PGC. This analytical platform will provide a powerful analytical tool for isomer-specific separation for glycan biomarker discovery and glycomic characterization of biopharmaceuticals.

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Characterization of structure isomers released from human serum using tandem MS

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Glycosylation is one of the most common post-translational modifications of proteins where glycans are attached to the protein chain. Glycan structures have many isomers due to numerous connectivity and branching possibilities. In General, structure isomers identification of glycan is performed by chromatographic separation techniques such as HPLC and CE. Glycans are highly amendable to mass spectrometric analysis and tandem MS. Tandem MS is a powerful tool to elucidate glycan structures. Here, we present MALDI-TOF/TOF tandem mass spectrometry to rapidly elucidate glycan structural isomers using high energy CID MS. In total, 32 glycan isomers corresponding to 24 glycan compositions have been characterized by MALDI-TOF/TOF MS. As an example, neutral N-glycan at m/z 1647.617[M+Na]⁺ corresponding to 4Hex, 4HexNAc, and 1Fuc is composed of four isomers. These isomers have been identified by different fragmentation pathways. Signature peaks which are uniquely presented in specific glycan structure we're used to distinguish these isomers. Antennary glycan suggest the attachment of the fucose residue to the antenna GlcNAc residue based on the m/z 372.118. Similarly, core fucosylated glycan present the attachment of fucose residue to the reducing end at the m/z 593.213. This is a rapid and new way to characterize structure glycan isomers by only ms.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Mimicking ECM incorporated lipid vesicles; Fibronectin network formation on liposomes

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We need to reduce the in vivo cell's complexity such as compositional heterogeneities and structural complexities, by developing "minimal cell model", to experimentally understand the interaction between cell membrane and ECM. Even though many researches on in vitro ECM are being studied, the fundamental mechanisms are fundamentally different from the reality. Using Giant unilamellar vesicles (GUV) suitable for bio-mimicking structure, novel artificial cell model, having an ideal native environment (geometrically and mechanically) is expected. Glycosaminoglycans (GAGs) receptors composed of negative functional groups, will induce the surface charge difference of liposomes, and the FN adsorption is consequently expected. The presence of heparin (Fibrillogenesis accelerator) & lateral diffusion (mechanical stretching) can be simultaneously occurred, and in vivo FN fibril formation can be simulated. The lipid vesicle incorporated with ECM network will provide the roles of ECM in the biological cells; cellular stability, migration and biological functions. FN-incorporated GUV may be very effective on cell-, tissue-, or organ healing process, if we find a way to transfer the FN-fibril on the live cell membrane. (in vivo application)

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Photo-induced proton gradient artificial cells composed of two different light-sensitive membrane proteins for utilizing entire visible light and enhancing functional efficiency

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Proteorhodopsin(PR) and Photosystem II(PSII) are light-sensitive integral membrane proteins which function critical biological processes in the cells. Each protein has been investigated each function and photo-dynamics. Proteorhodopsin is retinal-binding integral membrane protein that functions as light-driven proton pump which are activated by green light. Photosystem II is the integral membrane protein complex that performs splitting of water by absorbing blue and red light. These two proteins have characteristic wavelength absorption in visible light. To achieve complementary absorption efficiencies of sunlight, two radically different membrane proteins are reconstituted in single artificial membrane. Here, we investigated that artificial cells can utilize entire visible wavelength for proton gradients.

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Molecular imaging and quantification of biochemical environments inside lipid vesicles: application of visualized pH indicators

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Lipid vesicles are a basic tool of the artificial cell for studying cell metabolism, ion transport, as well as biochemical reaction in cells. Intracellular and intravesicular environments play significant roles in biological and physiological processes, e.g. cell function, ion transport and endocytosis. Therefore, there are a variety of methods such as microelectrodes and NMR to measure intracellular pH. Compare to these methods, fluorescent pH indicators are more sensitive, they can be used for precise real-time monitoring and they do not cause destruction of lipid membrane. FITC, pyranine and SNARF-1 are fluorescent dyes as pH indicators for quantitative proton translocation measurement. Pyranine dye has a dual excitation wavelengths and SNARF-1 has the fluorescence emission at two wavelengths. These ratiometric fluorescent pH indicators have proved effective methods for sensitive analysis because they are not influenced by temperature changes and photobleaching. They have been used to monitor the cytoplasmic environments of lipid vesicles or proteoliposomes in situ. Furthermore, fundamental understanding on application of visualized pH indicators and a light-induced proton trafficking mechanism will be discussed.

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Mechanical Properties of Phospholipid Vesicles Containing Cardiolipin

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A cell is the smallest and basic unit of all living organisms, which is surrounded by a cell membrane. The cell membrane not only separates the external and internal environment of cells, but helps maintain the structure of cells. We studied the mechanical properties of the cell membrane, which indicates how stable the cell membrane is, when the tension is applied. Especially, phosphatidylcholine (PC) is one of the major lipid components of the cell membrane and cardiolipin (CL) is a lipid found only in mitochondria inner membrane. We formed vesicles with these two lipids varying the compositions then, calculated the modulus of vesicles with micropipette aspiration equipment we developed recently. With this apparatus, we can grab a single cell, control the pressure and monitor a rupture of the vesicle simultaneously recording the whole process. In this study, how the existence of CL affects the cell membrane's activity will be discussed.

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Mimicking cytoplasmic environment thorough in vitro protein crystallization in an artificial cell

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Protein crystallization in living cells occurs as a native process. Protein crystallization in vivo is one of the most fascinating examples as biological self-assembly. Through the protein crystallization in the living cells, the cells can play roles such as protein storage, regulation of protein functions or plugging leaks etc. Unlike in vivo protein crystallization, the approaches to protein crystallization in vitro mainly have been focused on X-ray crystallography to find out structures and functions of the proteins. In this study, the main idea is to combine in vivo and in vitro protein crystallizations. One of the most challenging recent issues in bio-interfacial sciences is how to mimic in vitro the fundamental functions and structures of a living cell in artificially-constructed cell-like structures. Among these issues, the embodiment of cytoplasmic environments in an artificial cell is the hottest issue. Above all, it is so fascinating to verify the crowding effect as mimicking cytoplasmic environments using artificially constructed structure in vitro. The giant liposomes filled with gel-like substances such as the agarose, PEG, or dextran and protein crystallization inside that structure shows some abilities to realize how to mimic in vitro the fundamental functions and structures of a living cell in artificially-constructed cell-like structures.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Scopoletin induces autophagy via modulation of p53 and Sirt1 in IMR90 cells

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The recent evidences indicate that autophagy is associated with a number of processes including aging, muscular disorder and neurodegeneration in addition to longevity. The efficacy of scopoletin was investigated on induction of autophagy through histone deacetylation and p53 activation in human lung fibroblast cell line, IMR 90. In this study, it was discovered that scopoletin induced autophagy. It was also identified that the activation of p53 by scopoletin are related to the induction of autophagy. Furthermore, scopoletin modulates the expression of proteins related to autophagy. The expression levels of p-p53 and Ac-p53 was decreased in the presence of scopoletin. In contrast, the expression level of Sirt1 was increased in IMR 90 cells treated with scopoletin. In addition, the expression level of IGFBP-3 was increased in the presence of scopoletin. Moreover, SA- β -Gal staining, an aging marker was reduced by treatment with scopoletin. These results suggest that scopoletin promotes the induction of autophagy in IMR 90 cells through the enhanced activity of p53 and Sirt1.

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Customized Mesoporous Silica Nanoparticles (MSN)-Mediated Proteasome Delivery Promotes Tau Degradation through the Ubiquitin-Proteasome System

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The mesoporous silica nanoparticle (MSN) has been utilized as an effective drug delivery carrier, which may have potential to bring therapeutic benefits. Here, we report the first cellular delivery of 26S proteasomes ($\geq 3\text{MDa}$) conjugated with MSN and consequently enhanced proteasome activity which facilitate proteotoxic protein degradation. The surface of MSN was chemically engineered to have nickel ions to tether His-tagged proteasomes. Mammalian proteasomes were affinity-purified from HEK293-pre1-HTBH (tandem His-TEV-Biotin-His tags) cells using streptavidin. BET and BJH analysis show that MSN has enough pore size to contain the proteasome, even in the modified MSN with nickel. The surface charges of proteasomes measured by the zeta potential were converted from positive to negative, indicating that the proteasome with negative charges might be incorporated into the pores of MSN. A pull-down assay showed that the amount of conjugated proteasome was gradually increased in a higher MSN-proteasome mass ratio. There was virtually no cytotoxicity by proteasome-MSN complexes, and internalization of the particles was blocked by chlorpromazine. Proteasomes retained their activity after the endocytosis-mediated cellular uptake although they virtually lost the activity in low pH environments. We furthermore observed that proteasome-MSN complexes specifically targeted tau proteins overexpressed in cultured cell models, without detrimental nonspecific proteolysis. Our results show that not only the modified MSN can serve as an effective carrier for cellular proteasome delivery, but it might provide an effective strategy to reduce the level of proteotoxic proteins in cells, which potentially has therapeutic benefits for various diseases arisen from the deficient activity of UPS.

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장소: 창원CECO

발표코드: **BIO.P-588**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Computational study of HCV inhibitor screening

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About an 180million people worldwide are infected with the hepatitis C virus(HCV) leading cause of chronic liver disease. The complications of chronic HCV infection can be prevented by the combination treatment of pegylated interferon alfa and ribavirin. The standard of care(SOC) is peginterferonalfa-2a/-2b with ribavirin for 48 weeks or 24weeks in patients infected with HCV genotype1 or 2/3.and this treatment can cure half of the patients.But efficiency of the treatment is diverse for each different genotype. And sustained virologic response(SVR) rates shows lower than recent trials reported in the order of 67-69% and 67-75% for the combination of SOC with the protease inhibitors telaprevir and boceprevir in patients with HCV genotype 1 infection. Like this many researcher have an effort to develop new interferons, specifically targeted therapy against HCV,protease inhibitors, polymerase inhibitors, HCV entry inhibitors, host cell targeting inhibitors and etc. to improve the efficiency of antiviral treatment. We predicted the structure of compound using by computational method and selected some compounds among the several compounds by screening test. To confirm the effect of the compounds, we used APC140 cells harboring genotype 2a subgenomic replicon with Renilla luciferase reporter and NPTII selectable marker (from Apath). And we obtained inhibition percent and EC50 from the result of Renilla luciferase assay so we can choose the 8 compound of HCV inhibition. These compounds' range are 0.18~3.85 nM(EC50) and18.0~31.7 %(inhibition percent).

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장소: 창원CECO

발표코드: **BIO.P-589**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Probing the local environments surrounding proteins based on rotational viscosity sensors

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Motion of proteins in the cells depend on nature of the surrounding water structure over a protein. It would be interesting to ask how a protein feels its environment in the cells. Recently, a TIBET-based viscosity probe composed of coumarin and BODIPY moieties has been introduced so that its fluorescence spectra depend on polarity and viscosity of its environment. Upon interaction of proteins with this type of probes, spectrofluorometrical analysis was attempted in terms of the viscosity of the hydration shells surrounding proteins, implying that the local environments of proteins are dramatically heterogeneous.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Whitening effect of medicinal herbs in B16F1 cells

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Reactive oxygen species (ROS) leading to oxidation of lipid, protein and DNA are involved in melanin synthesis. Overproduction of melanin was known to cause melasma, age spot and freckle. The aim of this study is to investigate whitening and antioxidant effects of *Poria cocos*, *Glycyrrhiza uralensis*, *Ulmus macrocarpa* extracts or mixture (PGUE) in B16F1 cells. PGUE decreased DPPH radical, lipid peroxidation and tyrosinase activity. Moreover, PGUE inhibited superoxide dismutase-1 (SOD-1), tyrosinase related protein-1 (TRP-1) and TRP-2 protein expressions. These results suggest that PGUE has whitening effect and antioxidant effect, indicating that they are available for development of whitening cosmetics.

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장소: 창원CECO

발표코드: **BIO.P-591**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of lipid flip-flop

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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. It has long been believed that the exchange of lipids between the inner and outer leaflets of cellular membranes could only occur by a protein-mediated process. However, cells also use passive transport mechanism that facilitates the migration of lipids from one leaflet to the other without proteins. In this study, we aim at the mechanism of lipid flip-flop phenomenon at molecular level. We would like to investigate the effect of charge lipids and unsaturated lipids, which regulate many biological functions and are strongly related to the specific structure of bilayer membrane, 1) whether they cause the lipid disorder to facilitate the flip-flop, 2) how the negative charge is managed to move across the hydrophobic region in the intermediate structure. Our project is still undergoing the first stage, to prepare a well-organized bilayer structure by the Langmuir-Blodgett/Langmuir-Schaeffer method. The structures of lipid bilayers were characterized by X-ray reflectivity and Atomic Force Microscopy.

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장소: 창원CECO

발표코드: **BIO.P-592**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The anti-inflammatory effect of *Scutellaria baicalensis* through control of immune system in Raw264.7 cells

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Immune system protects the body from various diseases caused by bacterial infection and cancer by elimination of internal mutated cells. However, the abnormal immune system induces senile diseases like rheumatoid arthritis through chronic inflammation. Therefore, the purpose of this study is to investigate anti-inflammatory effect of *Scutellaria baicalensis* that contains baicalin as an effective gradient. First of all, MTT assay was carried out to evaluate the cytotoxicity of *Scutellaria baicalensis* hot water extracts (SBWE) in Raw264.7 cells. There was no cytotoxicity below 40 $\mu\text{g}/\text{mL}$ of SBWE. It was also observed that SBWE at 20 $\mu\text{g}/\text{mL}$ inhibited phagocytosis by 20 %. In addition, SBWE at 40 $\mu\text{g}/\text{mL}$ reduced the amount of nitric oxide produced by macrophage by 40 %. Furthermore, the content of tumor necrosis factor-alpha (TNF- α) was decreased in the presence of SBWE a dose dependent manner. SBWE also inhibited the production of interleukin-1 beta (IL-1 β) in a time course experiment. The expression level of cyclooxygenase-2 was remarkably decreased by treatment with SBWE at 20 $\mu\text{g}/\text{mL}$. Therefore, above results could provide an evidence that SBWE influence anti-aging through modulation of immune system.

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발표코드: **BIO.P-593**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Genotype Analysis of Estrogen Receptor α Gene Polymorphisms Associated with Endometriosis in Korean Women

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Endometriosis is common estrogen-dependent gynecological diseases related with interactions of dietary, genetic causes, social and environmental factors. The high prevalence approaches 5-15% in premenopausal women and 30% in infertile women and it is unusually occurred even after the onset of menopause. Estrogen receptor α is a higher affinity for estrogen, it is the predominant form in normal endometrium. Several single nucleotide polymorphisms (SNPs) in the estrogen receptor α gene have been identified. Especially, association between estrogen receptor α polymorphisms (PvuII and XbaI) and breast cancer, Parkinson`s disease, bone mineral density and ovarian cancer have identified. In addition, many epidemiological studies suggested that PvuII and XbaI polymorphisms of estrogen receptor α were associated with increased risk of endometriosis. Our present study, we investigated to association between estrogen receptor α polymorphisms (PvuII and XbaI) and endometriosis by PCR-RFLP method. Our data show that, mutant types of PvuII and XbaI polymorphisms had a high odds ratio compared with the wild type. The odds ratio of CC type of PvuII was 1.429 (OR= 1.429, 95% CI= 0.287-1.121, p-value= 1.000), AG type of XbaI was 1.796 (OR= 1.796, 95% CI= 0.611-5.276, p-value: 0.419), GG type of XbaI was 2.211 (OR= 2.211, 95% CI= 0.185-26.4, p-value: 0.607). In conclusion, we have found differences between cases and controls in the frequencies of the estrogen receptor α gene polymorphisms. However, statistical data is no associated with endometriosis due to small sample size.

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장소: 창원CECO

발표코드: **BIO.P-594**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of ABCG2 Gene Q141K Polymorphism Associated with Gout Patients in Korean

최영훈 조민호 윤일규 김진호 문명진 장원철^{1,*}

단국대학교 화학과 ¹단국대학교 자연과학대학

The gout is the most common cause of inflammatory arthritis in men over the age of 40 years. The prevalence and incidence of gout have increased in recent decades. The Gout is a disorder that is related to deposition of uric acid crystals caused by high level uric acid in the blood. The uric acid is the byproduct of purine nucleotide catabolism. ABCG2 protein included in ATP-binding cassette (ABC) transporters superfamily. The major role of ABCG2 proteins are transport diversity molecule across extra-intra cellular membrane and purine nucleoside analogues. ABCG2 protein is encoded to ABCG2 gene. ABCG2 gene is located in 4q22 and contains 16exons consisting 655 amino acids. Many single nucleotide polymorphisms in ABCG2 gene have identified. Among these SNPs, Q141K (rs2231142) polymorphism of ABCG2 gene was associated with gout in several epidemiological studies. In this study, we investigated to Q141K of ABCG2 gene associated with Korean gout patients by genotyped using the TaqMan assay.

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장소: 창원CECO

발표코드: **BIO.P-595**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Graphene Oxide/Metal Hybrids for Detection of Neurotransmitters

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Graphene oxide (GO) is able to emit photoluminescence (PL) in a visible range, which is susceptible to surroundings. Herein, we have studied the quenching kinetics of GO PL to metals, and designed GO/metal hybrids for the selective detection of neurotransmitters. GO/metal hybrids show different PL responses to several neurotransmitters such as dopamine, norepinephrine, epinephrine and ATP, which enables us to selectively recognize each one. GO/metal hybrids have been successfully applied to detection of a neurotransmitter, norepinephrine, secreted from living cells.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-596**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

RNA aptamer conjugated liposomes (aptamosomes) for efficient and specific delivery of anticancer drug to prostate cancer cell

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건국대학교 생명공학과

Nucleic acid aptamers are potentially useful for targeted delivery of drug-encapsulated liposome particles into cell or tissue of diseases. In this study, we report the novel design of aptamer conjugated liposomes (aptamosomes) that achieves selective strong binding and efficient delivery of anticancer reagent to the prostate cancer cell. Published PSMA RNA aptamer A9 which was well known PSMA (prostate-specific membrane antigen) specific RNA sequences was modified for annealing with complementary DNA linker which was labeled with thiol group and FITC. The modified thiol groups of DNA linkers were conjugated with maleimide group on the surface of PEGylated micelles. These PSMA aptamer conjugated micelles were fused with liposome through post-insertion method. The synthesized aptamosomes of nano scale (90~100 nm) specifically bind to the PSMA-positive LNCaP prostate epithelial cells, not to the PSMA-negative cancer cells. We demonstrated that doxorubicin-encapsulated aptamosomes were significantly more cytotoxic to the targeted LNCaP cells than to the non-targeted cancer cells. In addition, we also confirmed the efficacy of doxorubicin encapsulated aptamosome for targeting the tumors engrafted in nude mice. Thus, the PSMA-specific RNA aptamosomes are useful in delivery of anticancer drugs to the prostate cancer cells with a high specificity in vivo.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **BIO.P-597**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Manipulation of Self-shaping Protein Ribbons by Overlayered Carbon Nanotube Patterns

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The helical coiling of cucumber tendrils and opening of seed pod by transformation of an initially flat pod valve into a helix are self-shaping devices in nature. Inspired of these phenomena induced by different stretching and bending between bilayer of thin films, many researchers used partially cross-linked patterned hydrogels which respond to external stimulation such as temperature and pH for developing self-shaping devices. Our novel approaches are using double microcontact printing (μ CP) and sacrificial layer, which can manipulate the structural deformation of hybrids of hard (carbon nanotube(CNT), polystyrene sulfonate) and soft (fibronectin) materials at an interface. When they are detached from a surface, the soft layer easily contract and bend while the hard layer maintain their shape. Combination of these two dissimilar natures, we could successfully manipulate various 3D structures after we combine two materials in one system. None of structures never been observed since all the basic approaches using μ CP was only focused on the creation of replica on surface. Depending on the angles and contact area between two dissimilar materials, we could generate a whole new 3D nanostructure.

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장소: 창원CECO

발표코드: **BIO.P-598**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of agrichemical residues using cysteamine-modified CdTe quantum dots

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Human health is being menaced by numerous toxic chemicals. Agrichemicals are essential to farm, store and circulate agri-products, though they are highly toxicoids, even the slightest amount, which has lots of different kinds of constituents. Many analytical methods were studied for the detection only one or two kind of pesticides. However, the other types and thousands of agrichemical detection are yet unsatisfactory. Thus, a novel method is needed to detect lots of agrichemicals by a simple and sensitive system. CdTe quantum dots (QDs) were used to sense them by using a fluorescent spectroscopic tool. In this study, measurement of residual agrichemical residues in food was performed using surface-improved CdTe QDs with cysteamine. As a result, this novel method was able to detect many different kinds of agrichemicals at ppb level within only 10 min. Furthermore, we expect a possibility of sensing another type of agrichemicals.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-599**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid sterilization of pathogenic bacteria in the seawater using dielectric barrier device system

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Plasma, a unique state of matter with properties similar to those of ionized gas, is an innovative sterilization method characterized by its low toxicity and operation at room temperature. However, the study of plasma generations through the microbial inactivation in seawater containing the salt is not known and efficient yet. Thus, plasma device generated by a dielectric barrier discharge system was applied to inactivate pathogenic bacteria containing Halobacterium cells that live in seawater. This cleaning system against microbial contamination was investigated the sterilization efficiency by the operation of the plasma device in seawater with various concentrations of sodium chloride, in which the relative sterilization ratios via plasma exposure time. There are some errors by bubbles generated in the machine operation; however, the sterilization effect of near 80% was obtained within 20 min in all experiments. These results support the use of plasma for the aquacultural industry for removal of organic contaminants in seawater. It is anticipated that the plasma sterilization has a potential to improve the productivity of sea-food industry and to keep healthy environment in seawater.

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장소: 창원CECO

발표코드: **BIO.P-600**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid Diagnosis of Tuberculosis Using Quantum Nanoparticles and Recombinant Fusion Proteins

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중앙대학교 화학과

The most effective Tuberculosis control strategy will prevent the spread of tuberculosis disease by treatment of its patients and early-stage detection. Therefore, an ideal tuberculosis diagnosis is fast and cost-effective, whereas does not require complex equipment and facilities should be able to use easily. It must be performed with the best conditions to measure antigen-antibody interactions. However, there are several problems to overcome and to measure the benefits of the tuberculosis antigens. We detected target antigens, CFP-10 and Ag85, which are known specific secretory antigens from Mycobacterium tuberculosis. M. tuberculosis in culture media secretes a large quantity of toxic materials to human in the early preliminary study, and they can be proven to be detected in the urine and phlegm. Sandwich-assay method based on fluorescent nanoparticles can be used by the amplification effect of the detection signal using quantum nanoparticle. Quantum dots (QDs) are nanometer scale particles as semiconducting materials, traditionally chalcogenides of metals, which range from 2 to 10 nanometers in diameter. We studied for the optimization of antigen-antibody interaction using QDs and the production of recombinant fusion proteins as their antibodies. As a result, we developed a rapid diagnosis method for tuberculosis to detect multiple antigens from clinical specimens by using nanomaterials and its composites.

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장소: 창원CECO

발표코드: **BIO.P-601**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Combinatorial assay with luciferase and gold nanoparticle for detection of agrichemicals

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Agrichemicals are important substances to boost agricultural productivity-increase crop yield in the modern society. However, the residues of agrichemicals could cause serious health problems for human even at very low concentrations. Conventional instrument-based methods are the accurate quantitative analysis, however, they must cost a lot of money and are bulky and time-consuming. Thus, it is important to induce a simple and sensitive method for on-site detection of agrichemical residues. The luciferase is able to detect various agrichemicals because it has an inhibition effect against agrichemicals on the luciferase activity. Luciferase requires a luciferin substrate, ATP, oxygen, and Mg²⁺ ion to produce bioluminescent light. The catalytic reaction of luciferase alters a luciferin substrate and ATP to oxyluciferin and AMP. Gold nanoparticles (AuNPs) have been used for applications in biosensors due to their biocompatibility, outstanding biophysical and visible spectroscopic properties. Metal ions change the color and UV/Vis absorbance of AuNPs, whereas, the stability of AuNPs is preserved by ATP from the effect of metal ions. Thus, in the presence of agrichemicals, the catalytic reaction of luciferase do not occur, and then AuNPs are remained with its stability and color by ATP. On the other hand, when the agrichemicals do not exist, AMP produced by catalytic reaction of luciferase makes their color-change of AuNPs because of their aggregation. This rapid, sensitive and easy method is able to detect many types of agrichemicals.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-602**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and evaluation of an engineered molecule as a tool for the proteomic study

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대구대학교 과학교육학부/화학교육과 ¹대구가톨릭대학교 제약산업공학과

A novel substance has been designed, synthesized, and evaluated as a tool for the proteomic study. This new molecule consists of a biotin moiety at the one end and an azide-reactive chemical tag at the other end with a cleavable linker placed between these two entities. Biotin molecule is one of the most popular epitope tags for the detection and enrichment of molecules of interest, because of its strong interaction with streptavidin. However, their strong binding also exerts a negative effect when the bound biotinylated molecules are eluted from the streptavidin solid support. Harsh conditions required for interrupting the strong biotin:streptavidin interaction to release the bound molecules from the solid support, can lead to decomposition of the molecules, resulting in low product recovery. In order to tackle this problem, an engineered molecule, wherein a disulfide linker is inserted in the middle of the molecule to connect a biotin tag and an azide-reactive chemical tag, has been synthesized and examined for its utility as a tool in the proteomic study.

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장소: 창원CECO

발표코드: **BIO.P-603**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of the phosphorylation sites of protein kinase C delta

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Protein kinase C (PKC) is a multi-gene subfamily of serine-threonine kinases comprising of at least ten isoforms which play important roles in multitudes of cellular processes such as proliferation, differentiation, growth, and apoptosis. On the basis of the structural difference in the regulatory domain of the isoforms, PKC is divided into three classes (classical, novel and atypical PKCs). PKC delta is one of the important isoforms among the PKCs in regulating various cellular processes including cell survival and apoptosis. Studies have shown that activation of PKC delta is correlated with apoptosis in various cell types depending upon various stimuli. Phosphorylation of Thr505, Ser643 and Ser662 is crucial in activation of PKC delta. Furthermore, phosphorylation of tyrosine residues, in particular, that of Tyr311 is related with PKC delta activation and induction of apoptosis. We mutated Serine 662 to Alanine and generated hydrophobic motif phosphorylation-deficient mutant of PKC delta and studied the effect of this mutation in inducing apoptosis in L929 murine fibroblasts. We report that this mutation renders PKC delta apoptotically more active.

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발표코드: **BIO.P-604**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Single Molecule Optical Analysis of Various Yeast Mitochondria DNA Sizes

최소정 김용균 이진용 조규봉*

서강대학교 화학과

Saccharomyces cerevisiae is a yeast strain used for making wine and bread. Since it is a model organism for the study of eucaryotes, its genome has been fully sequenced that there are 16 chromosomes and a mitochondrial genome. However, a couple of previous studies reported that they found more sequences from mitochondrial DNA that was not previously sequenced. In addition, some other studies showed that mitochondrial DNA did not have the same size by using single DNA molecule experiment. Thus far, it is not clear how mitochondrial DNAs are different from each other in a yeast cell. Here we present their difference by using single molecule DNA analysis such as Optical Mapping, in which whole mitochondrial genomic DNAs are elongated and immobilized on the positively charged surfaces within a microfluidic device and digested by restriction enzyme such as EagI. Restriction enzyme digested barcode-like DNA patterns provides the information how mitochondrial genomic DNAs are different from each other.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **BIO.P-605**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single DNA Molecule Analysis for UV Resistant *Escherichia Coli*

김지수 이진용 조규봉*

서강대학교 화학과

Ultraviolet (UV) radiation is well known to cause DNA damages such as single strand breaks, and double strand breaks due to pyrimidine dimer. Interestingly, some species of bacteria have radiation resistance such as *deinococcus radioduran*. Recently, Harris et al developed four kinds of UV-resistant *E. coli* strains mutated from K-12 MG1655 strain. To characterize what makes these strain UV enduring, they used Pulse Field Gel Electrophoresis (PFGE) and sequencing. They reported recovery of UV-induced damage and they interpreted their result that UV-resistance is due to enhanced DNA repair mechanism. However, we suspect that DNA itself may have the characteristic of UV-resistance. Thus, here we performed single DNA molecule experiment to identify the resistance mechanism whether DNA itself is resistant or not by observing single-stranded breaks on the genomic DNA.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-606

발표분야: 유기화학

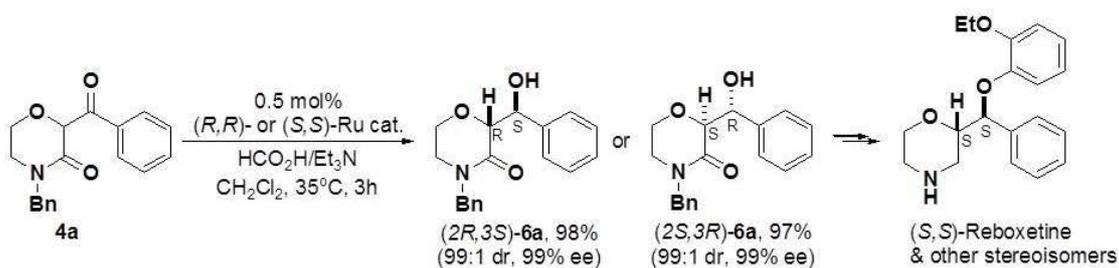
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dynamic Kinetic Resolution Based Asymmetric Transfer Hydrogenation of 2-Benzoyl-Morpholinones and Its Use in Concise Stereoselective Synthesis of All Four Stereoisomers of the Anti-depressant Reboxetine

손세미* 이현규¹

한국기술연합대학원대학교 의약및 약품화학¹ 한국화학연구원 한국화학물은행

Dynamic kinetic resolution driven, asymmetric transfer hydrogenation reaction of 2-benzoyl-morpholin-3-ones proceed efficiently to give the corresponding (2R,3S)- or (2S,3R)-2-(hydroxy-phenyl-methyl)-morpholin-3-ones with excellent level of diastereo- and enantio-selectivity, with simultaneous control of two contiguous stereogenic centers in a single step. This process is employed to prepare all four stereoisomers of the anti-depressant reboxetine



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-607**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An expedient synthesis of oxindole dimers by direct oxidative dimerization of oxindoles

이현주 임진우 김고훈 김재녕*

전남대학교 화학과

Oxindole dimers have been used as intermediates in the synthesis of various cyclotryptamine alkaloids. Thus, extensive studies have been carried out for the preparation of oxindole dimers. Rodrigo and co-workers reported a dimerization of oxindole anion with carbon tetraiodide *via* a radical anion chain mechanism. Inada and Morita reported an oxindole dimerization using cobalt(II) Schiff's base complexes. Some indirect synthesis of oxindole dimers has also been reported. An efficient direct synthesis of oxindole dimers was carried out from 3-substituted oxindoles *via* an oxidative dimerization using manganese(III) acetate or copper acetate/silver acetate system.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-608**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed domino cyclization (5-*exo*/3-*exo*), ring-expansion by palladium rearrangement, and aromatization: an expedient synthesis of 4-arylnicotinates from Morita-Baylis-Hillman adducts

김고훈 김세희 이현주 김재녕*

전남대학교 화학과

Poly-substituted pyridines are an important class of compounds due to their abundance in biologically important natural substances and their usefulness as synthetic intermediates in organic synthesis. Especially, the synthesis of functionalized pyridines with a carboxylic acid moiety at the 3-position (nicotinic acid derivatives) has received much attention due to their biological importance. The Morita-Baylis-Hillman (MBH) adducts have been used for the synthesis of various biologically important substances and synthetic intermediates. Various efficient protocols for the synthesis of pyridine and quinoline derivatives from the MBH adducts have also been developed by us and other groups. Various 4-arylnicotinate derivatives were synthesized *via* a palladium-catalyzed cascade reaction of *N*-(2-bromoallyl)-*N*-cinnamyl tosylamides in a one-pot in good yields. The reaction involved a domino 5-*exo*/3-*exo* carbopalladations, ring-expansion by palladium rearrangement, and an aromatization process.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-609**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed arylation of methyl 2-(acetoxymethyl)acrylate: a convenient synthesis of rearranged Morita-Baylis-Hillman acetates

김고훈 임진우 이현주 김재녕*

전남대학교 화학과

Very recently, a palladium-catalyzed chelation-assisted arylation of allyl acetate has been examined extensively to provide cinnamyl acetate *via* the selective β -H elimination process instead of β -acetoxy elimination. Many research groups have reported the arylation of allyl acetate with various arene sources; however, there is no precedent reports on the arylation of allyl acetate bearing an ester group at the 2-position *via* the selective β -H elimination process, to the best of our knowledge. Palladium-catalyzed arylation of methyl 2-(acetoxymethyl)acrylate has been carried out successfully with aryl iodides to afford the primary acetates of Morita-Baylis-Hillman adducts in good yields with high stereoselectivity under mild conditions (50 °C).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-610**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed arylation of α,β -unsaturated Weinreb amides

김고훈 김세희 임철희 김재녕*

전남대학교 화학과

Weinreb amides (*N*-methoxy-*N*-methyl amide) have been widely used as versatile synthetic intermediates in organic synthesis since their original discovery by Nahm and Weinreb. Weinreb amides could react with Grignard reagent, organolithium reagents, and LiAlH_4 to afford ketones or aldehydes in high yield *via* stable metal-chelated intermediates. Among the Weinreb amides, α,β -unsaturated analogs have received much attention because of their synthetic applications in organic synthesis and their interesting biological activity. Palladium-catalyzed arylation of α,β -unsaturated Weinreb amides has been examined to obtain β -aryl- α,β -unsaturated Weinreb amides. The chelation between the palladium center of an arylpalladium intermediate and Weinreb amide moiety facilitated both coordination and insertion steps.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-611**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2,2'-dipyrryl ketones from pyrrole-2-carboxylic acids with trifluoroacetic anhydride

김세희 임진우 유진 김재녕*

전남대학교 화학과

Dipyrryl ketone derivatives have been studied extensively due to their synthetic usefulness as precursors for the synthesis of porphyrin derivatives, Oxophlorin derivatives, and 10-oxo-Bilirubin. Dipyrryl ketones have been prepared usually by oxidation of the corresponding dipyrrylmethanes with cerium(IV) ammonium nitrate (CAN). Phosphoric acid-promoted acylation of pyrroles with mixed anhydride derived from pyrrole carboxylic acid has also been reported. We disclosed an efficient synthesis of 2,2'-dipyrryl ketones from pyrrole-2-carboxylic acids using TFAA. Simultaneous generation of both mixed anhydride and 2-unsubstituted pyrrole (*via facile* decarboxylation with *in-situ* generated TFA) made their cross reaction (intermolecular Friedel-Crafts acylation) possible and efficient.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-612**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient synthesis of 5-phosphorylated uracil derivatives: oxidative cross-coupling between uracil and dialkyl phosphite

김세희 임철희 김고훈 김재녕*

전남대학교 화학과

The synthesis of 5-substituted uracil and its derivatives has received much attention due to their diverse applications in pharmaceutical and molecular genetics. Among them the phosphorylation at the 5-position of uracil nucleus also received much attention. Most of the reported synthesis of these compounds has used a sequential halogen-metal exchange reaction and phosphorylation with phosphoryl chloride. However, the yields of phosphorylated products were very low (20-38%). Although a direct oxidative functionalization at the 5-position of uracil with various radical species has been reported, a direct phosphorylation with dialkyl phosphite has not been known, to the best of our knowledge. An efficient synthesis of 5-phosphorylated uracil derivatives has been carried out *via* an oxidative cross-coupling reaction between uracil derivatives and dialkyl phosphites in the presence of $\text{Mn}(\text{OAc})_3$ in AcOH .

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-613**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of poly-substituted benzene derivatives *via* [3+3] annulation protocol from Morita-Baylis-Hillman adducts

임진우 김세희 유진 김재녕*

전남대학교 화학과

Morita-Baylis-Hillman adducts have been used for the synthesis of various aromatic compounds including poly-substituted benzenes and phenols. The reaction of MBH adduct and 1,3-dimethylacetone dicarboxylate has been used for the synthesis of poly-substituted phenols bearing 2,6-dicarboxylates *via* the [3+3] annulation protocol. Glutaconates have been used in organic synthesis in order to introduce a three-carbon unit bearing two carboxylates at the 1,3-position. In these respects, the reaction of MBH adduct and diethyl glutaconate and MBH adduct provided an efficient preparation method of poly-substituted benzene derivatives bearing 1,3-dicarboxylates.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-614**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient synthesis of poly-substituted phenols and pyridines from Morita-Baylis-Hillman acetates and diethyl oxalacetate

유진 김고훈 김세희 김재녕*

전남대학교 화학과

Morita-Baylis-Hillman (MBH) adducts have been used for the synthesis of various aromatic compounds including phenols and pyridines. Poly-substituted phenols and pyridines are important due to their abundance in nature and biologically active substances. Various phenol derivatives were synthesized in a one-pot reaction from MBH acetates and sodium diethyl oxalacetate *via* a [4C+2C] cyclization protocol. In addition, some pyridine derivatives could also be synthesized using the same starting materials, by isolating the S_N2' reaction intermediate and performing the cyclization with NH₄OAc.

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장소: 창원CECO

발표코드: **ORGN.P-615**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An expedient synthesis of cinnamyl fluorides from Morita-Baylis-Hillman adducts

임철희 김세희 임진우 김재녕*

전남대학교 화학과

In contrast to the easy preparation of MBH bromides, the synthesis of MBH fluorides afforded a mixture of the corresponding primary and secondary fluorides. Ley and co-workers reported the fluorination of MBH adduct with DAST (diethylaminosulfur trifluoride), and a mixture of a primary and secondary allylic fluorides has been obtained. Brown and co-workers also examined the fluorination of MBH adduct, and they obtained secondary fluoride as a major product along with primary fluoride as a minor (5-10%). We disclosed an efficient synthesis of primary Morita-Baylis-Hillman fluorides. The synthesis was carried out *via* the bromination of a MBH adduct and the following fluorination with TBAF in a mixed solvent (*t*-BuOH/THF).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-616**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient synthesis of *o*-terphenyls from Morita-Baylis-Hillman adducts of cinnamaldehydes: a consecutive bromination, Wittig reaction, 6π -electrocyclization, and an aerobic oxidation process

임철희 김고훈 유진 김재녕*

전남대학교 화학과

Various chemical transformations of the Morita-Baylis-Hillman (MBH) adducts have been studied extensively during the last two decades. Among them the synthesis of aromatic compounds including poly-substituted benzenes has received a special attention. Very recently, we reported a synthesis of *p*-terphenyls by a Diels-Alder reaction of 1,3-diene that was prepared from MBH adduct of benzaldehyde. As a continuous work, an efficient synthetic method of *o*-terphenyls was developed from Morita-Baylis-Hillman adducts. The synthesis was carried out *via* a sequential bromination of MBH adducts, Wittig reaction with various aldehydes, 6π -electrocyclization, and a base-mediated aerobic oxidation process.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-617**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereoselective synthesis of benzofulvenes *via* a palladium-catalyzed cyclization of 1,3-dienes derived from Morita-Baylis-Hillman adducts

임철희 김고훈 임진우 김재녕*

전남대학교 화학과

Fulvene, benzofulvene and related derivatives have been used as building blocks for the preparation of metallocene catalysts, starting materials of polymers, discotic liquid crystals, and biologically interesting compounds. There have been reported numerous synthetic methods of fulvene derivatives including palladium-catalyzed synthesis. A facile synthesis of benzofulvenes was carried out starting from the Morita-Baylis-Hillman adducts of 2-bromobenzaldehyde. The synthesis was carried out *via* the sequential bromination, Wittig reaction with aldehyde, and Pd-catalyzed intramolecular Heck reaction. The stereochemistry of benzofulvenes was dependent on the reaction condition, especially on the kinds of base and reaction time, and the substituent of starting materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-618

발표분야: 유기화학

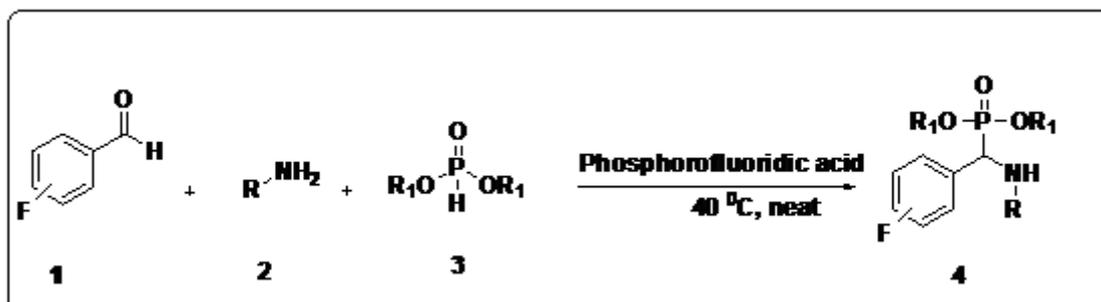
발표종류: 포스터, 발표일시: 수 16:00~19:00

Phosphorofluoric acid catalyzed three-component synthesis of α -amino phosphonates in one-pot

현동균 Atar Amol Balu 정연태*

부경대학교 이미지시스템공학과

A simple, efficient, and general method has been developed for the synthesis of fluorine containing α -aminophosphonates through a one-pot reaction of fluorine containing aromatic aldehydes with amines and phosphite in the presence of phosphorofluoric acid as a catalyst. As a consequence, efficient synthesis of novel fluorine containing derivatives of α -aminophosphonates was observed within short time periods in high yields under solvent-free reaction condition.



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발표코드: ORGN.P-619

발표분야: 유기화학

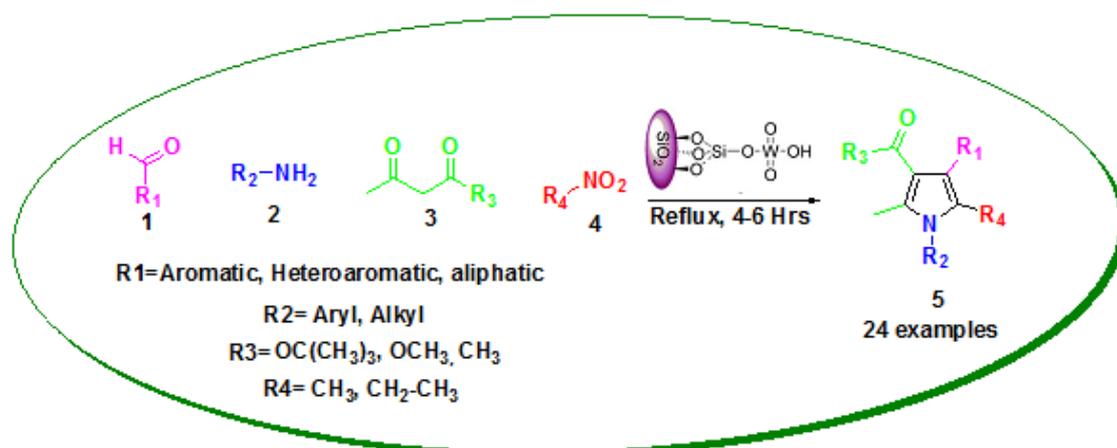
발표종류: 포스터, 발표일시: 수 16:00~19:00

Silica Supported Tungstic Acid-Catalyzed Four-Component Coupling Reaction of 1,3-Dicarbonyl Compounds, Amines, Aldehydes, and Nitroalkanes: A Simple and Direct Synthesis of Functionalized Pyrroles

Atar Amol Balu 정연태*

부경대학교 이미지시스템공학과

An efficient, high yielding, and expeditious method has been developed for the synthesis of diversity oriented pyrrole derivatives via a four component, one-pot cyclocondensation reaction of amines, aldehydes, α -methylene ketones and nitroalkanes using Silica supported tungstic acid as a heterogeneous catalyst for the first time. The scope of the domino reaction is successfully explored toward synthesis of highly aryl-substituted pyrroles. The reaction was conveniently promoted by Silica supported tungstic acid and the catalyst could be recovered easily after the reaction and reused without any loss of its catalytic activity. The advantageous features of this methodology are high atom-economy, operational simplicity, shorter reaction time, convergence, and facile automation.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-620

발표분야: 유기화학

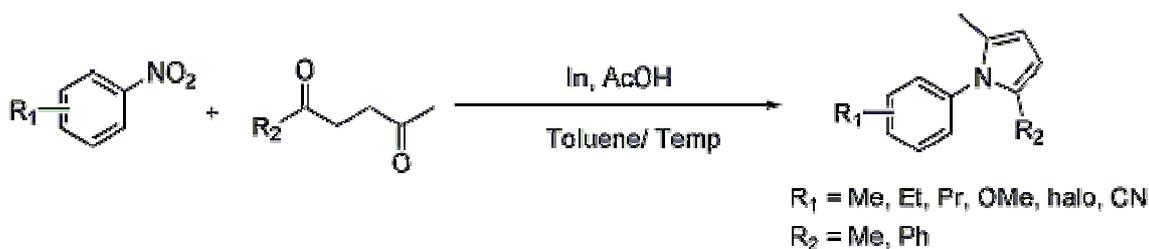
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot pyrrole synthesis via reduction-triggered intermolecular cyclizations of nitroarenes with 1,4-diketones

이현승 김병효*

광운대학교 화학과

Indium has been used in organic synthesis because it has reasonable reactivity, low toxicity and stability in the air or oxygen at room temperature. The first ionization potential of indium (5.8 eV) is similar to that of lithium and sodium, which makes indium as an effective single electron transferring reagent. Pyrroles have utilized in many research areas because of their broad applications as conducting polymers, pharmaceutical agents, and building blocks in natural products such as chlorophyll or hemoglobin. Thus, we examined one-pot intermolecular synthesis of nitroarenes with diketones toward pyrroles using indium in this study. To find out an optimized reaction condition, we tested various heterocyclizations of nitrobenzene under different conditions. As a result, nitroarene (1 equiv) with 1,4-diketone (1 equiv, 2,5-hexadione, 1-phenyl-1,4-pentanedione) in the presence of indium (4 equiv)/acetic acid (10 equiv) in toluene at 80 °C or reflux produced excellent yields of pyrroles (80-97%) mostly. In the case of *o*- or *p*-nitrobenzotrile, reaction rate was slow down with the low yield (40-70%) probably because of resonance stabilization effect of nucleophilic intermediates. In addition, we tried to elucidate the reaction mechanism. Plausible mechanism via SET reaction was proposed after various control experiments.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: ORGN.P-621

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New heteroleptic Ru(II) complexes containing 4,4'-bis(styryl)-2,2'-bipyridine ligand for electrochemiluminescence

박세주 김정옥 강창훈¹ 이원용^{1,*} 탁정애^{2,*} 김병효^{*}

광운대학교 화학과 ¹연세대학교 화학과 ²한양대학교 자연과학대학/화학과

Electrogenerated chemiluminescence (ECL) has been recognized as a sensitive and selective detection tool in life science. Recently, we have continuously studied on relationship between the ligand structures and ECL properties with newly prepared Ru(II) complexes. Ru(bpy)₃²⁺ based ECL reactions has been most widely studied because of its characteristics such as its chemical stability, intensity of luminescent emission and excited state reactivity, etc. In this study, we prepared several ligands and synthesized a different kind of new heteroleptic ruthenium(II) complexes using those ligands such as 4,4'-bis(styryl)-2,2'-bipyridine ligand and the other ligands we prepared. Then a series of novel Ru(II) complexes was synthesized, *i.e.* [Ru(4,4'-bis(styryl)-2,2'-bipyridine)₂ L]²⁺(PF₆⁻)₂ (L = 4,4'-dicarboxy-2,2'-bipyridine, 4,7-dicarboxy-1,10-phenanthroline, 4,7-bis(*E*-carboxyvinyl)-1,10-phenanthroline, 4,4'-bis(*E*-carboxyvinyl)-2,2'-bipyridine etc). Some complexes were synthesized in ethyleneglycol solvent while others were done in DMF solvent. When ethyleneglycol was used, ethyleneglycol was participated for esterification with acid-moiety of the ligand in complexes during the reaction. Spectroscopic properties of synthesized new Ru(II) complexes were studied in detail. Those Ru(II) complexes exhibited intense band at around 480 nm. Luminescence bands of those were observed at round 700 nm depending on the nature of the ligand. In addition, the ECL intensity was determined and some of those were higher than that of [Ru(bpy)₃]²⁺.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-622**

발표분야: 유기화학

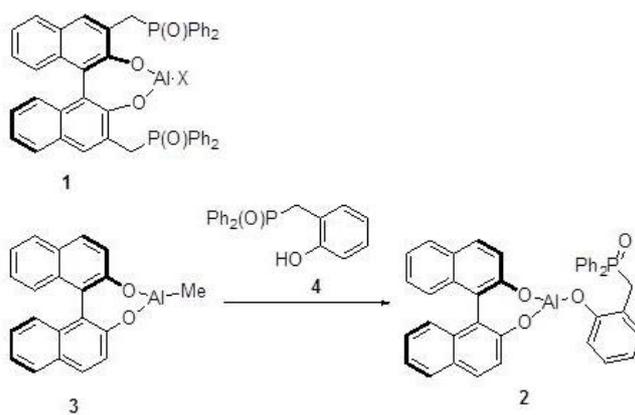
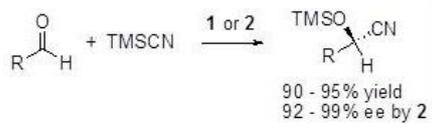
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Assembled Chiral Bifunctional Catalyst by a Metal Coordination Interactions: Application to the enantioselective Cyanosilylation

이기성 정낙철*

고려대학교 화학과

Bifunctional catalysts are among subjects of intensive research in recent years. These are considered as the mimic of the active sites of many enzymes. Among many successful examples reported so far, catalyst 1 bearing a pair of Lewis acid/Lewis base (LA/LB) is one of the notable one and exhibited its high efficiency in an asymmetric cyanosilylation of carbonyl compounds.¹ However, in most conventional bifunctional catalysts, including 1, a pair of Lewis acid/Lewis base (LA/LB) moieties were integrated into one molecule through covalent bonds. Under these circumstances, the trial to identify the catalyst having the best activity with the optimal proximity between Lewis acid and Lewis base moieties to avoid internal chelation would be a labor-intensive maneuver. Recently, a highly modular approach to assemble the LA/LB catalyst by a self-assembly of each part through the metal-organic coordination was devised and reported in the literature.² We also envisioned that a new bifunctional catalyst 2 could be obtained by self-assembly of binol-aluminum 3 and 2-methylenediphenylphosphine oxide phenols 4 in a modular manner. This method based on the self-assembly was so efficient in preparing the catalyst and could be done quickly. Especially, the optimization to identify the best catalyst could be carried out in a combinatorial manner. Catalyst 2 found by this method turned out to be an excellent catalyst for the enantioselective cyanosilylation of carbonyl. (Scheme 1) The details of the preparation of the catalyst by a modular self-assembly and the application of it to the enantioselective catalytic reaction will be described.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-623**

발표분야: 유기화학

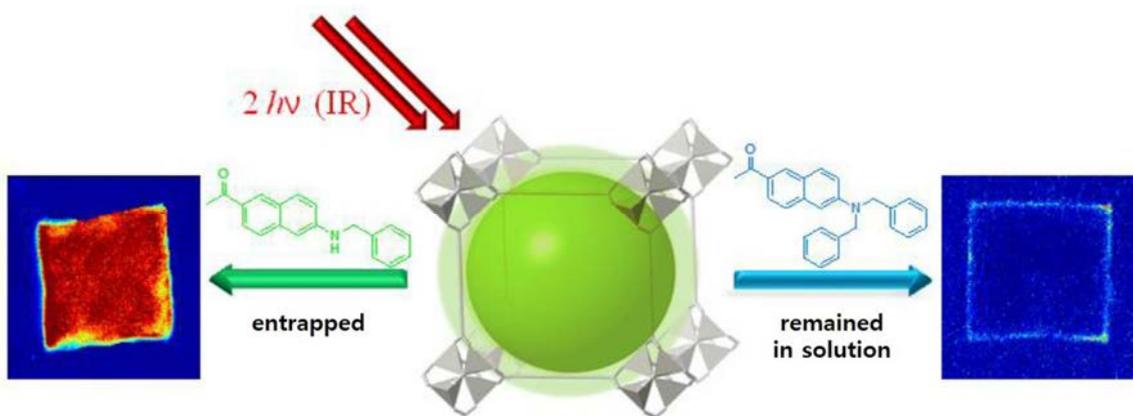
발표종류: 포스터, 발표일시: 수 16:00~19:00

Assessing the guest-accessible volume in MOF by two-photon fluorescence microscopy

신성민 이미선 정낙철*

고려대학교 화학과

Metal-organic frameworks (MOFs) are constructed using a modular approach, from organic links and metal ion units, controlling both their architecture and chemical functionality. The use of MOFs as a heterogeneous catalyst or a container, preferably asymmetric, is particularly intriguing, because there are serious demand for the selective preparation and/or separation of optically pure compounds. Despite impressive progress in the development of MOF catalysts, including chiral MOF for the enantioselective reaction, issues arose regarding chirality attenuation during the assembly of chiral MOF, and regarding the spotting the reaction site, whether on the surface or inside the MOF.¹ For responding the latter properly, it is important to know whether the porous materials have proper guest-accessible volume in them. Thus quick but direct methods to assess the void space of any porous materials are highly desirable, and it is envisioned that two-photon microscopy (TPM) could satisfy this demand. We have successfully devised a quick method to assess the guest-accessible volume of any porous materials in solution by taking advantage of two-photon fluorescence microscopy. With a toolbox of dyes, 2-amino-6-acyl naphthalene derivatives, having various sizes, the guest-accessible volume in three MOFs (MOF-5, KUMOF-2, and KUMOF-1, which had aperture diameters of 9.248 Å, 12.107 Å, and 16.018 Å) were determined. All data examined afforded an excellent correlation between the guest-accessible volume and the entrapped dye size. The details will be discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-624**

발표분야: 유기화학

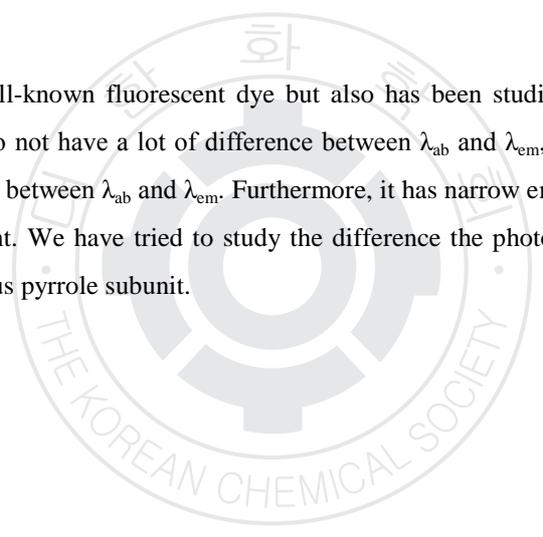
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, Synthesis and Characterization of BODIPY Derivatives

김철용 이정태*

한림대학교 화학과

BODIPY is not only a well-known fluorescent dye but also has been studied as a solar cell recently. Usually fluorescent dyes do not have a lot of difference between λ_{ab} and λ_{em} , given that, BODIPY has a relatively large Stokes-shift between λ_{ab} and λ_{em} . Furthermore, it has narrow emission bandwidth and high molar absorption coefficient. We have tried to study the difference the photophysical properties among these BODIPYs with various pyrrole subunit.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-625**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Enantioselective Synthesis of 2-Amino-4H-chromene Derivatives

서창원 이현아 김대영*

순천향대학교 화학과

The chromene core is present as a characteristic structural motif in a large number of natural products and biologically active molecules. We wish to report a binaphthyl-modified squaramide-catalyzed highly enantioselective Michael addition of 1,3-cyclohexanedione to benzylidenemalonitriles, to afford biologically valuable 2-amino-4H-chromene derivatives. This catalytic reaction at a low catalyst loading (0.5 mol%) was effective to give the Michael/cyclization adducts with high yields and excellent enantioselectivities (up to 99% ee) under mild reaction conditions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-626**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Friedel-Crafts Reaction of Naphthol with β , γ -Unsaturated α -Keto Esters Catalyzed by Binaphthyl-Modified Squaramide

이현아 김대영*

순천향대학교 화학과

The chromane and benzopyrane structures are present as a characteristic structural motif in a large number of natural products that possess a broad array of biological activities such as antimicrobial, antiviral, antitumor, and central nerve system activity. In this presentation, we wish to report organocatalytic enantioselective FC reaction of 1-naphthol to β , γ -unsaturated α -keto esters to afford biologically valuable chromane derivatives. The binaphthyl-modified squaramide organocatalyst showed excellent catalytic activity for this reaction to afford 3 in high yields with excellent enantioselectivities (up to 97% ee) under mild reaction conditions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-627**

발표분야: 유기화학

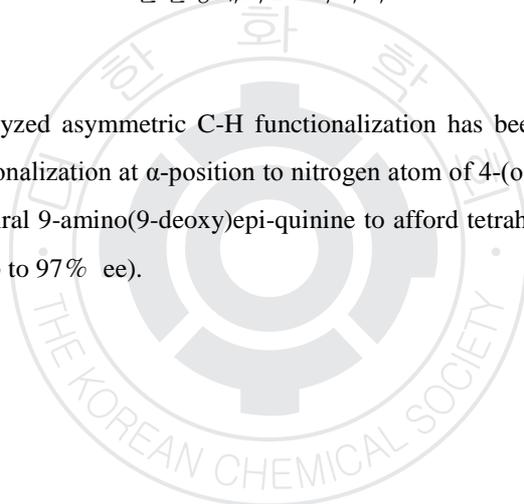
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Enantioselective Synthesis of Tetrahydroquinolines via 1,5-Hydride Transfer/Cyclization Sequences

김미현 김대영*

순천향대학교 화학과

Chiral primary amine catalyzed asymmetric C-H functionalization has been achieved. In this process, enantiotopic Csp³-H functionalization at α -position to nitrogen atom of 4-(*o*-(dialkylamino)phenyl)but-3-en-2-one is activated by chiral 9-amino(9-deoxy)epi-quinine to afford tetrahydroquinine derivatives with high enantioselectivities (up to 97% ee).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-628**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Oxidative Enamine Catalysis/1,5-Hydride Transfer/Cyclization Sequences: Enantioselective Synthesis of Tetrahydroquinolines

김미현 김대영*

순천향대학교 화학과

The development of C-C bond formation via C-H bond activation has become an area of intense interest in synthetic organic chemistry. Such reactions offer practical methods for the construction of structurally complex and biologically active organic molecules with atom- and step economy. The first organocatalytic enantioselective intramolecular oxidative enamine catalysis and 1,5-hydride transfer/ring closure reaction is described. This neutral reaction cascade allows for the efficient formation of ring-fused tetrahydroquinolines in high enantioselectivities.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-629**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Reduction of Chalcones and NMR Studies of Their Products

한인숙* 정은정¹

강원대학교 과학교육학부 ¹강원대학교 화학과

A series of chalcones, that is, α,β -unsaturated ketones, has been reduced selectively by Et₃SiH in the solution of acetic acid and trifluoroacetic acid to give the derivatives of 1,3-diphenylpropanone. On the other hand, the enone functional group was reduced to propane-1,3-diyl group in the absence of acetic acid to form 1,3-diarylpropane compounds from the chalcones. The m- and p-nitro substituted chalcones behaved exceptionally to the reducing conditions, forming 1-propanol derivatives. The ¹H and ¹³C NMR spectra of the series of 1,3-diarylpropanones and 1,3-diarylpropanes were studied in terms of substituent chemical shift effect to examine the possible correlation of the chemical shift values with the Hammett substituent constants.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-630**

발표분야: 유기화학

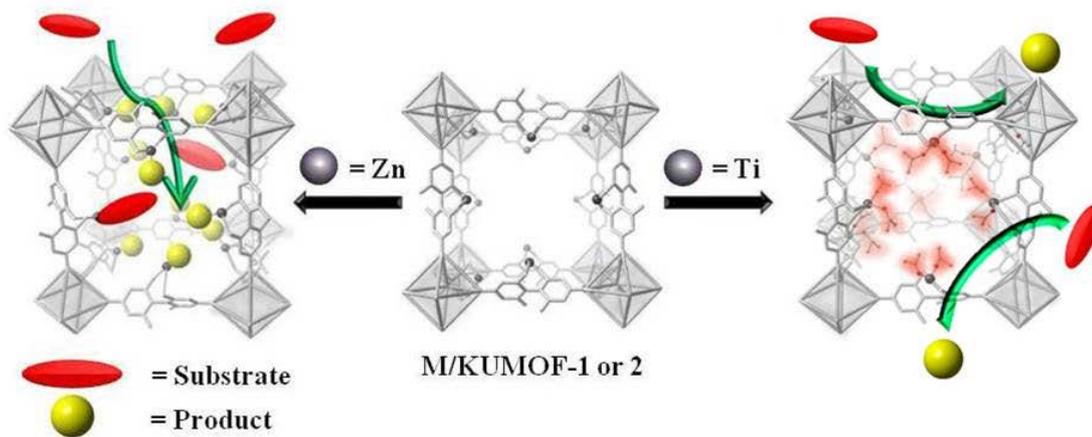
발표종류: 포스터, 발표일시: 수 16:00~19:00

Spotting of a reaction site in heterogeneous catalytic reaction by MOF

이미선 신성민 이혜민 정낙철*

고려대학교 화학과

Metal-organic frameworks (MOFs) are constructed using a modular approach, from organic links and metal ion units, and the use of MOFs as a heterogeneous catalyst or a container, preferably asymmetric, is particularly intriguing, because there are serious demands for the selective preparation and/or separation of optically pure compounds. There has been impressive progress in the development of MOF catalysts, including chiral MOF for the enantioselective reaction. We have also developed enantioselective heterogeneous catalysts based on chiral MOF. However, there is an issue seriously challenged by the researcher outside MOF field; questioning the real site of the reaction taking place. This issue is much more important than one might imagine because, if the most reactions are taking place on the surface of crystals with leaving the active sites inside MOF untouched, the legitimacy to use MOF as a heterogeneous catalysts would be damaged seriously. It is hard to justify the real advantages of MOF-based heterogeneous catalysts over the conventionally imbedded catalyst on solid supporter. Most researchers in this field have tried to provide the evidence for that the reaction utilized all the potential catalytic sites inside MOF. The most commonly employed approach, maybe the only as far as we know, is the comparison of reaction rates depending on the substrate size. But, we found that this approach is inappropriate. As long as the examined reactions are catalytic, the comparison data of reaction rates depending on the substrate size are not relevant to discern claims between the reactions taking place inside the MOF or on the surface. We have shown two distinctive cases in this poster. One has to use the entire reaction sites in the crystals, a case with Zn/KUMOF-1, and another uses only a portion of catalytic sites residing on the surface, a case with Ti/KUMOF-1. The conclusions were withdrawn based on the newly developed TPM study and chemical evidence. Full details will be discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-631

발표분야: 유기화학

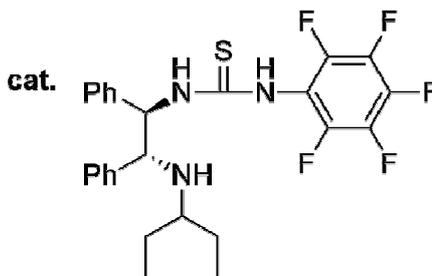
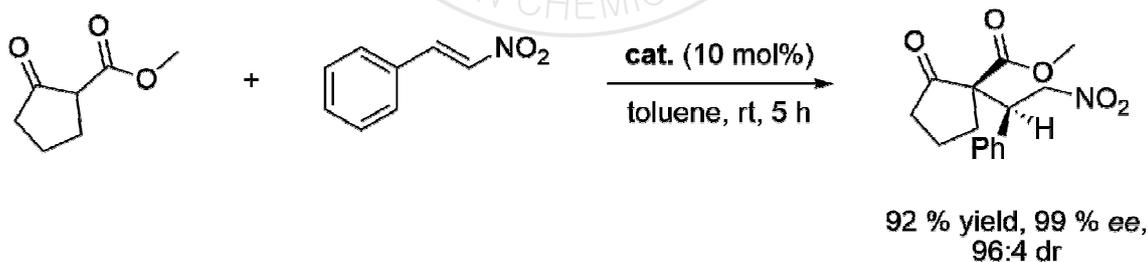
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Organocatalytic Michael Addition Reactions Using Chiral DPEN-derived Thioureas

이민지 이민호 하덕찬*

고려대학교 화학과

The Michael addition is widely recognized as one of the most general and versatile methods for formation of C-C bonds in organic synthesis. Efforts aimed at achieving asymmetric Michael addition by using powerful and environmentally friendly organocatalysts have been explored intensively in recent years. We synthesized hydrogen bonding catalysts bearing a thiourea moiety and an alkylamino group on a chiral scaffold. Among them, bearing pentafluorobenzene and 3-pentylamino group was revealed to be highly efficient for the asymmetric Michael of α -keto ester compounds to nitroolefins. The Michael adducts were obtained with high enantio- and diastereoselectivity.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-632**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of (10-(naphthalen-1-yl)-9-(phenanthren-9-yl)anthracen-2-yl)triphenylsilane

장재영 정용석*

충북대학교 화학과

청색발광은 풀칼라를 위한 전자발광 소자로의 응용에 매우 중요하다. 청색발광소자의 발광물질로서의 가능성을 확인하기 위하여 anthracene 의 2 번 위치에 triphenylsilyl group 을 9 번 위치에 phenanthrenyl group , 10 번 위치에는 naphthyl group 을 도입하였으며, 합성한 새로운 anthracene 유도체의 광학적·전기적 특성평가를 하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-633**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot, chemoselective and consecutive functionalization of bi-functional molecules using 2-substitued-pyridazinones

김보람 성기현 유기은 김점종¹ 윤용진*

경상대학교 화학과 ¹한국전자통신연구원 IT부품산업기술연구부

One-pot, efficient and green multi-functionalization is great importance in organic synthesis. Therefore, we attempt to develop an eco-friendly and atom-economical functionalization. According to recent our report, some 2-substitued-pyridazinones are chemoselective and also readily forms stable anion. Pyridazinone can act as a good leaving group, and is recyclable. In this poster, we describe the one-pot multi-functionalization of molecules involving —OH, —NH₂ and/or —SH group with 2-substitued-pyridazinones.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-634**

발표분야: 유기화학

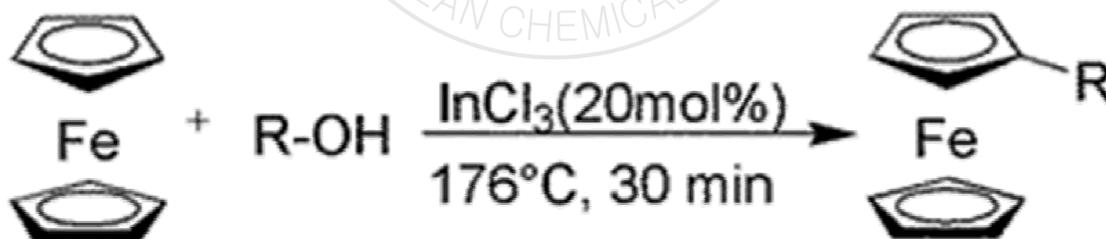
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of monosubstituted benzyl ferrocene derivatives

Razack Abdullah 홍인석*

공주대학교 화학과

A novel and efficient method was developed to synthesize monosubstituted ferrocene using allyl and benzyl alcohols by InCl_3 catalyzed Friedal Crafts alkylation. The strategy of molten ferrocene in the reaction condition, enhanced the activity of catalyst and reactivity of allyl and benzyl carbocations. Furthermore, the reaction duration was reduced to (30mins) 12 fold as compared to those proceeded in the presence organic solvents. To the best of our knowledge this is the first report to use ferrocene as a solvent. This synthetic protocol is quiet simple and yields were up to 92% which offer great potential in developing new synthetic routes for ferrocene derivatives. Scheme:



R =allyl and benzyl derivatives of alcohol.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-635**

발표분야: 유기화학

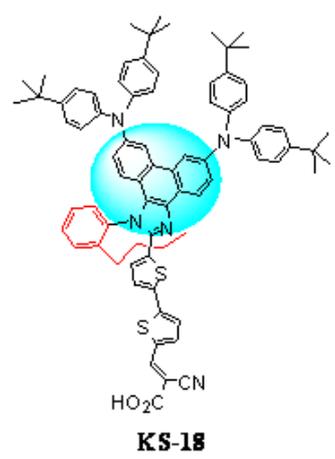
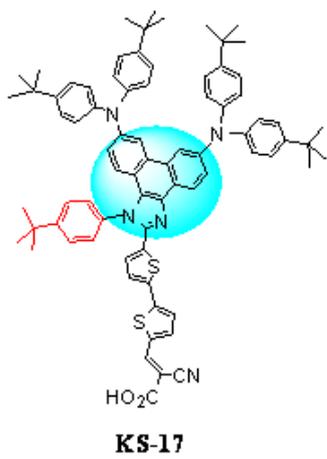
발표종류: 포스터, 발표일시: 수 16:00~19:00

Phenanthroimidazole as a linker in Dye-sensitized Solar Cell

이상희* 이유석 김동희 Mannix Balanay

군산대학교 화학과

Novel dye KS-17 and KS-18 containing phenanthroimidazole as a linker were synthesized. They have two donor groups and planar phenanthroimidazole group can transfer electron efficiently from two donor groups to cyanoacrylic acid. KS-17 showed serious aggregation problem in DSSC. To reduce the aggregation problem of KS-17, in KS-18, n-butyl group was introduced to ortho position of phenyl moiety instead of para position in KS-17. The synthesis and photovoltaic performance in DSSC will be described.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-636**

발표분야: 유기화학

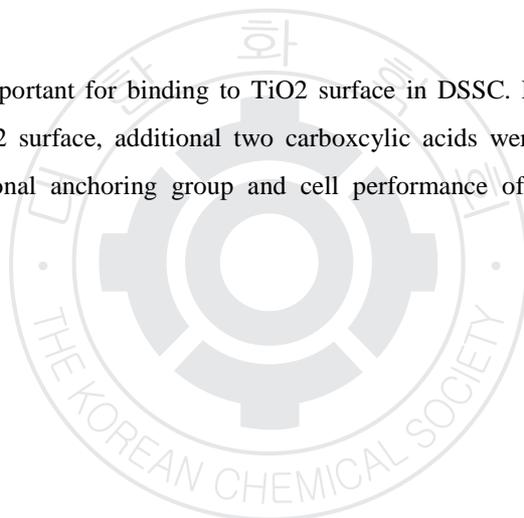
발표종류: 포스터, 발표일시: 수 16:00~19:00

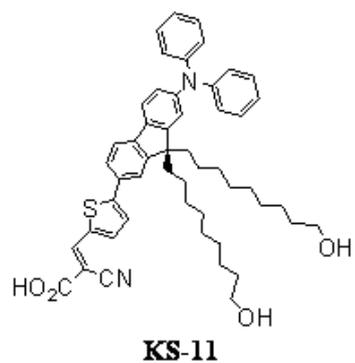
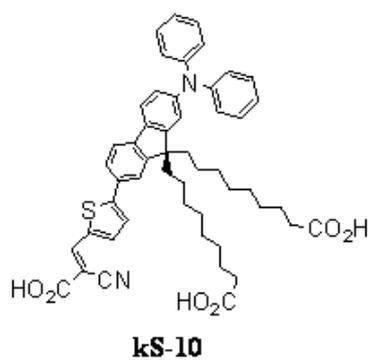
Tripodal dye for Dye sensitized Solar Cell

이상희* 이정구 유수창 김동희

군산대학교 화학과

Carboxylic acid is very important for binding to TiO₂ surface in DSSC. For strong binding and rigid orientation of dye on TiO₂ surface, additional two carboxylic acids were introduced (KS-10). The synthesis, effect of additional anchoring group and cell performance of KS-10 and KS-11 will be described.





일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-637**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A highly selective fluorescent turn-on probe for Al³⁺ via Al³⁺-promoted hydrolysis of ester

김보연 김홍석*

경북대학교 응용화학과

The developments of turn-on fluorescent probes that operate through chemical reactions triggered by the target analytes have attracted attention. Previously, the synthesis and Zn²⁺ or Cu²⁺ sensing properties of several thiazole based chemosensors were reported. A new reactive and highly selective fluorescent chemosensor (1) based on thiazole was synthesized for the quantification of aluminum ions in ethanol. The mechanism of fluorescence was based on the aluminum-promoted hydrolysis of the ester moiety and subsequent complexation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-638**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aluminum selective naphthol-based ‘turn-on’ thiazole fluorescent chemosensor

김보연 김홍석*

경북대학교 응용화학과

Aluminum is the third most prevalent element and the most abundant metal in the earth's crust, representing approximately 8.3% of total mineral components. Due to its reactivity, it is widely dispersed in the environment around us in modern society: in water treatment, in food additives, aluminum-based pharmaceuticals, occupational dusts, and of course as the production of light alloy used in container and cooking utensils. Two new reactive and highly selective turn on fluorescent chemosensors based on the position of ring annulation of the naphthalene ? thiazole moiety for aluminum ions in ethanol, were synthesized and investigated.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-639**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Biologically Active Natural Component 4-Hydroxyderricin Through Water-Accelerated [3,3]-Sigmatropic Rearrangement

윤현호 이재준 전종갑*

한림대학교 화학과

Angelica keiskei has been used in traditional medicine, food and beverages, and exhibited various biological activities, such as antitumor, antibacterial, antioxidant, antidiabetic, antiallergic, antimetastatic, antiulcer, hypotensive, lipid regulatory, and cancer chemopreventive effects. The plant has been reported to contain chalcones, flavanones, and coumarines. Two types of polyphenolic chalcones, 4-hydroxyderricin and xanthoangelol, are especially rich in the plant. Sugamoto reported the synthesis of 4-hydroxyderricin via [1,3]-sigmatropic rearrangement of chalcone ether using montmorillonite K10 which showed relatively low rearrangement yield, and this is the only reported total synthesis of 4-hydroxyderricin as far as we know. We recently developed the water-accelerated [3,3]-sigmatropic rearrangement reaction for licochalcone A synthesis and showed advantages promising higher yield and preventive effect to abnormal rearrangement which was known disadvantage of [3,3]-sigmatropic rearrangement reactions. We report the effective total synthesis of biologically active natural product 4-hydroxyderricin.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-640**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Licochalcone Analogues with Increased Anti-Inflammatory Activity

김철기 윤소라 전종갑*

한림대학교 화학과

Licochalcones have been reported to have various biological activities. However, most of licochalcones also showed cytotoxicity even though their versatile utilities. Licochalcones B and D, which have common substituents at aromatic ring B, are targeted to modify the structure at aromatic ring A for inflammatory studies. Licochalcone derivatives thus prepared are compared for their suppression ability of nitric oxide (NO) production.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-641**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Anthracene Based Organic Light Emitting Diodes and their Physical Properties

정진형 정용석*

충북대학교 화학과

OLED 에서의 블루 컬러는 디스플레이의 색을 내는 데 있어 매우 중요하다. 그렇기에 anthracene 을 기반으로 한 새로운 형광 물질을 합성하였다. 이 신규화합물은 anthracene 의 9 번 위치에 fluorenyl group, 10 번 위치에 phenanthrene 을 도입하였고, 또한 triphenylsilyl group 을 도입하여 화합물을 완성하였다. 합성한 물질을 발광 소자로 만들어 전기/광학적 특성을 평가하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-642**

발표분야: 유기화학

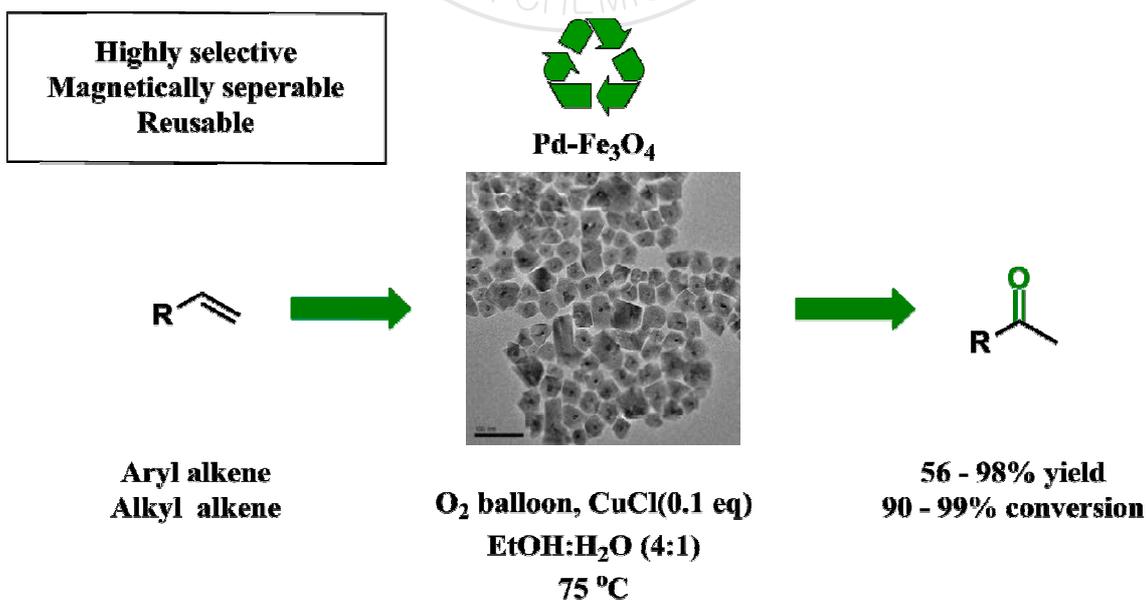
발표종류: 포스터, 발표일시: 수 16:00~19:00

Wacker Oxidation of Terminal Olefins Using Magnetically Reusable Pd-Fe₃O₄ Heterodimeric Catalyst

변상문 정주영 권정민¹ 현택환² 김병문*

서울대학교 화학부 ¹서울대학교 화학과 ²서울대학교 화학생물공학부

Wacker oxidation is a powerful process converting a terminal olefin to a methyl ketone. We describe herein a new highly selective and environment-friendly Wacker oxidation process employing Pd-Fe₃O₄ heterodimeric crystals as a catalyst. Various reaction conditions were investigated for the determination of optimal reaction conditions. Consistently high yields and excellent reaction selectivities of the desired Wacker product were detected in almost all the reactions employing the Pd-Fe₃O₄ nanocatalyst in an optimal condition in EtOH-H₂O under 1 atm O₂. This operationally simple oxidation protocol allows reusing of the Pd-Fe₃O₄ after the reaction through the use of an external magnet.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Orientated Isomerization of Allylic Alcohols Mediated by Organolanthanide Catalysts

김판수 손수진 서성용*

부경대학교 화학과

We report here the catalytic isomerization of aryl-substituted allylic alcohols mediated by lanthanide alkoxo complexes. The conversion yields allylcarbinols as the products of the olefin isomerization process, but with different olefinic positions than those afforded by typical transition metal catalysts. The average isolated product yields in these reactions are 65~81%. The catalytic cycle and the source of the unusual olefinic positioning are proposed to involve a strong interaction between the Lewis acidic La³⁺ ion and the substrate hydroxyl group.

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장소: 창원CECO

발표코드: ORGN.P-644

발표분야: 유기화학

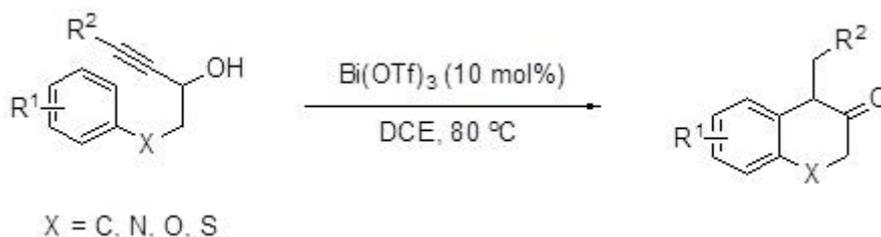
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-Tetralone Derivatives via Bismuth-Catalyzed Intramolecular Hydroarylation and Isomerization of Propargylic Alcohols

윤지희 박정민 김재현 이구연*

강원대학교 생명건강공학과

Substituted 2-tetralone have played an important role in organic synthesis because they are highly reactivity and suitable as starting materials for a wide range of compounds with biological activities, as well as being the precursors of several biologically active natural products. However, in comparison with 1-tetralones, 2-tetralones are often very expensive, less stable, and much more difficult to be synthesized. Herein, we have developed that bismuth catalyzed intramolecular cyclization of aryl propargyl alcohols to provide an efficient method for 2-tetralones. 5-Phenylpent-1-yn-3-ol was treated with 10 mol% of Bi(OTf)₃ to give 1-methyl-2-tetralone in good yield. This highly efficient transformation involves intramolecular hydroarylation, isomerization, and tautomerization in the same flask.



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발표코드: ORGN.P-645

발표분야: 유기화학

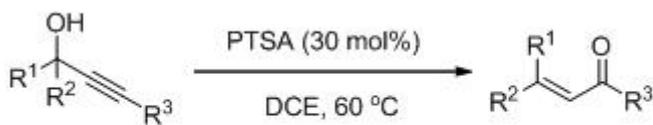
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Conjugated Enons via Brønsted Acid-Catalyzed Meyer-Schuster Rearrangement of Propargyl alcohols

박정민 윤지희 김재현 이구연*

강원대학교 생명건강공학과

α,β -Unsaturated carbonyl compounds are useful building block in organic synthesis and key structural units in a large number of biologically active natural products. Such species are usually obtained by using Meyer-Schuster rearrangement, in which a formal isomerization of propargyl alcohols. Such reaction has received considerable interest in recent years, and numerous organometallic complexes have been used to catalyze or promote this reaction. We have shown that p-TsOH can be very effective catalyst to promote such a reaction, and various propargylic alcohols have been proved to tolerate this reaction and produce the corresponding unsaturated carbonyl compounds. Reactions proceeded smoothly in DCE at 60 °C to provide the corresponding α,β -unsaturated carbonyl compounds in excellent yields.



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발표코드: **ORGN.P-646**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodamine Cyclic Hydrazide as Fluorecent Probe for the Detection of Hydroxyl Radical

김민정 태진성*

연세대학교 화학과

We have developed a new rhodamine 6G fluorescent probe for monitoring $\cdot\text{OH}$ (hydroxyl radical). The mechanism for sensing $\cdot\text{OH}$ is based on the oxidative C-H abstraction reaction of rhodamine cyclic hydrazide, which is the first example in the rhodamine fluorescent probes. The probe exhibits excellent selectivity for $\cdot\text{OH}$ with virtually no interference by other ROS/RNS species. We examined the ability to quantify $\cdot\text{OH}$ in vitro. When probe is treated with $\cdot\text{OH}$, the fluorescence intensity was linearly proportional to the molar equivalents of $\cdot\text{OH}$, and probe showed strong fluorescence in the presence of $\cdot\text{OH}$ at pH 4-10. So, we then investigated biological imaging of intracellular hydroxyl radical. Fluorescent imagings of A549 and RAW264.7 cells are also successfully demonstrated to detect intracellular $\cdot\text{OH}$ in live cells. We expect that this imaging technique will serve as a practical tool for $\cdot\text{OH}$ -related biological studies.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-647**

발표분야: 유기화학

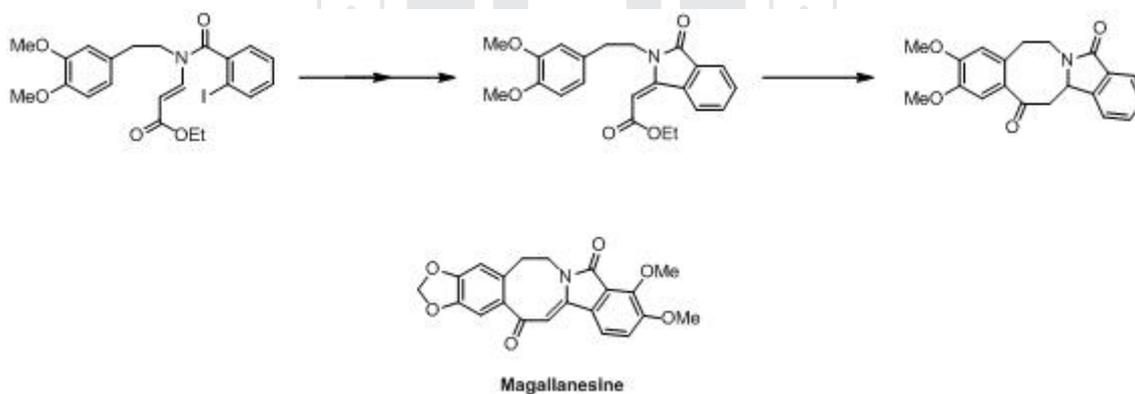
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study of an isoindolobenzazocine alkaloid, magallanesine

서성예 김건철*

충남대학교 화학과

Magallanesine, the first known isoindolobenzazocine alkaloid, was isolated from *Beberis Darwinii*. In this study a isoindolobenzazocine derivative has been synthesized by intra-molecular Heck reaction and intra-molecular Friedel-Craft type reaction. Using this method, we are going to synthesize magallanesine.



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장소: 창원CECO

발표코드: **ORGN.P-648**

발표분야: 유기화학

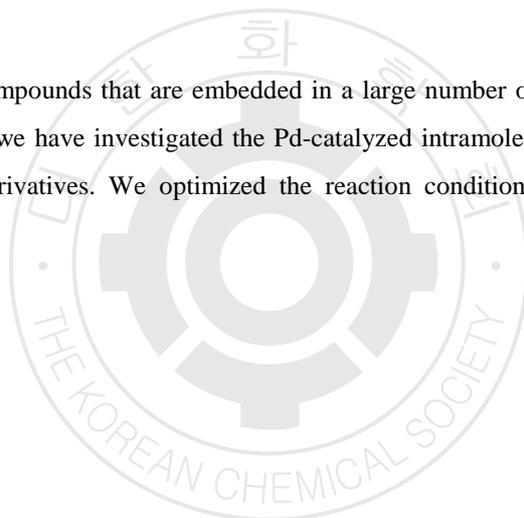
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Indole Synthesis

강다영 이소라 윤소원*

한양대학교 화학과

Indoles are heterocyclic compounds that are embedded in a large number of pharmaceutically bioactive natural products. Recently we have investigated the Pd-catalyzed intramolecular cyclization reaction for the synthesis of indole derivatives. We optimized the reaction conditions by screening a variety of reaction parameters.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-649**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of α -aminophosphonates via radical addition to hydrazones

이준혁 장두옥*

연세대학교 화학과

The synthesis of α -aminophosphonates exhibiting high bio-activity has recently attracted a lot of attention. Especially, the search for a general method of synthesis of α -aminophosphonates from hydrazones of α -keto ester still remains of current interest. However, little has been reported on the synthesis of α -aminophosphonates using radical reaction. We developed an effective synthetic route to afford α -aminophosphonates via radical addition to C=N bond. Treatment of hydrazones derived from α -keto phosphonates with various alkyl halides, diphenylsilane, and triethylborane gave the corresponding α -aminophosphonates in high yields.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 유기화학

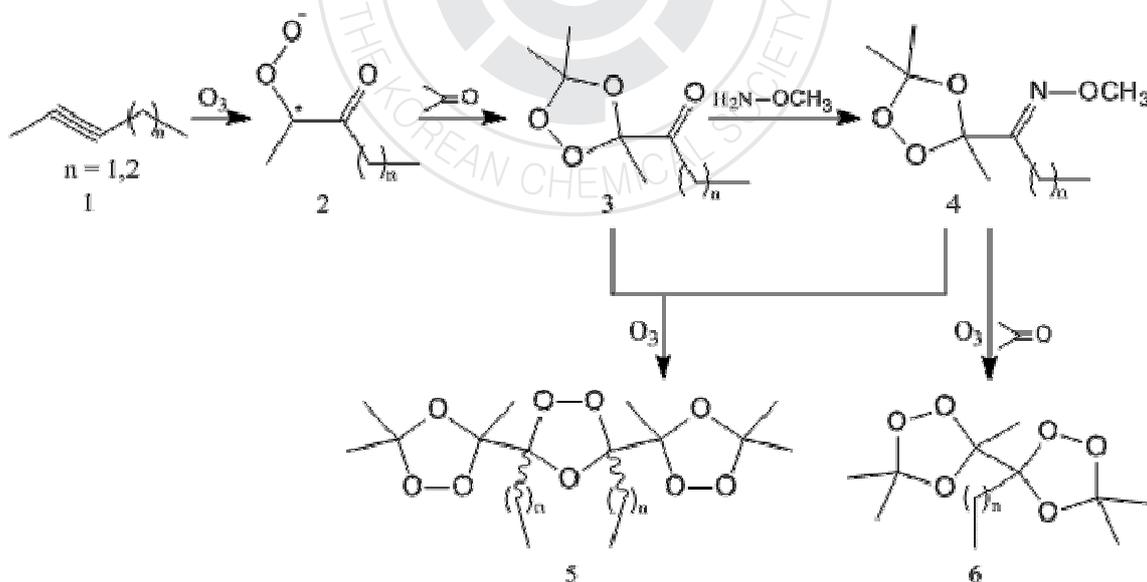
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ozonides from Cozonolyses of 2-Alkynes and Carbonyl Compounds

김서초 곽형민 구분석 정인찬*

한서대학교 화학과

Ozonolyses of 2-Pentyne or of 2-Hexyne in the presence of Carbonyl Compounds afforded the corresponding labile α -Oxonozonides, which could be stabilized and, hence, isolated by subsequent conversion into α -Methoximino Derivatives. All of the Oxonozonides have been characterized by positive Peroxide Tests, and their ^1H and ^{13}C NMR Spectra.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 유기화학

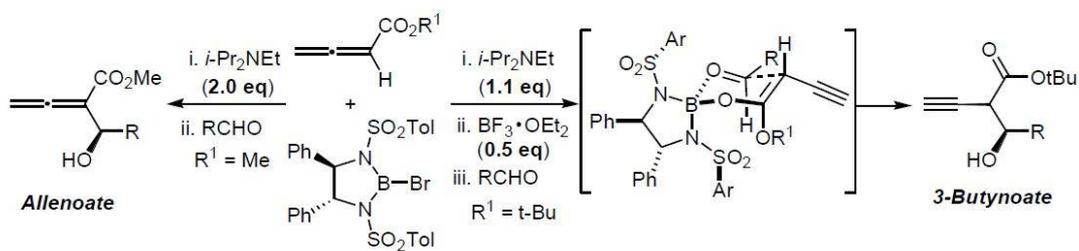
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Stereoselective Aldol Reaction of Allenates with Aldehydes for the Synthesis of threo 3-Butynoate Aldol Adduct

김현아 유찬모*

성균관대학교 화학과

Asymmetric aldol reactions have been regarded as one of the most efficient methods to construct chiral pools. Recently, we have developed a new adol method of allenolate in forming 2-hydroxy allenolate in high levels of enantioselectivity. During this investigations, we envisioned that the realization of alkynyl adduct without isomerization might be possible. After conversion of allenolate to borone enolate in the presence of chiral bromoborane complex, addition of trifluoroborane complex followed by aldehyde resulted in the formation of alkynyl aldol adduct without any allenyl species. We would like to present herein the scope of reaction, stereoselectivity, mechanistic pathway and its applications to lignan synthesis.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: ORGN.P-652

발표분야: 유기화학

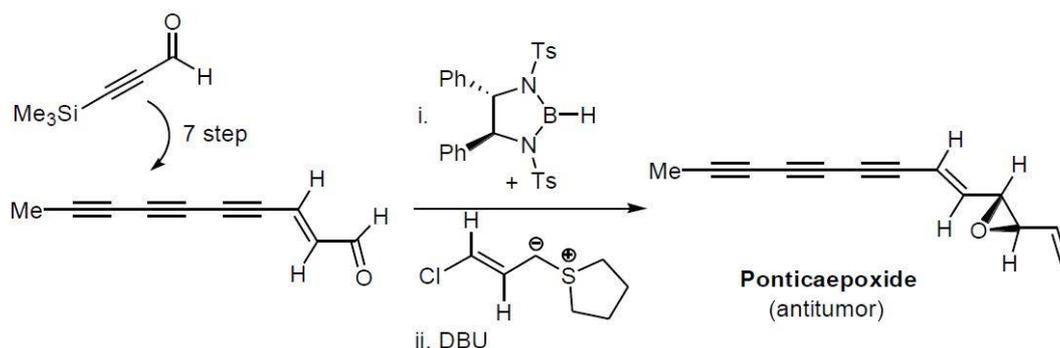
발표종류: 포스터, 발표일시: 수 16:00~19:00

Chloroallylic Transfer Reactions for the Enantio- and Diastereoselective Synthesis of 3-Vinyloxiranes: Synthesis of Annuadiepoide

방지윤 유찬모*

성균관대학교 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity in the production of enantiomerically pure compounds is of considerable current interest in synthetic chemistry. In light of widespread advances in synthetic methods for the synthesis of chiral substances, the allylic transfer reactions of carbonyl functionalities using chiral auxiliaries or catalysts led to significant developments in the area of asymmetric synthesis. Recently, we have developed a new chloroallylboration for the synthesis of enantiomerically enriched vinyl chlorohydrins and vinyl oxiranes. We would like to present herein synthetic application for the synthesis of naturally occurring ponticaepoxide.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 유기화학

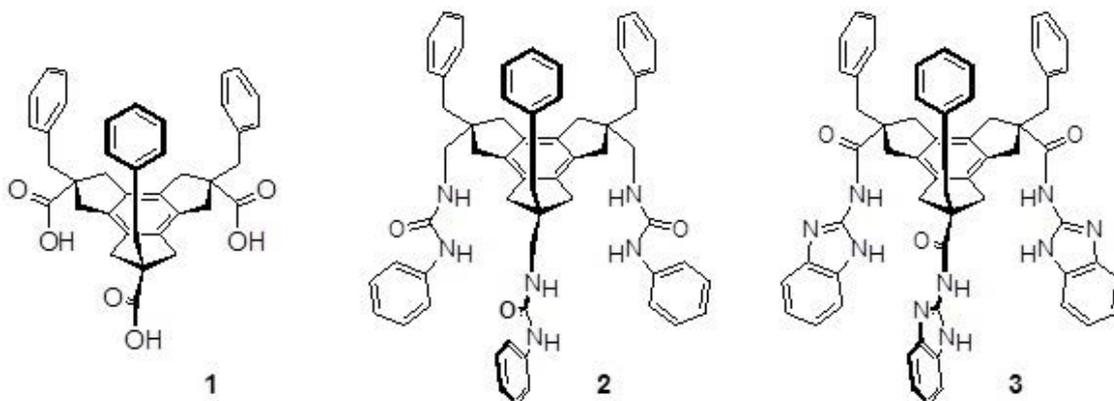
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel C_{3V} -Symmetric Tripodal Anion Receptor; Synthesis and Anion Recognition of *cis,cis,cis*-2,5,8-Tribenzyl-2,5,8-tri[*N*-(1*H*-benzo[*d*]imidazol-2-yl)carbamoyl]trindane

김원 최홍진*

경북대학교 응용화학과

A novel C_{3V} -symmetric tripodal anion receptor **3** with guanidine recognition motif, was synthesized from *cis,cis,cis*-2,5,8-tribenzyltrindane-2,5,8-tricarboxylic acid (**1**) with 2-aminobenzimidazole in 80% yield via its imidazolide intermediate. The C_{3V} -symmetric tripodal receptor **2** with three urea recognition motif fixed in same side of trindane molecular plane (all-*syn* form) have shown to bind effectively with C_{3V} -symmetric anion guests such as F^- , Cl^- , Br^- , I^- , $H_2PO_4^-$, HSO_4^- , NO_3^- , HCO_3^- ions. The urea binding motifs are known to recognize anions effectively through hydrogen-binding to anion. The new guanidine moieties in benzoimidazolyl groups which are structural analogue of urea binding motif are expected to show a good anion recognition properties. The structural determination and anion recognition by NMR titration will be presented.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-Catalyzed C-H Amination for the Synthesis of Indoles

정은주 고태윤 윤소원*

한양대학교 화학과

Indoles are ubiquitous structural motifs in biologically active compounds and natural product. Therefore, the chemical synthesis of indoles moieties has attracted the attention of organic chemists. In recent years, the construction of the indole skeleton based on transition-metal-catalyzed reactions, in particular on the Pd-catalyzed processes, has aroused great attention. In this context, we have been interested in development of a new synthetic method using Pd-catalyzed C-H amination of (*Z*)-*N*-protected dehydroamino acids. We will demonstrate our findings regarding the *N*-protecting group effect and various reaction parameters.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereoselective Synthesis of Chiral Pyrrolizine-Based Triheterocycles by An Organocatalytic Cascade Reaction

이효준 조창우*

경북대학교 화학과

The construction of polyheterocyclic skeletons has been the focus of intensive research effort because of their diverse structural features and interesting biological activities. In particular, the development of efficient routes for the asymmetric synthesis of stereogenic complex molecules including chiral polyheterocycles from simple starting materials in a single step has become a challenging topic in modern organic chemistry. In this regard, we recently reported organocatalytic asymmetric cascade aza-Michael-aldol reactions of α,β -unsaturated carbonyl compounds with pyrroles as *N*-centered heteroaromatic nucleophiles to provide a variety of chiral pyrrolizines. Owing to the importance of pyrrolizines in the development of pharmaceuticals, we planned to prepare chiral pyrrolizine-based polyheterocycles as a unique and potential skeleton of pharmaceutical agents. Herein, we report the organocatalytic asymmetric cascade aza-Michael-aldol reactions of α -branched α,β -unsaturated aldehydes with trifluoroacetylpyrroles as *N*-centered heteroaromatic nucleophiles that afford highly functionalized chiral pyrrolizine-based triheterocycles having two quaternary stereocenters of three consecutive stereocenters. Concomitantly, two sequential Suzuki cross-couplings of the chiral pyrrolizine-based triheterocycles with different aryl boronic acids provide unsymmetrically diarylsubstituted chiral pyrrolizine-based triheterocycles in a highly chemoselective controlled manner.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Asymmetric Aza-Michael Reactions of Pyrazole with α,β -Unsaturated Ketones

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 itself, without any derivatization, as the *N*-centered heteroaromatic nucleophile remains unexplored in organocatalytic asymmetric aza-Michael reactions, in spite of the importance of pyrazole as optically pure *N*-heteroaromatic pharmacophores in biologically active natural products. Here, the first use of pyrazole itself as the *N*-centered heteroaromatic nucleophile in the organocatalytic asymmetric aza-Michael reactions of α,β -unsaturated ketones will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of 2-Isoxazolines by an Organocatalytic Cascade Reaction

은미경 조창우*

경북대학교 화학과

2-Isoxazolines are an important class of heterocyclic compounds that show a variety of remarkable biological activities and thus have found application in the development of pharmaceuticals. Recently, the development of organocatalytic asymmetric cascade reactions has received much attention, because they provide powerful tools for the concise construction of complex structures from simple precursors in a single step. Herein, we report the asymmetric synthesis of 2-isoxazolines by the organocatalytic cascade oxa-Michael/imine cyclization reactions of (*E*)-tert-butyl 2-methyl-4-oxo-4-(hetero)arylbut-2-enoate as the substrates with hydroxylamine as the nucleophile.

일시: 2013년 10월 16~18일(수~금) 3일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereoselective Synthesis of Chiral 2-Substituted-3,3-dinitroazetidines

윤희석 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-dinitroazetidine 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-dinitroazetidines via diastereoselective aza-Henry Reactions with *N*-sulfinylimines.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cinchona-based Primary Amine-catalyzed Stereoselective Aza-Michael Reactions

안준기 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.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-660**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasound-mediated gene and drug delivery using a microbubble-liposome particle system

윤영일 조희상¹ 윤태종^{2,*}

서울대학교 나노융합¹ 차의과대학교 의생명과학과² 차의과학대학교 바이오산업응용학과

Microbubble (MB) structures are useful contrast agents in ultrasound imaging (US). Here, we present a functional MB-liposome complex particle, termed the Pop-particle, and describe its preparation, targeting of cancer cells, and transportation of various bioactive materials by flash stimulation. Organic dyes incorporated into Pop-particles after antibody modification were selectively imaged in cancer cells. Pop-particles loaded with plasmid DNA exhibited higher transfection efficiencies in cancer and primary cell lines than commercialized agents. Moreover, successful delivery of the anticancer drug doxorubicin and short interfering RNA (siRNA) to cancer cells via the Pop-particle system led to apoptotic cell death under external ultrasound stimulation. Pop-particles containing both doxorubicin and siRNA exhibited dramatic therapeutic effects in a rabbit renal tumor model. Thus, this biocompatible Pop-particle system was able to function as a delivery system for both US contrast agents for angiogenesis imaging and therapeutic materials such as anticancer drugs and siRNA for gene therapy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-662**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

NHC-Catalyzed Asymmetric Oxidative Cyclization Reactions of *o*-Alkenylbenzaldehydes under Aerobic Conditions

송형섭 장영호 윤소원*

한양대학교 화학과

N-Heterocyclic carbenes (NHCs) have become an important and powerful class of organocatalysts with widespread applications in a variety of synthetic transformations. Recently, we developed a highly effective NHC-catalyzed oxidative cyclization of *o*-alkynylbenzaldehydes that enabled the easy preparation of a diverse array of phthalides and isocoumarins. Chiral 3-substituted phthalides are important classes of naturally occurring lactones that have been found to exhibit a wide range of biological indications and to be versatile building blocks for the synthesis of bioactive compounds. In light of our recent success in NHC-catalyzed oxidative cyclization of *o*-alkynylbenzaldehydes, we investigated an NHC-catalyzed asymmetric oxidative cyclization of *o*-alkenylbenzaldehydes to afford stereocenter-containing phthalides.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-663**

발표분야: 유기화학

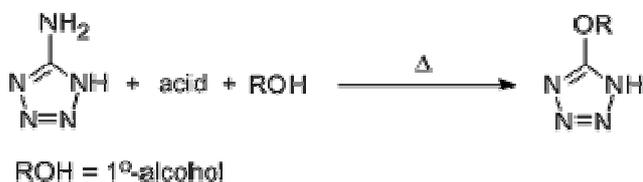
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis of 5-alkoxytetrazole by substitution of amino group of 5-aminotetrazole

이세진 임영권^{1,*}

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Tetrazole derivatives have similar acidity to the carboxylic acid group, and are more stable metabolically. Therefore, replacement of carboxylic acids by tetrazoles in biologically active compounds has been widely applied in research areas of medicinal chemistry. Also it frequently used as high energy density materials (HEDMs) because those have high nitrogen content and thermal stability despite large positive enthalpies of formation. There have been reported various reactions to prepare 5-substituted tetrazoles by substitutions of 5-halotetrazoles, C-H activation reactions of 5-H tetrazoles, and cyclization reactions of nitriles with azide. However, most reactions started with 1-alkylated tetrazoles because acidic proton of the tetrazoles disturbed formation of 5-substituted tetrazoles. In addition, there are few ways for preparations of 5-alkoxytetrazoles without substituted alkyl group that can be achieved by the reaction between 5-halo 1- or 2-alkylated tetrazoles and alcohols on basic condition. Herein, preparation of 5-alkoxytetrazoles with facile reaction condition will be presented.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2,5-Disubstituted Dihydrofuran-3(2*H*)-ones via [2,3]- Sigmatropic Rearrangement of Oxonium Ylides Generated from α - Oxo Gold Carbenes

배주희 태진성*

연세대학교 화학과

The gold-catalyzed oxidation of alkynes into α -oxo gold carbenes has been a key strategy in a variety of transformations, such as cyclopropanation, C-H insertion, O-H insertion, and dipolar cycloaddition. Recently, The Zhang group reported the synthesis of four- and five-membered oxacycles by intramolecular O-H insertion of α -oxo gold carbenes. O-H insertion reactions of the α -oxo gold carbenes yield the substituted dihydrofuran-3(2*H*)-ones. However, intramolecular trapping of α -oxo gold carbenes by the allyl ether oxygen could lead to the formation of the oxonium ylides. Subsequent [2,3]-sigmatropic rearrangements are expected to give the substituted dihydrofuran-3(2*H*)-ones. We have developed a flexible and general solution for the synthesis of various 2,5-disubstituted dihydrofuran-3(2*H*)-ones via [2,3]-sigmatropic rearrangements of oxonium ylides generated from α -oxo gold carbenes which are formed by the gold-catalyzed intermolecular oxidation of the allyl homopropargyl ethers with *N*-oxide. The synthetic utility of the present method has been proved by the concise formal synthesis of (\pm)-kumausallene.

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장소: 창원CECO

발표코드: **ORGN.P-665**

발표분야: 유기화학

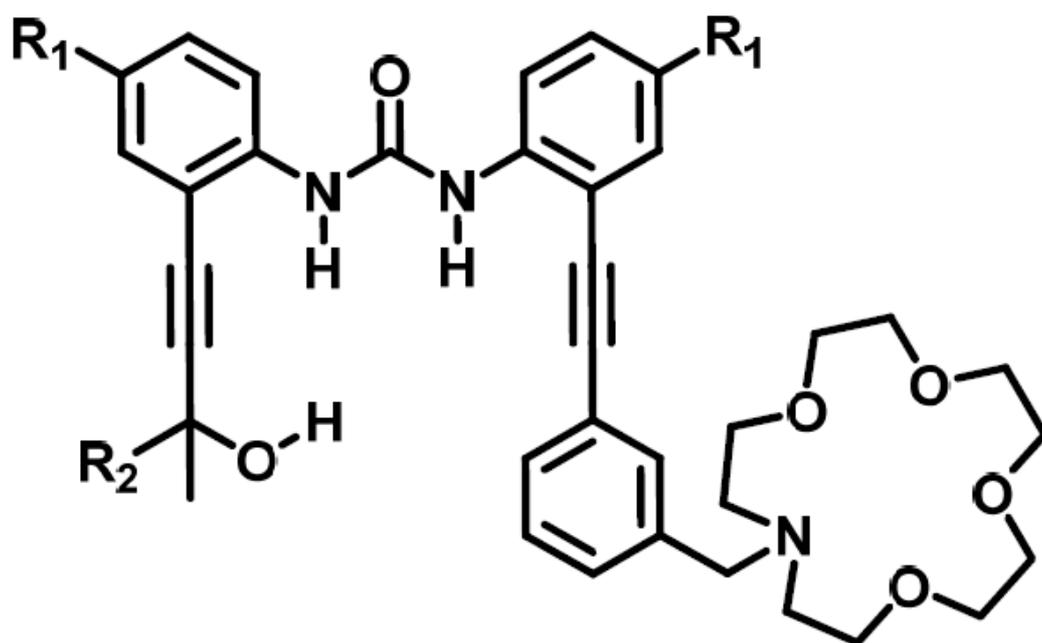
발표종류: 포스터, 발표일시: 수 16:00~19:00

A ditopic receptor capable of transporting both cations and anions across a lipid membrane

이정하 정규성*

연세대학교 화학과

Ditopic receptors based on the dipenylurea scaffold have been prepared which have hydrogen bonding sites for anion binding and crown ethers for cation coordination. The substituents (R1 and R2) in the receptors are systematically varied to reveal contributing factors to the transport activity, such as binding affinity, lipophilicity, hydrophilicity, mobility, etc. The binding properties are investigated using ¹H NMR spectroscopy and the transport abilities across a POPC lipid membrane are measured by ion-selective electrodes. Details will be described in the presentation. Keywords : Salt transport; Ditopic receptor; Lipid membrane; Crown ether



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Structure Characterization of 3',6'-Bis(diethylamino)-2-(phenylamino) spiro[isindoline-1,9'-xanthen]-3-one

Muhammad Saleem Razack Abdullah 김종혁¹ 김문환² 이기환*

공주대학교 화학과 ¹한국화학연구원 화학분석센터 ²한국화학연구원 화학물질연구단

In the present study, the characteristic of a non-fluorescent spiro form rhodamine B phenyl hydrazide was studied and the results showed that it has a sensitive response to nitrite ion. The reaction of nitrite ion with rhodamine B hydrazide, a colorless, non-fluorescent compound results in a dramatic increase in fluorescence intensity of the reaction mixture. Based on this phenomenon, a novel fluorescent probe for nitrite ion was developed. The objectives of the present study are to evaluate the ability of rhodamine B phenyl hydrazide as a probe for nitrite ion detection and its potential used in biological and natural water systems.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-667

발표분야: 유기화학

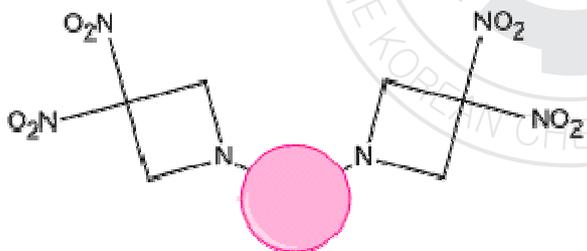
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on synthesis of Dinitroazetidine derivatives as High Energy Plasticizers

최재이 고훈영* 이희윤¹ 문지수²

인하대학교 화학과 ¹한국과학기술원(KAIST) 화학과 ²인하대학교 화학

Energetic plasticizers are defined as the functional materials having a positive heat of explosion. It is applicative as propellant and explosive formulations in order to modify their properties. It is essential to design and synthesize new plasticizers for enhanced flexibility and elasticity. Several new substituted dinitro-azetidines were designed and synthesized.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-668**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Potassium alkenylaryltrifluoroborates from haloaryltrifluoroborates via Mizoroki-Heck reaction

김태정 정규혁¹ 송중호¹ 함정엽*

한국과학기술연구원(KIST) 천연의약센터 ¹강릉원주대학교 화학신소재학과

Organotrifluoroborate salts have been used as important coupling partners in the Suzuki-Miyaura cross-coupling reaction due to their inherent stability to both air and moisture as well as their easy handling. Moreover, their remarkable tolerance to harsh conditions in a number of reactions has allowed the preparation of functionalized trifluoroborates that may not be synthesized from the corresponding boronic acids or boronate esters. For example, functionalizations of organotrifluoroborates such as epoxidation, dihydroxylation, oxidation, metalation, [3+2] cyclization, and nucleophilic substitution were successfully performed without loss of the BF₃K group. In particular, Molander and co-workers demonstrated the synthesis of alkenylaryltrifluoroborates via Wittig and Horner-Wadsworth-Emmons olefination of the corresponding organotrifluoroborates. Although a number of di- or trisubstituted olefins was successfully prepared in moderate to excellent yields via direct olefination of organotrifluoroborates, these previous methods have limitations, resulting from the inseparable mixture of *E/Z* isomers and stoichiometric amounts of the phosphate [(EtO₂)P=O(OLi)] by-products. With these considerations in mind, we report herein the preparation of potassium alkenylaryltrifluoroborates using arylolefins or activated olefins as electrophiles via a Pd-catalyzed Mizoroki-Heck reaction and the further functionalization of these alkenylaryltrifluoroborates under microwave irradiation.

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발표코드: **ORGN.P-669**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Potassium (1-Organo-1H-1,2,3-triazol-4-yl)trifluoroborates from Ethynyltrifluoroborate via Regioselective One-Pot CuAAC Reaction

정규혁 김태정¹ 최필주 이명재 함정엽^{1,*}

강릉원주대학교 화학신소재학과 ¹한국과학기술연구원(KIST) 천연의약센터

Being one of the most important structural motifs for the development of potentially bioactive molecules and new materials, 1,4-disubstituted 1,2,3-triazoles are widely used in various fields such as organic synthesis, medicinal chemistry, and materials science. However, despite significant recent improvements, the diversity of 1,2,3-triazoles that can be obtained through the CuAAC reaction is limited by the availability and high price of the terminal alkyne derivatives from commercial sources. Moreover, some low-molecular-weight alkynes are difficult to handle because of their low boiling points. Therefore, new facile and efficient methods to obtain multifariously C4-functionalized triazole compounds are still of synthetic interest. A novel series of 1,4-disubstituted 1,2,3-triazole-containing potassium trifluoroborates were prepared from the corresponding organohalides with potassium ethynyltrifluoroborate via regioselective one-pot Cu-catalyzed azide-alkyne cycloaddition (CuAAC) reaction in good to excellent yields. Further succeeded in Suzuki-Miyaura cross-coupling reaction of these organo 1,2,3-triazol-4-yltrifluoroborates with aryl and alkenyl bromides using of PdCl₂(dppf)/CH₂Cl₂/TBAB system under microwave irradiation.

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발표코드: **ORGN.P-670**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Coumarin-Based Ratiometric Fluorescent Probe for Biothiols

임수연 김해조^{1,*}

한국의국어대학교 화학과 ¹한국의국어대학교 자연과학대학 화학과

Biothiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) are involved in a myriad of vital cellular processes, including redox homeostasis [1] and cellular growth [2]. It serves many cellular functions, including the maintenance of intracellular redox activities, xenobiotic metabolism, intracellular signal transduction, and gene regulation [3]. Therefore, it is important to develop fluorescent probe for detection these biothiols. Herein we report an aminocoumarinyldisulfide probe 1 which displays a ratiometric fluorescence change to afford the quantitative detection of biothiols by a thiol-induced disulfide cleavage reaction. When GSH was added, a ratiometric fluorescence change of 1 were observable so that micromolar concentration of Cys was detectable by the naked eye. Reference[1]. Dalton, T. P.; Shertzner, H. G.; Puga, A. *Annu. Rev. Pharmacol. Toxicol.* 1999, 39, 67. [2]. (a) Wood, Z. A.; Schroeder, E.; Harris, J. R.; Poole, L. B. *TransBiochem. Sci.* 2003, 28, 32. (b) Carnel, R.; Jacobsen, D. W. *Homocysteine in Health and Disease*, Cambridge University Press, UK, 2001.[3]. Krauth-Siegel, R. L.; Bauer, H.; Schirmer, R. H. *Angew. Chem. Int. Ed.* 2005, 44, 690.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bisbromoaceylfluorescein-Based Fluorescence Turn-On Probe for Cys over Hcy/GSH

홍금희 김해조^{1,*}

한국의국어대학교 화학과 ¹한국의국어대학교 자연과학대학 화학과

Biothiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) play important roles in such processes as redox homeostasis [1] and cellular growth [2] in a biological system. An abnormal level of biothiols is an indicator of human diseases like cancer and AIDS. [3] However, The discrimination of biothiols with a similar functionality is a difficult goal to achieve. Recently, we report a selective fluorescent probe for Cys over Hcy and GSH by introducing a kinetic and thermodynamic discrimination strategy during the probe-cysteine cyclization step. The probe showed a selective and sensitive response to cysteine over homocysteine and glutathione in aqueous buffer through a rapid cyclization reaction . When cysteine was added, a fast fluorescence turn-on change of probe was observed, thus allowing cysteine to be discriminated from other biothiols and micromolar concentrations of cysteine to be detected by the naked eye. [4]References[1]. (a) Dalton, T. P.; Shertzer, H. G.; Puga, A. *Annu. Rev. Pharmacol. Toxicol.* 1999, 39, 67. (b) Mathews, C. K.; van Holde, K. E.; Ahern, K. G. *Biochemistry*; Addison-Wesley Publishing Co.: San Francisco, 2000. [2]. (a) Wood, Z. A.; Schroeder, E.; Harris, J. R.; Poole, L. B. *Trans-Biochem. Sci.* 2003, 28, 32. (b) Carmel, R.; Jacobsen, D.W. *Homocysteine in Health and Disease*; Cambridge University Press: Cambridge, 2001.[3]. (a) Townsend, D. M.; Tew, K. D.; Tapiero, H. *Biomed. Pharmacother.* 2003, 57, 145. (b) Herzenberg, L. A.; De Rosa, S. C.; Dubs, J. G.; Roederer, M.; Anderson, M. T.; Ela, S. W.; Deresinski, S. C.; Herzenberg, L. A. *Proc. Natl. Acad. Sci. U.S.A.* 1997, 94, 1967. [4]. Hong, K.-H.; Lim, S.-Y.; Yun, M.-Y.; Lim J.-W.; Woo, J.-H.; Kwon, H.; Kim, H.-J. *Tetrahedron Lett.* 2013, 54, 3003

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Fluorescein Monoaldehyde with Disulfide Functionality for the Selective Detection of Cys and Hcy in HEPES Buffer

이희진 김해조*

한국외국어대학교 자연과학대학 화학과

Thiol-containing amino acids (AAs) such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) play an important role in many biological processes including cellular redox homeostasis [1]. The lack of Cys induced many health disorders such as hematopoiesis reduction, retarded growth, hair depigmentation, liver damage, skin lesion, and cancer [2]. On the other hand, elevated total homocysteine (Hcy) levels are related to cardiovascular diseases [3] and coronary heart disease [4]. Therefore, the rationally designed fluorescent probes capable of the selective detection of the biothiols were of growing interest [5]. Herein, we report a fluorescent probe based on disulfide-containing fluoresceinylaldehyde, which displayed the selective recognition of Cys and Hcy over GSH with high fluorescence turn on response in HEPES buffer. The probe displayed highly selective responses to cysteine (Cys) and homocysteine (Hcy) over glutathione (GSH) due to the rapid ring formation reaction of Cys and Hcy with the aldehyde group of probe and the concomitant cleavage of the disulfide group followed by the subsequent intramolecular cyclization. The fluorescent probe also exhibited a highly sensitive fluorescence turn-on response to Hcy with the detection limit of 2.4 μM Hcy in HEPES buffer. References [1]. Chen, X.; Zhou, Y.; Peng, X.; Yoon, J. Chem. Soc. Rev., 2010, 39, 2120. [2]. Shahrokhian, S. Anal. Chem., 2001, 73, 5972. [3]. Klee, G. G. Clin. Chem., 2000, 46, 1277. [4]. Clarke, R., Smith, A. D., Jobst, K. A., Refsum, H., Sutton, L., Ueland, P. M. Arch. Neurol., 1998, 55, 1449. [5]. Wang, W., Rusin, O., Xu, X., Kim, K. K., Escobedo, J. O., Fakayode, S. O., Fletcher, K. A., Lowry, M., Schowalter, C. M., Lawrence, C. M., Fronczek, F. R., Warner, I. M., Strongin, R. M. J. Am. Chem. Soc., 2005, 127, 15949.

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장소: 창원CECO

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Coumarinyloxime-Based Colorimetric and Fluorometric Probe for the Selective Detection of Cyanide

나상윤 김해조^{1,*}

한국의국어대학교 화학과 ¹한국의국어대학교 자연과학대학 화학과

Cyanide anions (CN⁻) are extremely toxic to living organisms, and a trace amount of intake of the cyanide anions can therefore result in death [1]. Nevertheless, cyanides are industrially useful materials and are still widely employed for various uses such as synthetic resins, medicines, pesticides, fertilizers, and in gold extraction. The World Health Organization (WHO) sets the maximum permissible level of cyanides in drinking water at 1.9 μM [2]. Therefore, the selective and sensitive detection of cyanide is very important for environmental protection, food analysis and even anti-terrorism [3]. Herein, we report a coumarinyloxime-based fluorescent probe (1) for cyanide. The probe has shown a highly selective and sensitive response to the cyanide anion over other various anions with a submicromolar limit of fluorimetric detection (LOD = 0.49 μM). When CN⁻ was added to 1, probe 1 showed dramatic fluorescence and color changes, which were easily observable with the naked eye in aqueous solvent. References [1]. Kulig, K.W.; Cyanide Toxicity, U.S. Department of Health and Human Services, Atlanta, 1991 [2]. Guidelines for Drinking-water Quality, World Health Organization, Geneva, 1996[3]. Young, C.A.; Tidwell, L.G.; Anderson, C.G.; Cyanide: Social, Industrial and Economic Aspects, Warrendale The Minerals, Metals and Materials Society Press, 2001?

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장소: 창원CECO

발표코드: ORGN.P-674

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Mechanism Study on $\text{RuCl}_3 \cdot (\text{H}_2\text{O})_x$ Catalyzed Olefination

김세진¹ 서현옥¹ 나영임² 한소엽^{2,*}

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이화여자대학교 화학나노과학과, 촉매반응·합성연구센터

We have developed an efficient catalytic system to form alkenes by the addition reaction of aldehydes to alkynes using the $\text{RuCl}_3 \cdot (\text{H}_2\text{O})_x$. To understand the role of the catalyst, we extensively studied the reaction mechanism of decarbonylative olefination. The result of our study will be discussed at the presentation in details. This work is supported by the NRF (WCU project R33-10169)



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발표코드: ORGN.P-675

발표분야: 유기화학

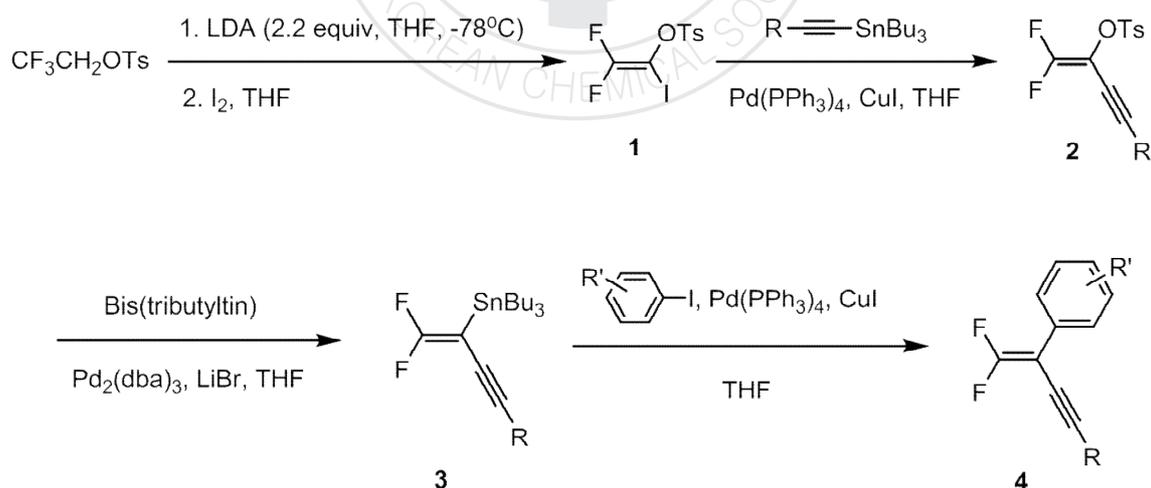
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of 1,1-difluoro-2-tributylstannylenynes and their reactions

김주희 정인화^{1,*}

연세대학교 화학과 ¹연세대학교 화학및의화학과

2,2-Difluoro-1-iodoethenyl tosylate **1** was synthesized in 80% yield from the reaction of 2,2,2-trifluoroethyl tosylate with 2.2 equiv of LDA at -78°C, followed by treatment with iodine. Alkynylation reaction of **1** with alkynylstannanes afforded 1,1-difluoroenynes **2** in 52~73% yields. Stannylation of **2** with bis(tributyltin) reagent in the presence of Pd₂(dba)₃ and LiBr in THF provided 1,1-difluoro-2-tributylstannylenynes **3** in 30~44% yield. The cross-coupling reactions of **3** with aryl iodides provided 1,1-difluoroenynes **4**. The scope and limitation of these reactions will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-676**

발표분야: 유기화학

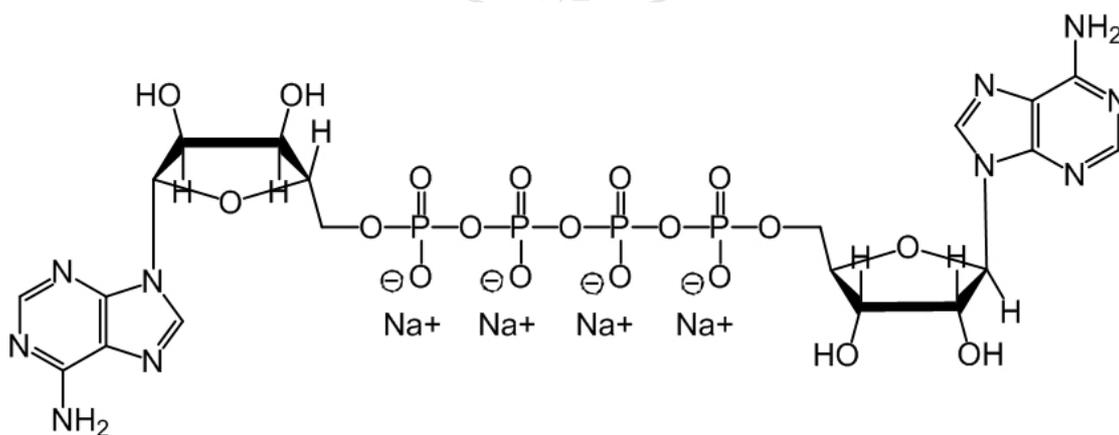
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Development for the preparation of Dinucleoside oligophosphate (NpnN)

고덕환 강용한*

한양대학교 응용화학과

Diadenosine oligophosphate (ApnA) is made up of two adenosine moieties joined by a 5P-5P linkage with a chain from two to six phosphodiester linkages. ApnA has discovered by P. Zamecnik and his co-workers in the mid-sixties. Recently, ApnA has emerged as intracellular and extracellular signalling molecules implicated in the maintenance and regulation of vital cellular functions and is considered as a second messenger. A high-yield synthesis for NpnN and their analogues would facilitate studies of their possible medical applications. We have developed the route for the preparation of Ap4A and Ap4G that makes the trimetaphosphate in a more efficient method.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-677

발표분야: 유기화학

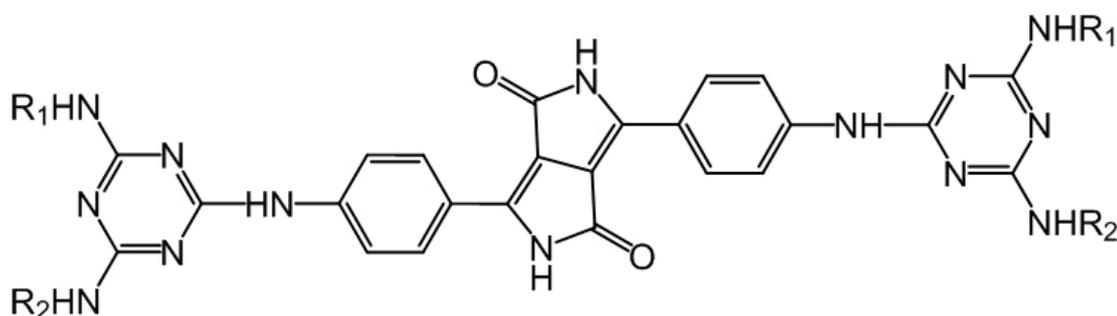
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of 3,6-bis[4-(2,4-substituted-1,3,5-triazin-6-yl)- amino]phenyl-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione as the Derivatives of DPPs

김주영 이은영 강용한*

한양대학교 응용화학과

In 1974, Farnum, et al. briefly reported their attempt on the synthesis of 2-azetines by the reaction of benzonitrile with ethyl bromoacetate. The desired reaction failed and instead, the diphenyl DPP, 3,6-diphenyl-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione, was isolated in 5-20% yield. Now DPPs are used as pigments in paints, plastics, fibers, and inks. In this research, derivatives of 3,6-bis[4-(2,4-substituted-1,3,5-triazin-6-yl)amino]phenyl-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione were synthesized and studied using optical characterization (absorption and fluorescence).



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: ORGN.P-678

발표분야: 유기화학

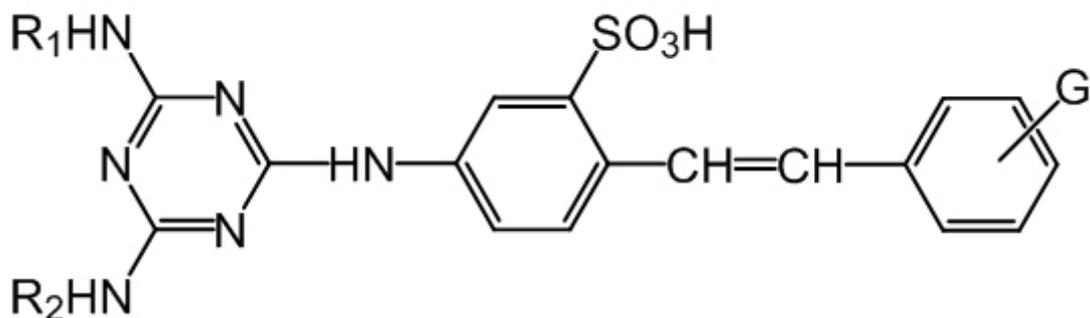
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of 4-(2,4-substituted-1,3,5-triazin-6-yl)aminostilbene-2-sulfonic acid derivatives as the Fluorescent Whitening Agent

김성래 정진성 강용한*

한양대학교 응용화학과

Disodium 4,4'-bis(triazinylamino)stilbene-2,2'-disulfonate derivatives are most widely used as the fluorescent brighteners for the whitening both cotton and wool. The whiteness of stilbene derivatives were increased by a process of absorbing ultraviolet ray (330~380nm) and emitting visible blue lights (400~450nm). This research relates to synthesis of p-nitro-substitutedstilbene-2-sulfonic acid derivatives and its application as dye intermediates. Various p-nitro-substitutedstilbene-2-sulfonic acid derivatives are prepared from the reaction of 4-nitrotoluene-2-sulfonic acid with aryl aldehydes then converted to 4-(2,4-substituted-1,3,5-triazin-6-yl)aminostilbene-2-sulfonic acids.



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발표코드: **ORGN.P-679**

발표분야: 유기화학

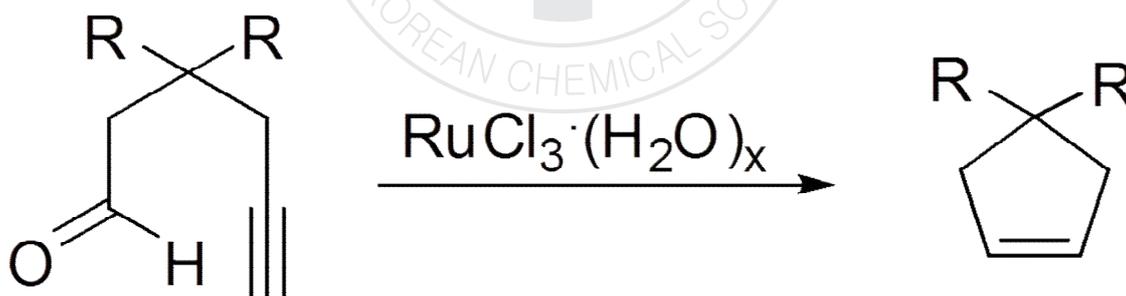
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on a Ru-Catalyzed Intramolecular Olefination

문지현 서현옥 김세진¹ 나영임² 한소엽^{2,*}

*이화여자대학교 화학나노과학과 ¹이화여자대학교 화학나노과학과, 촉매반응·합성연구센터 ²
이화여자대학교 화학나노과학과, 촉매반응·합성연구센터*

We have explored an efficient intramolecular olefination between aldehyde and alkyne moieties to form corresponding cycloalkene by using ruthenium(III) chloride hydrate as a catalyst. The optimized condition of intramolecular decarbonylative olefination has been thoroughly studied. Through our presentation, we will show the result in details. This work is supported by the NRF (WCU project R33-10169)



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발표코드: **ORGN.P-680**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of butyrylcholinesterase inhibitors using S-allyl cysteine derivatives

김범철 이승환¹ 임용배² 박정호^{3,*}

한밭대학교 생명공학과 ¹한밭대학교 응용화학과 ²한밭대학교 응용화학 ³한밭대학교 응용화학생명공학부

Recently, the molecular hybridization, the combination of appropriate pharmacophores onto one compound, has been developed to quickly find out promising drug candidates. It may overcome the recent problems in the pharmaceutical field such as appearing diseases having multiple pathogenic factors and drug resistant organisms. Hybrid compounds may have advantages over their parent molecules in having new biological activities. Therefore, we have tried to look for novel compounds to inhibit BuChE and they can be a candidate drug to treat AD patient. Although garlic (*Allium sativum*) has showed several benefit effects such as bactericidal, bacteriostatic, antimicrobial, antiviral, antisclerotic, antihypertensive, anti-aggregation and anticancer activity, it has showed some adverse reactions. In order to eliminate these adverse reactions, garlic was aged to result in 'aged garlic extract' (AGE). AGE showed beneficial activities for AD such as antioxidant and A β lowering properties. S-allyl cysteine (SAC) is one of the major components of AGE. A series of S-allyl cysteine (SAC) derivatives were synthesized and their in vitro cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated. Even though SAC itself didn't show any inhibitory activity against cholinesterase (ChE), all hybrid molecules including isopropyl ester selectively inhibited BuChE over AChE (more than 60 fold).

일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-681**

발표분야: 유기화학

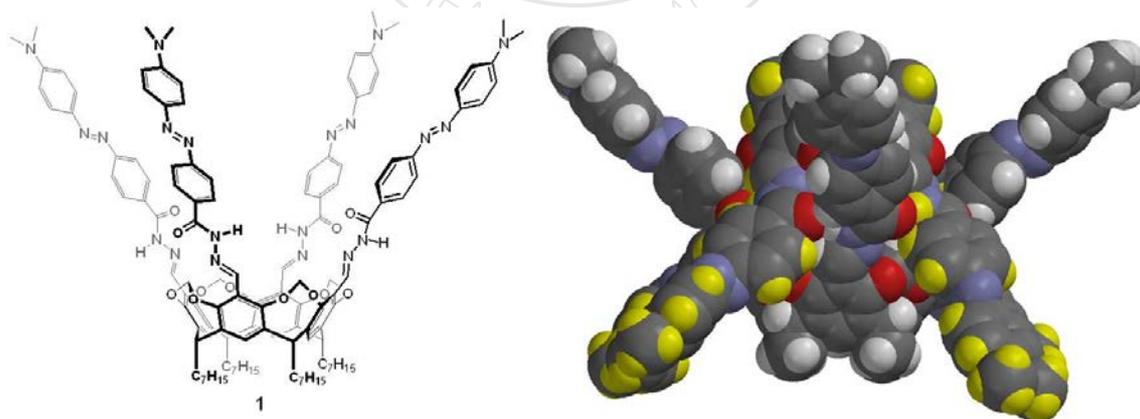
발표종류: 포스터, 발표일시: 수 16:00~19:00

Chromogenic Molecular Capsule for Naked-Eye Detection

박주완 박연실 백경수*

승실대학교 화학과

A new chromogenic self-assembled molecular capsule was developed by the introduction of four azobenzene moieties on the upper rim of a amidoimino-cavitand based on resorcin[4]arene. Cavitand 1 self-assembled to molecular capsules I_2 in the presence of suitable guests via the eight intermolecular N-H...O=C hydrogen bonds. The capsular complex $G@I_2$ showed a large bathochromic shift as well as hyper-chromic effect upon the addition of organic acid. The color change from deep yellow to violet can be observed by naked eyes. The synthesis and atomic force microscopy (AFM), UV-Vis, ^1H NMR spectroscopic studies on this chromogenic molecular capsule will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-682**

발표분야: 유기화학

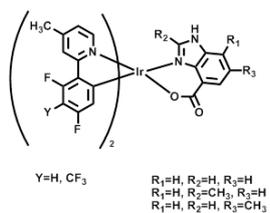
발표종류: 포스터, 발표일시: 수 16:00~19:00

Heteroleptic Blue Phosphorescent Iridium(III) Complexes Containing Main Ligand, 2-Phenylpyridines and Ancillary Ligand, Methylbenzimidazole 4-Carboxylates

김지나 유현지 윤웅찬*

부산대학교 화학과

Phosphorescent iridium complexes attract more attention as emitting-materials for OLEDs because their highly efficient phosphorescence which originates from strong spin-orbit coupling leads to high internal quantum efficiencies in devices. In particular, Ir(ppy)₃ (ppy : 2-phenylpyridine) and its derivatives have attracted much attention because systematic fine control of the emission color can be possible by introduction of substituents or extension of π -conjugation on the main and (or) ancillary ligands. Based on the earlier observations, we designed new iridium complexes which consist of main ligand, 2-(2',4'-difluorophenyl)-4-methylpyridine and 2-(2',4'-difluoro-3'-trifluoromethylphenyl)-4-methylpyridine, and ancillary ligand, 2-, 6-, and 7-methylbenzimidazole 4-carboxylate. The main ligands were prepared by utilizing a Suzuki coupling reaction and the new three ancillary ligands were prepared following a modified method of the reported. With the main ligands and ancillary ligands, the designed six heteroleptic iridium complexes were prepared by a conventional reaction of chloro-bridged main ligand dimers and the ancillary ligands. Their structures were fully characterized by ¹H-, ¹³C-NMR, and high resolution mass spectroscopy. The iridium complexes exhibit absorptions at 441~449 nm caused by MLCT*³ and strong blue emissions in the wavelength region of 459~467 nm (CH₃OH) and 466~476 nm (film) with moderately high quantum efficiencies (Φ 0.12~0.28). (This work was supported by a 2-Year Research Grant of Pusan National University)



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-683

발표분야: 유기화학

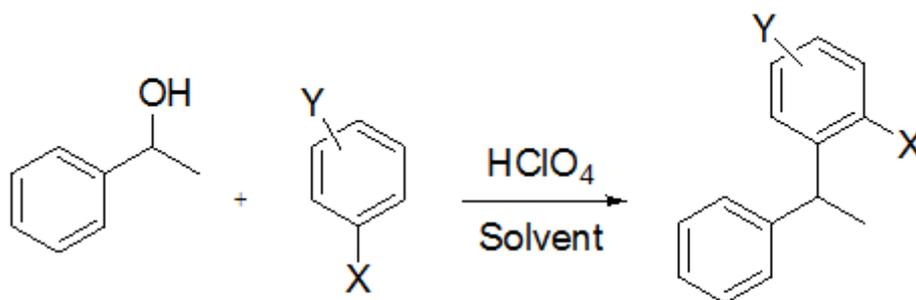
발표종류: 포스터, 발표일시: 수 16:00~19:00

Friedel-Crafts reaction of 1-phenylethanol with phenol derivatives in presence of perchloric acid

이영은 안현석 shabbir saira¹ 백정현¹ 이학준^{1,*}

한양대학교 바이오테크놀로지학과 ¹한양대학교 응용화학과

Friedel-Crafts reaction is widely used to introduce C-C bond formation in organic synthesis. Typical catalysts of Friedel-Crafts reaction are AlCl₃ or FeCl₃. We tried the reaction using perchloric acid as catalyst in order to perform the reaction effectively. Perchloric acid has some advantages such as easy to handling, cost effectiveness, clean synthetic methods so, we could find the reasonable reaction condition. In this study, the reaction of 1-phenylethanol with phenol derivatives was carried out in various polar aprotic solvent and we controlled temperature condition and equivalents of perchloric acid. The case of Tolterodine which was reported previously in our group was also applied and we performed to confirm the process improvement. We expect that it can be applied in the synthesis of useful pharmaceutical ingredients.



X = OH, OCH₃, CH₃, NH₂
Y = OH, F, Cl, Br, CH₃, NO₂

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-684

발표분야: 유기화학

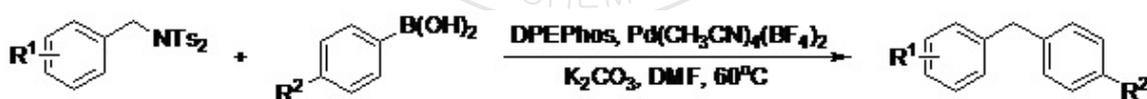
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Palladium-Catalyzed Reaction of Benzyl N,N-Ditosylimides with Arylboronic Acids

윤상은¹ 홍명찬¹ 이신영¹ 이용우² 이학준^{2*}

한양대학교 바이오테크놀로지학과¹ 삼화페인트공업(주) 정밀화학팀² 한양대학교 응용화학과

The Tsuji-Trost reaction is a palladium-catalyzed cross coupling reaction of carbon nucleophile with π -allylpalladium complexes. Various allylic substrates such as halides, acetates, ethers, sulfones, carbonates, alcohols, and phosphates have been studied for Tsuji-Trost reaction. Recently, Some examples of Tsuji-Trost reaction using the benzylic halides and carbonates as pseudo allylic substrates have been reported. Our group already showed that allyl N,N-ditosylimide can be applied to Pd(0)-catalyzed reaction. Here, we present that the coupling reaction of benzyl N,N-ditosylimides can be proceeded with arylboronic acids in the presence of Pd catalyst.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-685

발표분야: 유기화학

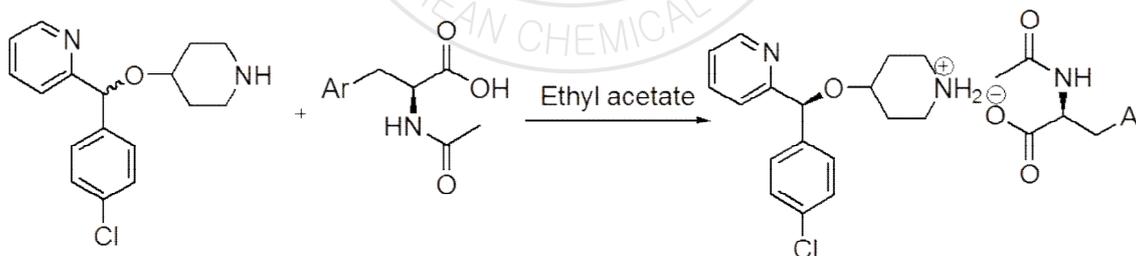
발표종류: 포스터, 발표일시: 수 16:00~19:00

Chiral Resolution of rac-2-[(4-Chlorophenyl)(4-piperidinyloxy)methyl]pyridine for the Synthesis of Anti-histamine Drug, Bepotastine

이신영 안현석 이학준^{1,*}

한양대학교 바이오테크놀로지학과 ¹한양대학교 응용화학과

(S)-Bepotastine is one of the non-sedative anti-histamine drugs, that shows lower blood brain barrier (BBB) permeability. Chiral resolution of racemic mixture is an applicable method for large scale process. In this study, we obtained (S)-2-[(4-chlorophenyl)(4-piperidinyloxy)methyl]pyridine [(S)-CPMP] which is an important intermediate for the synthesis of (S)-Bepotastine by the chiral resolution of rac-CPMP with N-acetyl-L-aminoacid.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-686

발표분야: 유기화학

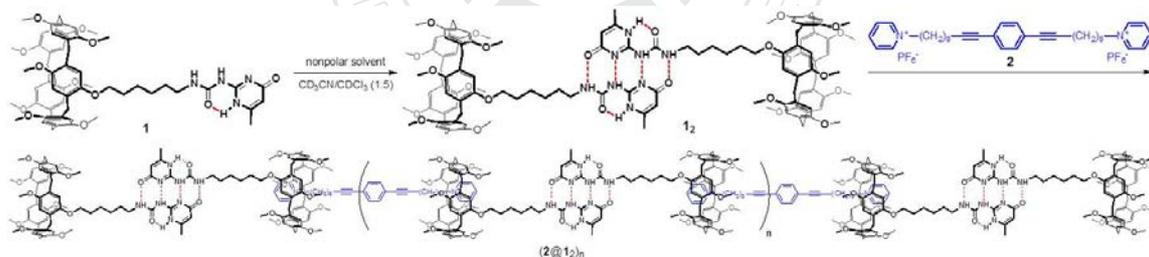
발표종류: 포스터, 발표일시: 수 16:00~19:00

The formation and structure of self-assembled supramolecules based on Copillar[5]arene

황성민 박연실 백경수*

승실대학교 화학과

Copillar[5]arene **1** mono-substituted with ureido-4[1H]-pyrimidone itself forms stable dimer **1₂** by quadruple hydrogen bonds, and the dimer **1₂** can self-assemble into supramolecular structures through cation- π interactions when di-cationic bridging guests **2** are present. The characteristics of these self-assembled supramolecular structures were studied by ¹H NMR and atomic force microscopy (AFM).



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: ORGN.P-687

발표분야: 유기화학

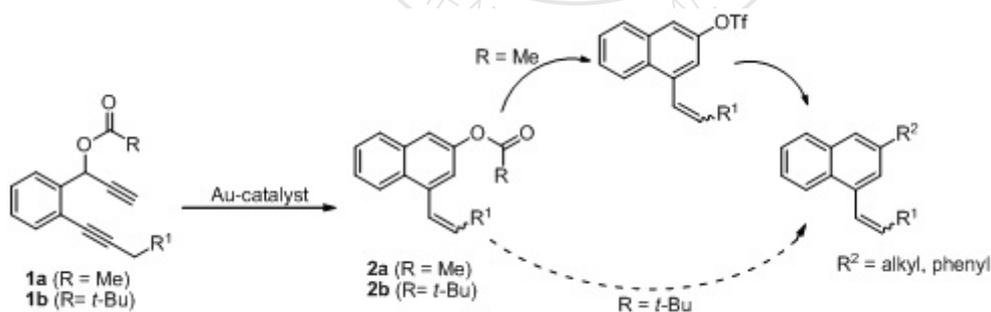
발표종류: 포스터, 발표일시: 수 16:00~19:00

Au(III)-catalyzed cyclization of 1-(2-(1-ynyl)phenyl)prop-2-ynyl acetate to 2-acetoxynaphthalene and its application

정은영 김지희 오창호*

한양대학교 화학과

We have synthesized [6,6]-bicyclic compounds(2a-b) bearing various substituents via gold(III)-catalyzed dual activation of propargylic carboxylate and another triple bond in substrates(1a-b). The resultant acetate groups(2a), after changing to OTf groups, have been functionalized by using various coupling reactions (sonogashira reaction, suzuki reaction, heck reaction). Alternatively, the pivalate(1b) could be cyclized in the same manner to give 2b which is known directly to undergo C-C bond formations like Heck reaction.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-688**

발표분야: 유기화학

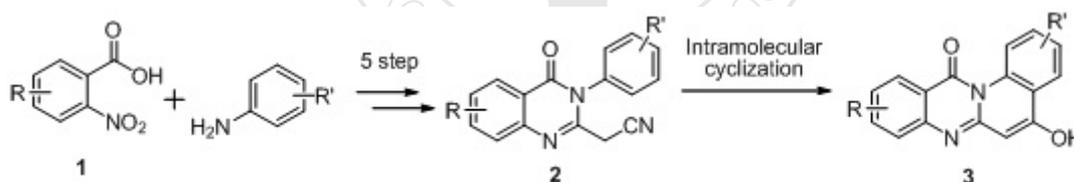
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 5-hydroxy-12H-quinolino[2,1-b]quinazolin-12-one derivatives

박종률 유진 오창호*

한양대학교 화학과

Heterocyclic 5-hydroxy-12H-quinolino[2,1-b]quinazolin-12-one systems (3) are interesting compounds because of their broad-ranging biological activities and working as variety colored compounds. We have developed an efficient synthesis for a variety of 5-hydroxy-12H-quinolino[2,1-b]quinazolin-12-one derivatives. The key precursors 2 were prepared from 2-nitrobenzoic acid derivatives 1 in five steps, and cyclized under acid-catalysis to give 3 in good yields.



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발표코드: **ORGN.P-689**

발표분야: 유기화학

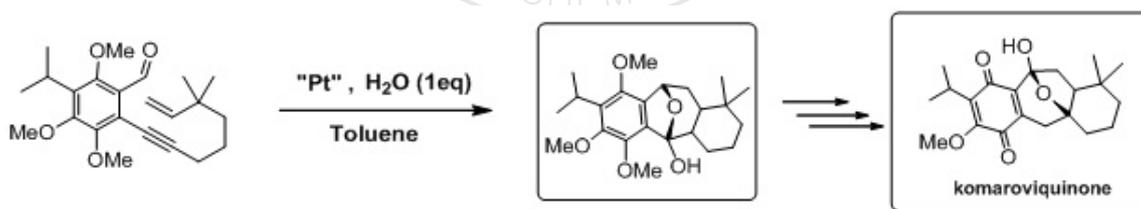
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study of komaroviquinone via Pt-catalyzed [6,7,6] tricyclic hydrative cycloaddition

김소영 PIAOLANHUA 오부근 오창호*

한양대학교 화학과

Komaroviquinone is a nature product which was isolated from uzbek plants “Buzbosh”(Dracocephalum komarovi). “Buzbosh” showed strong in vitro trypanocidal activity against epimastigotes of Trypanosoma cruzi. Our group reported Pt-catalyzed hydrative cycloaddition of o-alkynylbenzaldehydes with an unsaturated bond. This Pt-catalyzed hydrative cycloaddition has successfully served to synthesis of faveline Methyl Ether as a key step. Encouraged by this result, we planned to synthesize komaroviquinone by utilizing Pt-catalyzed hydrative cyclization as a key step. The general scheme is shown as follows.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-690**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative C-H Activation/Cyclization for the Synthesis of Phosphaisocoumarins and Phosphorous 2-Pyrones Catalyzed by Rhodium

박영철 박상준 유은정 이필호*

강원대학교 화학과

The rhodium-catalyzed cyclization of phosphinic acids and phosphonic mono-esters with alkynes has been developed. The oxidative annulation proceeded with complete conversion of phosphinic acid derivatives and allowed for the atom economic preparation of useful phosphaisocoumarins with high yield and selectivity. The reaction is tolerant of extensive substitution on the phosphinic acid, phosphonic mono-esters and alkynes, including halides, ketone, and hydroxyl group as substituents. Also, we found that alkenylphosphonic mono-esters proceed to give a wide range of phosphorus 2-pyrones through oxidative annulations with alkynes. Mechanistic studies revealed the C-H bond metalation to be rate-limiting step.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-691**

발표분야: 유기화학

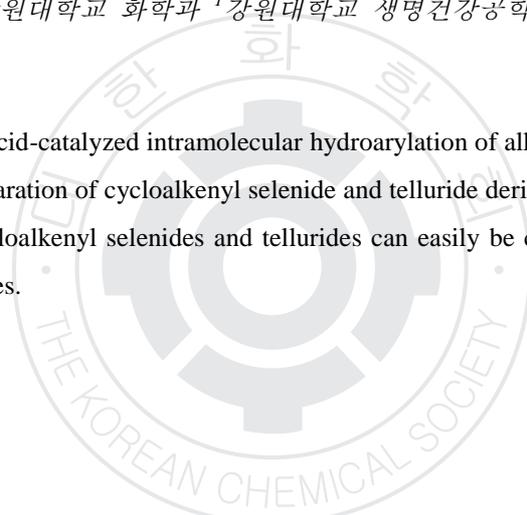
발표종류: 포스터, 발표일시: 수 16:00~19:00

Brønsted Acid-Catalyzed Intramolecular Hydroarylation of Alkynyl Selenides and Tellurides

엄다한 박상준 박영철 이구연¹ 이필호*

강원대학교 화학과 ¹강원대학교 생명건강공학과

Trifluoromethanesulfonic acid-catalyzed intramolecular hydroarylation of alkynyl selenides and tellurides was developed for the preparation of cycloalkenyl selenide and telluride derivatives through a selective 6- and 7-*endo* mode. The cycloalkenyl selenides and tellurides can easily be converted to a wide range of other valuable functionalities.



일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-692**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative Arylation of Phosphoramidate by Palladium-Catalyzed C-H Bond Cleavage

Bathoju Chandra Chary 김성각* 박영철¹ 이필호^{1,*}

Nanyang Technological University, Singapore ¹강원대학교 화학과

In the past several decades, transition metal-catalyzed cross-coupling reactions have been well developed and widely applied in organic synthesis, which provides useful methods to construct complicated scaffolds. But it is well known that traditional cross-coupling involves two kinds of fully functionalized starting materials, including organic halides and organometallic reagents. So taking the place of either C-X or C-M or both with C-H is an ideal design to make cross-coupling more efficient and cleaner. A highly efficient Pd-catalyzed *ortho*-arylation is reported using phosphoramidate directing group for the first time. Remarkably, the nature of a new directing group drives selective C-H bond activation to afford diverse *N*-aryl phosphoramidates in good to excellent yields at room temperature.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-693**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of 4,6-Disubstituted Phosphorus 2-Pyrones through Gold-Catalyzed Sequential Alkyne Activation

모준태 강동진 엄다한 김성홍¹ 신서현 이필호*

강원대학교 화학과 ¹한국기초과학지원연구원 대구분소

Organophosphorus compounds continue to receive widespread attention due to their ubiquity in biological systems and their potential to serve as novel pharmaceuticals. 2-Pyrones are an important structural motif found not only in valuable biologically active compounds but also in diverse synthetic intermediates. Since there is a remarkable similarity in reactivity and bioactivity between the carbon species and their phosphorus counterparts, we imagined phosphorus 2-pyrones to have potential bioactivities similar to those of the 2-pyrones reported. Herein, tandem gold-catalyzed addition of alkynyl phosphonic acid monoethyl esters to terminal alkynes and cyclization were developed for the synthesis of 4,6-disubstituted phosphorus 2-pyrones in one reaction vessel based on the concept of sequential alkyne activation. Alkynyl enol phosphonates were selectively obtained through the gold catalyzed addition reaction in presence of a catalytic amount of triethylamine. Also, gold-catalyzed cyclization of alkynyl enol phosphonates was successful in giving a variety of 4,6-disubstituted phosphorus 2-pyrones.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-694**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium-Catalyzed Oxidative Coupling of Phosponamide and Phosphinamide Group via C-H Activation and Annulation

박상준 서보람 신서현 손정유 김예린 이필호*

강원대학교 화학과

The site-selective formation of carbon-carbon bonds through Catalytic C-H functionalization has developed its effect on economically attractive strategy in the synthesis of organic molecules. Rhodium catalysts in particular are prominent in the area of formation of C-C bonds that proceed with C-H functionalization for their high functional group tolerance and wide range in utility of synthesis. Recently, our group have focused on phosphoryl-related compounds as the directing group for C-H activation. therefore, In regard to new directing group with desired synthetic features, we drew attention to the phosphonamide and phosphinamide moiety. We have developed an efficient rhodium-catalyzed oxidative coupling via C-H activation and annulation using arylphosponamides and arylphosphinamides under aerobic conditions, which produced benzazaphosphole 1-oxides and phospha-isoquinolin-1-oxides with high selectivity, a wide substrate scope and an excellent functional group tolerance.

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장소: 창원CECO

발표코드: **ORGN.P-695**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Vinyl Sulfides and Amines through Catalytic Intramolecular Hydroarylation in the Presence of FeCl₃ and AgOTf

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Synthetic method was developed for the preparation of vinyl sulfides and vinylamines from arylalkynyl phenyl sulfides and sulfonamides. Under mild conditions, a catalytic intramolecular hydroarylation reaction was carried out in the presence of FeCl₃ and AgOTf (OTf = trifluoromethanesulfonate) in 1,2-dichloroethane. A variety of 1,2-dihydronaphthalenes, 2H-chromenes, and 1,2-dihydroquinolines containing a phenylsulfenyl or N-phenyl-N-tosyl group on the sp²-hybridized benzylic carbon were prepared in good to excellent yields. The present method could be extended to the preparation of dihydropyrano[2,3-g]chromenes through a twofold Fe-catalyzed hydroarylation by a selective 6-endo mode.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium-Catalyzed Oxidative Cyclization of Arylphosphonic Acid Monoethyl Esters with Alkenes

류태규 김재은 박영철 김상혁 김철의 이필호*

강원대학교 화학과

C-H bond functionalizations catalyzed by transition metals have demonstrated to be a very streamlined method for the formation of C-C and C-heteroatom bonds. In particular, *ortho* C-H bond functionalizations can be accomplished by the employment of a variety of directing groups with the aid of coordination of transition metals. In a number of directing groups for C-H bond functionalizations, nitrogen-containing compounds, carboxyl and hydroxyl ones have been broadly investigated. We report for the first time rhodium-catalyzed tandem oxidative alkenylation and intramolecular *oxa*-Michael reaction using arylphosphonic acid monoethyl esters and alkenes under aerobic conditions, which produced benzoxaphosphole 1-oxides in good to excellent yields.

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발표코드: **ORGN.P-697**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative *ortho*-Alkenylation of Arylphosphine Oxides by Rhodium-Catalyzed C-H Bond Cleavage

모준태 임수진 박상준 류태규 김상혁 이필호*

강원대학교 화학과

C-H activation reaction catalyzed by transition metals has emerged as an atom- and step- economical synthetic method and its synthetic applications have been proved in the preparation of natural products, pharmaceuticals, and organic materials. Recently, we have focused on phosphoryl-related compounds as the directing group for C-H activation. However, the employment of arylphosphine oxide as directing group have been rarely reported. Therefore, development of new C-H activation using phosphorus-related directing group have been rarely reported. We have developed an efficient rhodium-catalyzed oxidative *ortho*-alkenylation of arylphosphine oxides with activated as well as non-activated alkenes with functional group tolerance. Current efforts are directed toward the development of efficient reactions using phosphorus-related functional group and their application.

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장소: 창원CECO

발표코드: **ORGN.P-698**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydroarylation of Aryl Alkynylphosphonates for the Synthesis of Phosphacoumarins Catalyzed by Gold

김철의 류태규 김상혁 이구연¹ 이창희 이필호*

강원대학교 화학과 ¹강원대학교 생명건강공학과

Organophosphorus compounds have been received continuous interests due to their frequency in living systems and their chance to function as novel biological active compounds. Therefore, development of new synthetic method of heterocyclic compounds bearing phosphorus atom is crucial. we foresee that the phosphacoumarin, which may be recognized as a phosphorus-containing analog of coumarin, would have pharmacological activities similar to those of coumarins described. As a consequence, we were attracted in expanding an efficient procedure for the synthesis of a number of phosphacoumarins with the purpose of making focused chemical libraries. we have developed an intramolecular hydroarylation of easily accessible aryl alkynylphosphonates catalyzed by gold/silver catalyst in the presence of TfOH in selective 6-*endo* mode, thus providing an effective and distinctive method for preparing phosphacoumarins having a range of functional groups.

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장소: 창원CECO

발표코드: **ORGN.P-699**

발표분야: 유기화학

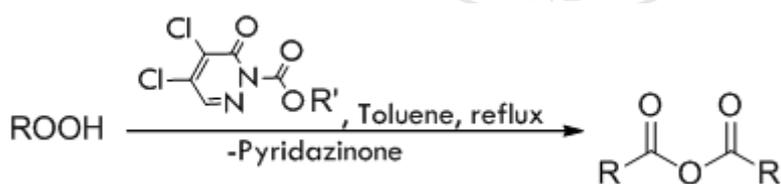
발표종류: 포스터, 발표일시: 수 16:00~19:00

Conversion of Carboxylic Acid to Anhydride Using 2-Alkoxy-carbonyl-4,5-dichloropyridazin-3(2H)-ones

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2-Substituted-pyridazin-3(2H)-ones are useful the electrophilic agents and synthones for the functionalization of the electron rich compounds and active methylenes. Recently, Lee, et al. reported on facile and selective synthesis of carbamates and ureas using phenyl 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylate as carbonyl source. Phenyl 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylate is stable in air and in organic solvents at high temperature, and is prepared easily from cheap and commercially available 4,5-dichloropyridazin-3(2H)-one. Herein, we present a convenient synthetic method of anhydride from carboxylic acid using 2-alkoxy-carbonyl-4,5-dichloropyridazin-3(2H)-ones.



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발표코드: **ORGN.P-700**

발표분야: 유기화학

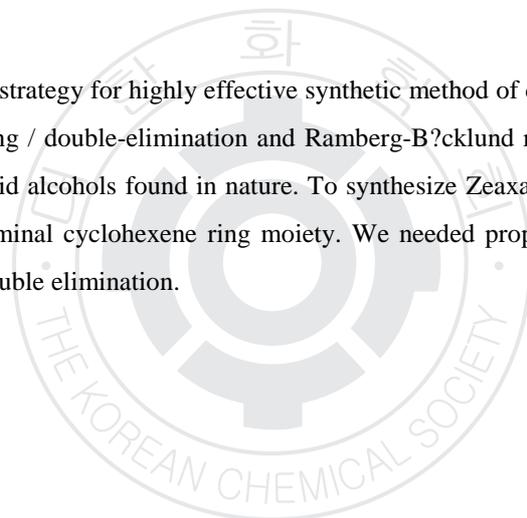
발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on effective synthesis of carotenoid Zeaxanthin

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Our group has developed a strategy for highly effective synthetic method of carotenoid compounds on the basis of the sulfone coupling / double-elimination and Ramberg-B α cklund reaction. Zeaxanthin is one of the most common carotenoid alcohols found in nature. To synthesize Zeaxanthin required the controlled allylic oxidation in the terminal cyclohexene ring moiety. We needed proper protection, coupling with C10 di-aldehyde and the double elimination.



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발표코드: **ORGN.P-701**

발표분야: 유기화학

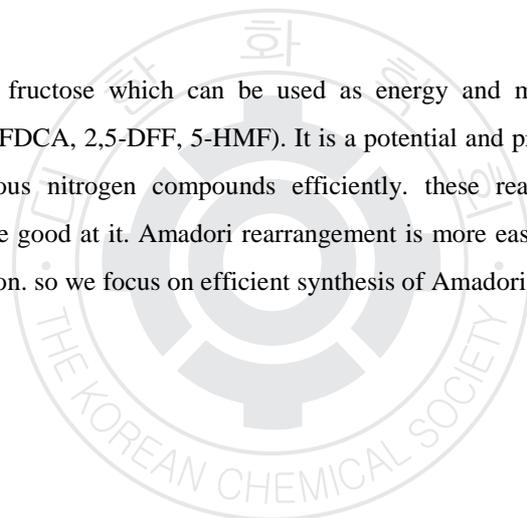
발표종류: 포스터, 발표일시: 수 16:00~19:00

study of N-glycosylation and Amadori reaction of glucose

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Biomass such as glucose, fructose which can be used as energy and medicinal material is sort of commodity chemicals (2,5-FDCA, 2,5-DFF, 5-HMF). It is a potential and promising object to synthesize of glucose attaching various nitrogen compounds efficiently. these reactions, N-glycosylation and Amadori rearrangement, are good at it. Amadori rearrangement is more easier to use medicinal material than N-glycosylation reaction. so we focus on efficient synthesis of Amadori rearrangement.



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발표코드: **ORGN.P-702**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Research of the synthetic method and electric characteristics of the Unnatural Carotenoids

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The carotenoids which take the form of a polyene hydrocarbon chain are an important class of organic molecules with delocalized π -electrons, which show electric conductance. We have demonstrated the synthetic route of natural carotenoids and then made the unnatural carotenoid wires containing various aromatic substituents by using the synthetic route. The unnatural conductive carotenoids can be disconnected into Allylic sulfone and Dialdehyde unit containing aromatic substituents. These subunits can be assembled by the following reactions ; sulfone-mediated coupling reaction, protection of alcohol, and double elimination. We have measured the conductance of unnatural carotenoid by using AFM/STM equipment. As a result, the conjugated polyene chains of the unnatural carotenoids can improve electronic characteristics compared with the natural carotenoids.

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발표코드: **ORGN.P-703**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Research on synthetic method of Unnatural carotenoid

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We plan to synthesize the conjugated polyene chain containing phenyl substituents. It is postulated that two phenyl substituents in 1,6-position are orthogonal to conjugated polyene chain which can coordinate with specific metal ions. In our protocol, we utilized sulfone mediated chemistry including coupling reaction between the allylic sulfone and allylic aldehyde. And then subsequent double elimination, we can get fully trans conjugated carotene compound. In order to synthesize the unnatural carotenoids, it is necessary to design efficient building blocks. Allylic sulfone unit containing phenyl substituents can be readily prepared from acetophenone derivatives via indium mediated addition and oxonia-cope rearrangement. Allylic aldehyde unit can be easily obtained. Based on our design, it is feasible to synthesize the conjugated polyene chain with di phenyl substituents.

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발표코드: **ORGN.P-704**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Regioselective construction of 1- α -tocopheryl-2-glyceride for the synthesis of self-assembled membrane

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Phosphatidylcholine is one of the main components of cell membranes. A general phosphatidylcholine is composed of a choline head group that is hydrophilic part and two fatty esters being hydrophobic tail group. We decide to replace one of the ester by α -tocopherol, which is a well known anti-oxidant. We have synthesized 1- α -tocopheryl-3-glyceride by using acetic acid through the regioselective ring opening reaction of the α -tocopherylglycidylether, followed by the esterification using various carboxylic acid. Then 1- α -tocopheryl-2-glyceride can be obtained by reduction. Phosphatidylcholine part were synthesized by transferring the hydroxy to the polar group. We synthesized various 1- α -tocopheryl-2-glycerides, which would be efficiently utilized for the formation of diversely substituted phosphatidylcholine derivatives.

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발표코드: **ORGN.P-705**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantiopure Gamma Amino Acid of gauche-gauche Conformation: Synthesis of Linear Hybrid Peptides and Foldameric Properties

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The diversity of sizes, shapes and arrangements available with non-natural monomers offers a myriad of opportunities for designs of molecular interaction modules supported by foldamer frameworks. The creation of these frameworks has already resulted in many intellectually useful and functionally interesting molecules. The design and synthesis of foldamers from gamma amino acids is a recent trend. Sugar Amino Acids (SAAs) are enantiopure sugar moieties containing amino and carboxyl group. Herein, we want to report the synthesis of linear hybrid peptides containing enantiopure gamma amino acids of gauche-gauche conformation to study their folameric properties.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The novel oxidation method of 1, 3-dicarbonyl derivatives catalyzed by Mn(OAc)₃ and the application on cyclic compound synthesis

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The organic compounds with cyclic skeleton are of great importance and usage in medical, chemical and material industry. It is known that furan is frequently used as a starting material for the synthesis of other specialty chemicals and polycyclic ring structures in medical chemistry to develop multi-functional drugs. Mn(OAc)₃ can initiate carbon radical formation of 1,3-dicarbonyl compounds and subsequent cyclization. However, in our reaction system, the Mn(OAc)₃-triggered carbon radical trapped one molecular of oxygen from the air instead of carrying out the radical addition reaction to unsaturated bond. After the sequence of deacetylation, double bond migration and hydroxylation, various polycyclic structures and aromatic furan derivatives were successfully accomplished from different 1, 3-dicarbonyl resources.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Peptoid-based ApoE/A β Binding Inhibitors

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이화여자대학교 화학·나노과학과

Alzheimer's disease (AD) is the progressive neurodegenerative disease and the accumulation and aggregation of amyloid- β (A β) as plaques in the brain are pathological hallmarks of AD. Generally, the rates of AD increase dramatically with aging. Thus, it's critically needed to develop treatments for AD. Current treatments can only temporarily slow down the progressing of AD symptoms, i.e., there is no cure. A β is a 39- to 43-aa peptide, which is derived from cleavage of the transmembrane amyloid precursor protein and A β 40 and A β 42 are two major variants in humans. The fibril formation of A β homologous peptides can be promoted by A β pathological chaperone proteins such as apolipoprotein E (ApoE). Inheritance of ApoE4 allele is the important risk factor for AD. ApoE and A β bind in vivo and in vitro, emphasizing the importance of the ApoE/A β interaction for the modulation of aggregation and clearance of A β . Thus, blocking the ApoE/A β interaction has been considered a novel therapeutic approach for AD. Residues 12-28 of A β were identified to be the binding motif for ApoE on A β , and a synthetic peptide homologous to 12-28 aa sequence of A β (A β 12-28) was demonstrated to be a competitive inhibitor of ApoE/A β interaction. However, peptides are sensitive to proteases and have poor cell permeability and poor bioavailability. Therefore, we envisioned to develop more effective inhibitors with better pharmacokinetic properties and biological activities for blocking the ApoE/A β interaction by using peptidomimetic approach. In this study, we synthesized a series of peptoid-based chemical tools in both linear and cyclic forms as possible ApoE/A β inhibitors because peptoids possess many characteristic advantages over peptides.

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발표코드: **ORGN.P-708**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed *ortho*-Olefination of Aryl Hydrogen Phosphates Using a New mono-Phosphoric Acid Directing Group

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Nanyang Technological University, Singapore ¹강원대학교 화학과

Over the years, chemists have pursued their ways to activate and functionalize inert C-H bond. In the latest fashion, such C-H activation reactions are impressively enhanced by the use of directing groups or ligands to control the selectivity. Most widely used directing groups in Pd(II)-catalyzed C-H activation reactions utilize carboxylic derivatives along with N-heterocycles. The phosphoric acid and its derivatives are important constituents of living organisms and also have been widely exploited as organic catalysts and coupling partners in Pd-catalyzed cross-coupling reactions. A highly efficient Pd-catalyzed *ortho*-alkenylation is reported using mono-phosphoric acid-directing group for the first time. This phosphoric acid-directing group is successfully utilized for the synthesis of various alkenylated products and offers a new way to transition metal-catalyzed C-H activation.

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발표코드: **ORGN.P-709**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Tandem Gold-Catalyzed Hydrosilyxylation-Aldol and -Mannich Reaction

류태규 박영철 박상준 정연석 이필호*

강원대학교 화학과

Aldol and Mannich reaction rely on the activation of carbonyl compounds by transforming them into enolates or their derivatives. These moieties have been synthesized from the carbonyl compounds by deprotonation with bases or deprotonation-enolate trap with electrophiles. However, because sensitive functional groups are not tolerable under these conditions, enolates or enol derivatives must be synthesized apart in advance of the addition of electrophiles in the following step, indicating that the selective preparation of an enolate from another precursor in lieu of carbonyl compounds is very important. Thus, we have tried to develop synthetic methods of enol derivatives from easily accessible noncarbonyl precursors. Tandem gold-catalyzed hydrosilyxylation-aldol and hydrosilyxylation-Mannich reaction were developed through the formation of enol silyl ether catalytically generated in situ from alkynylaryloxysilanols in 6-*exo* mode in one reaction vessel.

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발표코드: **ORGN.P-710**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Phosphaisocoumarins through Rhodium-Catalyzed Oxidative Annulation Using Alkynes and Arylphosphonic Acid mono-Esters

박영철 진인철 류태규 박상준 이필호*

강원대학교 화학과

A rhodium-catalyzed cyclization using alkynes and arylphosphonic acid monoesters for the synthesis of phosphaisocoumarins is reported. A range of substrates were selectively cyclized in high yield with functional group tolerance. Additionally, unsymmetrical alkynes are applied in high efficiency and regioselectivity. Further studies to examine differences or similarities between the reaction of aromatic acids and phosphonic acids and expand the synthetic scope of this reaction are currently underway.

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장소: 창원CECO

발표코드: ORGN.P-711

발표분야: 유기화학

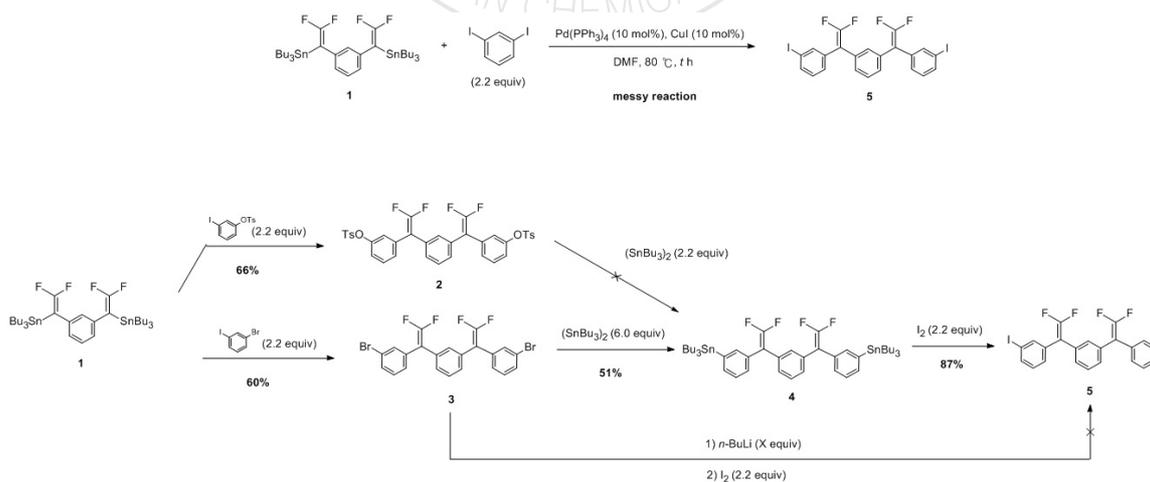
발표종류: 포스터, 발표일시: 수 16:00~19:00

An attempt to synthesis of 1,3-bis(2,2-difluoro-1-(3-iodophenyl)vinyl)benzene

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연세대학교 화학과 ¹연세대학교 화학및의화학과

Cross-coupling reaction of 1,3-iodobenzene with stannane reagent 1 to give 1,3-bis(2,2-difluoro-1-(3-iodophenyl)vinyl)benzene resulted in the formation of messy reaction mixture. Several approaches to synthesis of compound 5 were attempted. Cross-coupling reaction of 1 with 3-iodophenyl tosylate in the presence of catalysts provided the coupled product 2, but further stannylation of 2 did not afford the compound 4. However, the reaction of 1 with 1-bromo-3-iodobenzene gave the compound 3 which underwent stannylation to give the compound 4. Finally, iodination of 4 provided the final compound 5. Direct preparation of 5 from the compound 3 was unsuccessful.



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장소: 창원CECO

발표코드: ORGN.P-712

발표분야: 유기화학

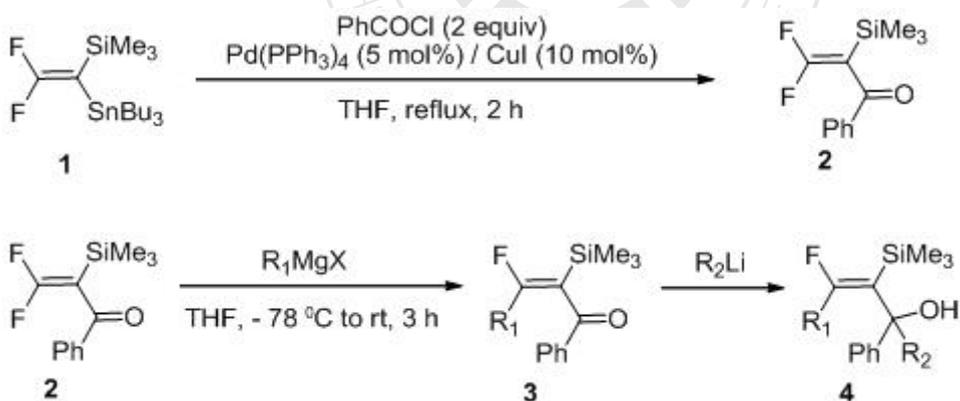
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of 1,1-difluoro-2-(trimethylsilyl)enone and its reactions

정여진 정인화^{1,*}

연세대학교 화학과 ¹연세대학교 화학및의화학과

1,1-Difluoro-2-(trimethylsilyl)enone **2** was prepared in 30 % yield from acylation reaction of 1,1-difluoro-2-(trimethylsilyl)ethenyl tributylstannanes **1** with 2 equiv of benzoyl chloride in the presence of Pd(PPh₃)₄ (5 mol%) and CuI (10 mol%) in THF at reflux temperature for 2 h. When **2** was reacted with various Grignard reagents in THF at -78 °C, the products **3** were obtained via addition and elimination reaction. The reaction of **3** with alkyl lithium afforded the 1,2-addition products **4**.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-713

발표분야: 유기화학

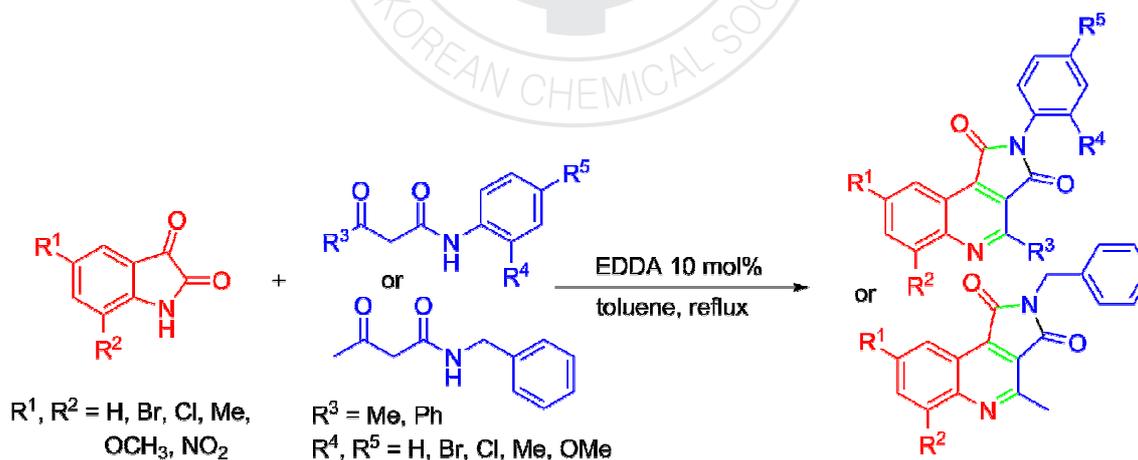
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Cascade Reaction for the Synthesis of Novel and Diverse Pyrrolo[3,4-c]quinoline-1,3-dione Derivatives

하립개 이용록*

영남대학교 화학공학부

We present herein an efficient and novel one-step synthesis of pyrrolo[3,4-c]quinolinedione derivatives using ethylenediamine diacetate (EDDA)-catalyzed cascade reactions of isatins and β -ketoamides. It is the first direct conversion of isatins to pyrrolo[3,4-c]quinolinedione derivatives via C-N bond cleavage and isatin ring expansion. Furthermore, this protocol provides a one-step route to the synthesis of biologically interesting complex molecules that are generally prepared by multi-step reactions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-714**

발표분야: 유기화학

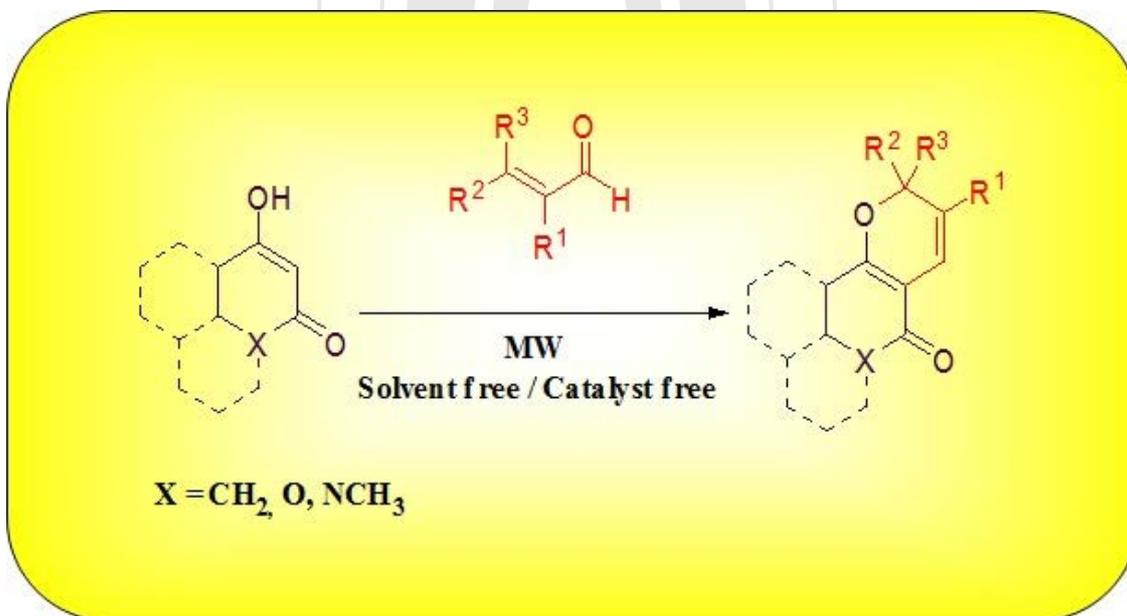
발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalyst- and Solvent-Free One-pot Synthesis of 2H-pyrans

NAUSHADALIEDAYADULLA 이용록*

영남대학교 화학공학부

Herein we present one-pot synthesis of a variety of 2H pyrans using microwave irradiation under solvent- and catalyst-free conditions. This method offers the advantages of a green approach, high yields, and short reaction times. Sixteen compounds were obtained in good to excellent yields using this procedure.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-715**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Computational study of a gold-catalyzed intermolecular coupling reaction

김현우 이영호 이영민*

포항공과대학교 화학과

Gold(I) catalyst has gained much attention due to its capability of activating carbon-carbon triple bonds in mild conditions. This alkyne activation has contributed to developments of many gold(I)-catalyzed reactions. However, intermolecular reaction with high regioselectivity is still a challenging subject in devising new gold-catalyzed reactions and only a limited number of intermolecular reactions can be carried out with this catalyst. Recently, it was reported that a gold(I) catalyst can direct intermolecular coupling between alkynoates and allylic ethers with good regioselectivity. The importance of controlling the regioselectivity in intermolecular reactions warrants more detailed mechanistic studies regarding the involved process. Here, we present our computational investigation on a representative example of this reaction to account for its regioselectivity. We found that intermolecular interaction of reactants activated by the catalyst can induce the regioselectivity even when there are two reaction pathways with similar energy barriers.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-716

발표분야: 유기화학

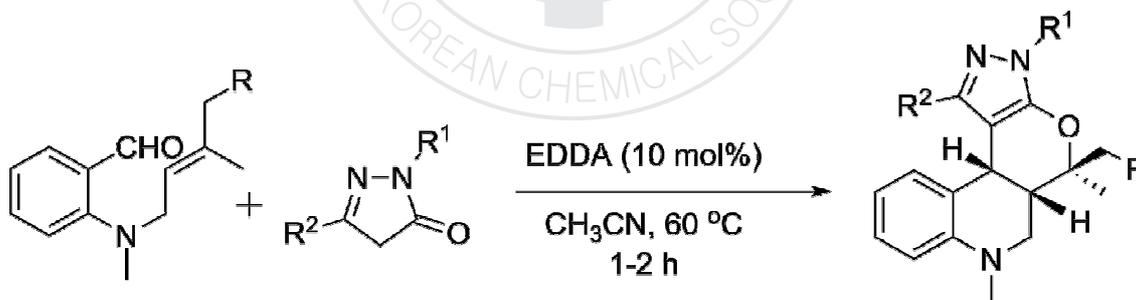
발표종류: 포스터, 발표일시: 수 16:00~19:00

EDDA-Catalyzed Domino Knoevenagel/ Hetero Diels-Alder Reaction for the Synthesis of Tetrahydroquinolines bearing Pyranopyrazoles

PANDIT RAMESHWAR PRA 이용택*

영남대학교 화학공학부

We present herein ethylenediammonium diacetate (EDDA)-catalyzed domino Knoevenagel/ hetero Diels-Alder reaction of substituted aminobenzaldehydes and pyrazolones for the synthesis of tetrahydroquinolines bearing pyranopyrazoles. This methodology provides a rapid synthetic route to a variety of diverse tetrahydroquinolines bearing pyranopyrazoles. The benefits of the methodology include use of non-toxic organocatalyst, short reaction time, high yields and simple workup procedure.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-717

발표분야: 유기화학

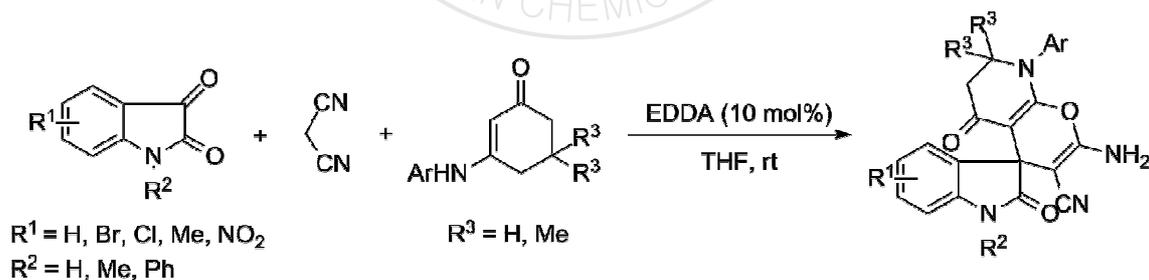
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Diverse Spirooxindole Derivatives Bearing Hexahydroquinolines by Ethylenediamine Diacetate-Catalyzed Multi-Component Reactions

강소량 이용록*

영남대학교 화학공학부

We describe the herein an efficient and one-pot synthesis of a variety of spirooxindole derivatives bearing hexahydroquinolines by Ethylenediamine Diacetate(EDDA)-catalyzed reaction of isatins with malononitrile and enaminones. Spirooxindole derivatives have received considerable attention as leading pharmaceutical compounds because of their pivotal roles in various biological activities such as diuretic, analgesic, myorelaxant, anticoagulant, antibacterial, antimicrobial, anticancer, anti-inflammatory anti-tumor, and anti-HIV.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-718**

발표분야: 유기화학

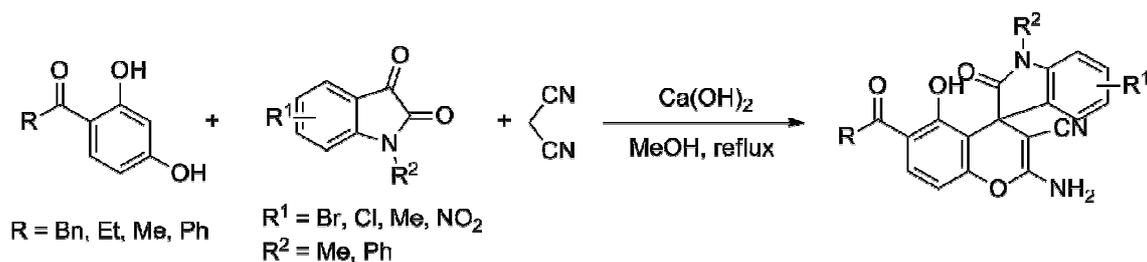
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Synthesis of Diverse 2-Amino-5-Hydroxy-4H-Chromene Derivatives with a Spirooxindole Nucleus by Ca(OH)₂-Mediated Three-Component Reactions

박지향 이용록*

영남대학교 화학공학부

2-Aminochromenes are important heterocyclic compounds with a number of biological and pharmacological properties such as antimicrobial, antiviral, anticonvulsant, antiproliferative, antitumor and anti-cancer. We present herein an efficient one-pot synthesis of biologically interesting 2-amino-5-hydroxy-4H-chromene derivatives bearing spirooxindole skeletons by Ca(OH)₂-mediated three-component reaction of substituted resorcinols with isatins and malononitrile. This simple method provided a variety of biologically interesting diverse 2-amino-5-hydroxy-4H-chromene derivatives in moderate yields under mild reaction conditions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-719

발표분야: 유기화학

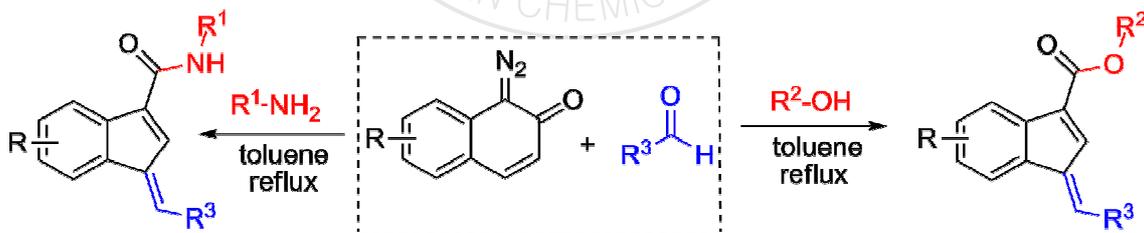
발표종류: 포스터, 발표일시: 수 16:00~19:00

First One-Pot Synthesis of Novel and Diverse Indene Derivatives by Catalyst-Free Thermal Cascade Reactions of 1-Diazonaphthalen-2(1H)-ones

소마이마가크리쉬나 이용록*

영남대학교 화학공학부

We present herein a novel one-pot cascade approach to the synthesis of a variety of 1H-indene-3-carboxamide and 1H-indene-3-carboxylate derivatives by the thermal cascade reactions of 1-diazonaphthalen-2(1H)-ones using a Wolff rearrangement/ketene addition/aldol condensation. This catalyst-free multicomponent coupling reactions provide a rapid approach to the synthesis of various functionalized indene derivatives, which were widely used in the synthesis of natural products and pharmaceuticals.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-720

발표분야: 유기화학

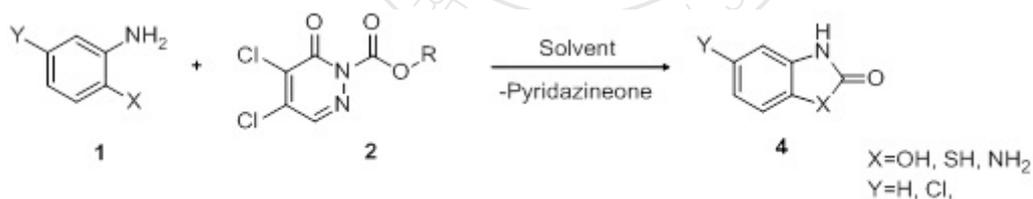
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Benzo[d]azol-2(3H)-ones Using Aryl(or alkyl) 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylates

유기은 성기현 김보람 김점종¹ 윤용진*

경상대학교 화학과 ¹한국전자통신연구원 IT부품산업기술연구부

Benzo[d]azol-2(3H)-one derivatives are widely used in medicinal chemistry. Benzo[d]azol-2(3H)-one derivatives were synthesized using highly toxic reagents such as phosgene, urea and CO. Thus, we design a synthetic method of benzo[d]azol-2(3H)-one derivatives using Aryl(or alkyl) 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylates as acyl source. Aryl(or alkyl) 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylates are inexpensive, stable and easily preparation. Herein, we present a method of benzo[d]azol-2(3H)-one derivatives using Aryl(or alkyl) 4,5-dichloro-6-oxopyridazine-1(6H)-carboxylates.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-721**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Photoremovable Protecting Group Using Intramolecular Charge Transfer

한관우 박봉서*

동국대학교 화학과

For the last two decades, we have witnessed a surge of photoremovable protecting groups(PPG), which are also known as photocages. Among those, substituted phenacyl photocages have received much attention not only due to many advantages in application over other PPG's, but also due to many interesting aspects in their reaction mechanisms. We have recently discovered that photoinduced releasing of a departing group in a phenacyl PPG can be greatly accelerated by the intramolecular charge transfer. The new PPG consists of a phenacyl group attaching an electron/proton donor pendant at the para position of the phenyl ring. Mechanistic details of photochemistry of the new PPG will be discussed together with a new reaction discovered in this research

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-722**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Amphiphilic Diblock Dendrimers Containing Carbazole as a Core Chromophore

최인화 이재욱* 한승철 윤성희

동아대학교 화학과

In the convergent synthesis of the dendrimers, two feasible methods are the fusion of two dendrons and the stitch of multi-functional group with dendrons. We have developed the fusion and stitching methods for the synthesis of symmetric and unsymmetric dendrimers and diblock codendrimers using click chemistry between an alkyne and an azide. The well-known click chemistry which is useful tool for synthesis of dendrimers, is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition proved to be an ideal reaction in very good to excellent yields. Taking advantage of these facts, we will present the efficient strategy for the convergent synthesis of amphiphilic diblock dendrimers having the core chromophore via the double click chemistry. The absorption and emission of the dendrimers will be disclosed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-723**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Fréchet-type Dendrimer Using Homo-coupling Reaction of the Terminal Alkyne-focal Dendrons

최인화 윤성희 이재욱* 한승철

동아대학교 화학과

The homo-coupling of terminal alkynes is a straightforward method for the synthesis of buta-1,3-diyne, which are important building blocks in the organic synthesis of natural products, pharmaceuticals, organic/inorganic composites, and polymers. Since Rossi's group used a palladium/CuI catalytic system to catalyze the homo-coupling of terminal alkynes, this method has attracted a great deal of interest due to its mildness and wide-ranging substituent tolerance. Taking advantage of these facts, herein we will present the efficient strategy for the convergent synthesis of emissive Fréchet-type dendrimers containing a chromophore by fusion method through homo-coupling of dendrons with a profluorophore at core.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-724

발표분야: 유기화학

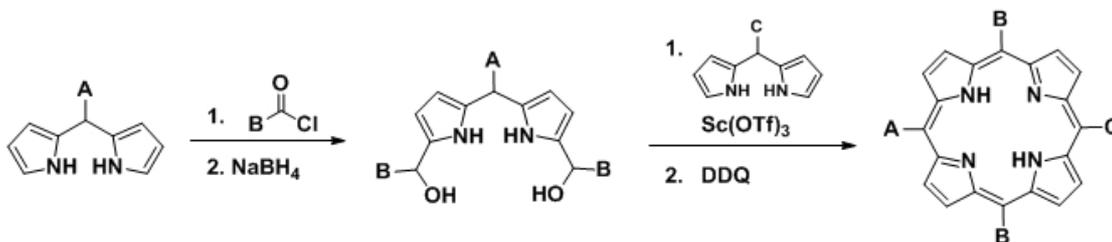
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photoelectronic Properties of Porphyrin with Donor-Acceptor for Bulk Heterojunction Organic Solar Cells

전예슬 황광진^{1,*} 권기혁¹

홍익대학교 화학시스템공학과 ¹홍익대학교 바이오화학공학과

A series of porphyrin derivatives with the electron-donating or accepting groups at meso-position have been designed and synthesized for use as bulk heterojunction organic solar cells. Based on the MacDonld-type [2+2] condensation of the dipyrromethane-diol and a dipyrromethane as key step, we synthesized AB₂C porphyrin derivatives. The porphyrin structures were confirmed by ¹H-NMR and by FAB mass data. Their photoelectronic properties, planned to be discussed were studied by UV-Vis absorption, PL, and CV.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-725**

발표분야: 유기화학

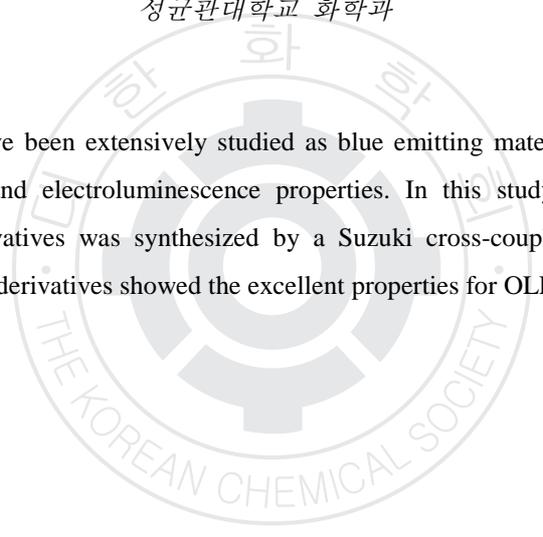
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel blue organic-light emitting materials of anthracene derivatives with aryl amine groups

이슬비 송지영 윤승수*

성균관대학교 화학과

Anthracene derivatives have been extensively studied as blue emitting materials in OLEDs because of their photoluminescence and electroluminescence properties. In this study, a series of anthracene-arylamine-anthracene derivatives was synthesized by a Suzuki cross-coupling reaction or Buchwald reaction. These anthracene derivatives showed the excellent properties for OLED applications.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-726**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

9-(1-naphthyl) anthracene derivatives for blue organic light-emitting diodes

박수나 김혜정 윤승수*

성균관대학교 화학과

Organic light-emitting diodes (OLED) have gained much attention due to its potential applications in organic flat-panel displays and solid-state lighting. For full-color displays, it is required to high EL efficiencies of red, green and blue emitters. However, blue emitters are still needed to be improved efficiencies and color purity. In this study, we have designed and synthesized blue emitters based on 9-(1-naphthyl) anthracene groups using Suzuki cross coupling reaction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-727**

발표분야: 유기화학

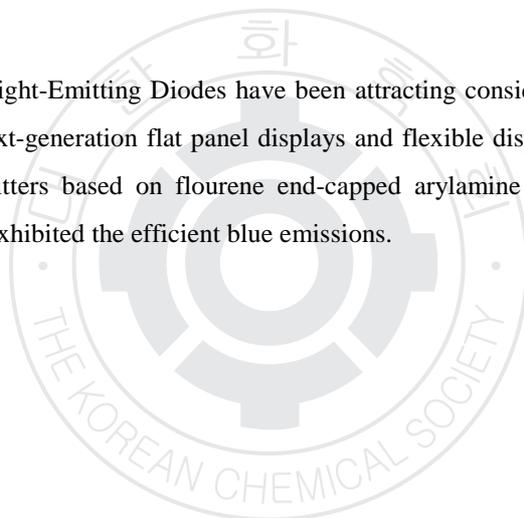
발표종류: 포스터, 발표일시: 수 16:00~19:00

Blue Fluorescent Emitters Based on Fluorene for OLEDs

김현구 윤진영 전학림 윤승수*

성균관대학교 화학과

Many studies of Organic Light-Emitting Diodes have been attracting considerable attention due to their potential applications in next-generation flat panel displays and flexible displays. In this study, we have synthesized three blue emitters based on fluorene end-capped arylamine groups by Horner-Emmons reactions. These materials exhibited the efficient blue emissions.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-728**

발표분야: 유기화학

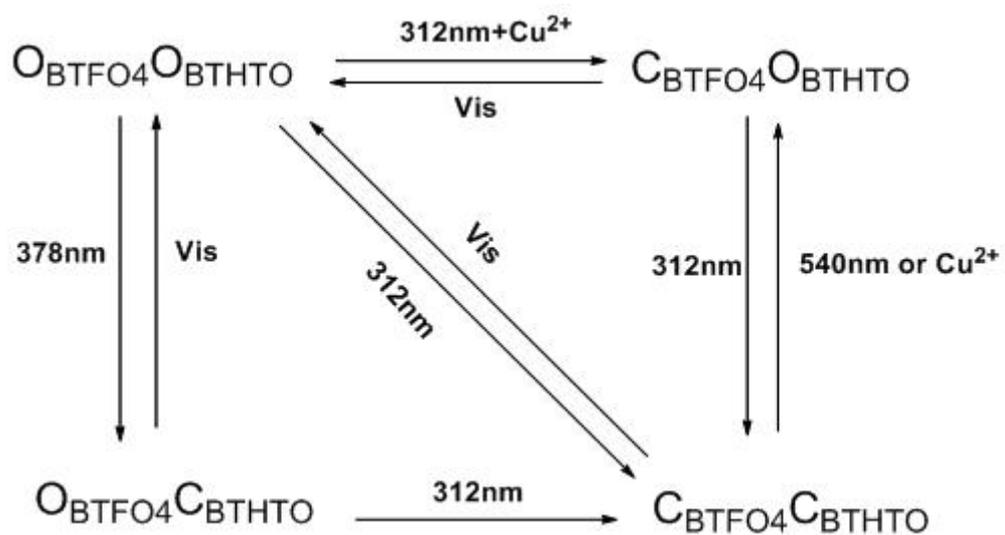
발표종류: 포스터, 발표일시: 수 16:00~19:00

Multifunction Molecule Logic Device Based on Diarylethene Derivatives Dimer

Ai Qi 강혁모 여주희 안광현*

경희대학교 응용화학과

Diarylethene derivatives (DTE) are photoswitchable, bistable chromophores which can implement binary logic operations. Herein, we report a molecule consist of two diarylethene derivatives (BTFO₄ and BTHTO) that are stimulated by light of different wavelengths and Cu(II). All the four isomers could be characterized, which is rarely found in literature. The dimer, which share a common initial state OBTFO₄OBTHTO, can allow the design of simple Boolean logic gates and more complex logic devices with light of different wavelengths and Cu(II) as inputs and absorption and emission properties at different wavelengths as outputs. References:1. J. Andreasson, U. Pischel, S.D. Straight, T. A. Moore, A.L. Moore, and D. Gust, J. Am. Chem. Soc. 2011, 133, 11641?116482. A. Perrier, F. Maurel, and D. Jacquemin, Acc. Chem. Res., 2012, 45 (8), 1173?1182



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-729**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study on the Synthesis of Quinazolinones from Anthraniloyl hydrazine and Aldehydes

최순규* 양정우 김인식^{1,*} 정대일* 한정태^{2,*}

동아대학교 화학과 ¹동아대병원 산업의학과 ²영동대학교 뷰티케어과

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. Many of the literature synthetic methods for elaboration of this simple ring structure are, however, time consuming, tedious and often low yielding. Recently, the synthesis of 2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids has been described and their catalystfree 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(DPP) as a catalyst.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-730**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis of Benzoimidazole from Benzylamine and Diamines

이용균* 김아영 이연진* 정대일* 한정태^{1,*}

동아대학교 화학과 ¹영동대학교 뷰티케어과

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 contrast to oxygen, which in a biradical in the ground state, sulfur is less reactive. Consequently, the reaction using sulfur presents a low risk of explosion, shows different and interesting reactivities and selectivities even without metal catalyst, and does not require pressurized reactors. Herein, we report a chemoselective method for an oxidative coupling reaction of alkylamine with various diamines for the formation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-731**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-substituted 4-phenylquinoline derivatives under microwave irradiation

김성태 이용균* 정대일* 한정태^{1,*}

동아대학교 화학과 ¹영동대학교 뷰티케어과

Quinolines are well known not only for their significant biological activities but also for their formation of conjugated molecules and polymers that combine enhanced electronic, optoelectronic, or nonlinear optical properties with excellent mechanical properties. Recently, much attention has focused on microwave assisted organic reaction in the absence of solvent. Often, thermal demanding reactions take hours in solution, and may require repetitive treatments with excess reagents to drive them to completed in minutes. We report that Synthesis of 4-phenylquinolines and (5Z,11Z)-6,12-diphenyldibenzo[b,f][1,5]diazocines under microwave irradiation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-732**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study on the Synthesis of 2-amino-4-arylthiazoles from Thiourea and Ketones with Iodine

송주현* 김수완 정대일* 한정태^{1,*}

동아대학교 화학과 ¹영동대학교 뷰티케어과

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 pharmacoactive protecties 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 rapid 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.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-733

발표분야: 유기화학

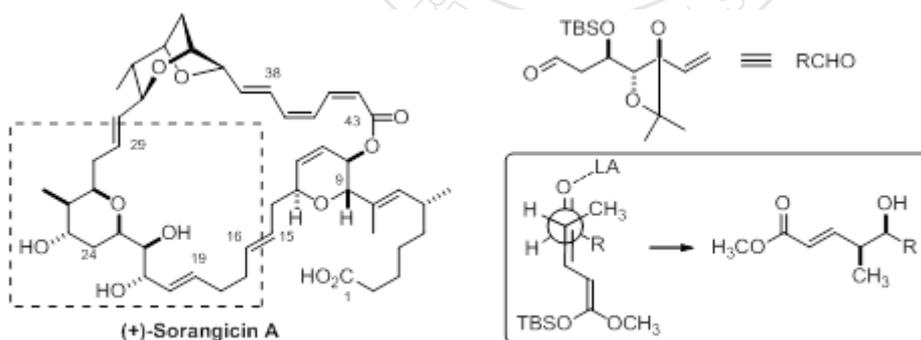
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of the C16-C29 Subunit of Sorangicin A via the Mukaiyama Aldol Reaction

이유진 최일영¹ 이효원*

충북대학교 화학과 ¹한국화학연구원 의약화학연구센터

Our synthetic efforts toward the subunit of C16-C29 comprising a tetrahydropyran subunit of potent antibiotic macrolide sorangicin A utilizing the Prins reaction as well as the Evans protocol of aldol reaction will be disclosed. Now we modified the previous reaction pathway utilizing the vinylogous Mukaiyama aldol reaction as a key reaction to improve the efficiency. The strategy for the Michael reaction toward a tetrahydrofuran ring using *E*-unsaturated ester was switch to the *Z*-isomer for the improvement. The details of the synthetic route will be revealed



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-734**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the reaction of phthalaldehydic acid and surfobenzaldehyde sodium salt with ketones

이도훈* 권연근 정대일* 한정태^{1,*}

동아대학교 화학과 ¹영동대학교 뷰티케어과

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-dimensional molecular frameworks which potentially might preserve the 'privileged' status of their aromatic precursors. Herein, we report an approach to the synthesis of isoindolo[2,1-a][1,5]benzodiazepin-12-one derivatives. Phthalaldehydic acid has been prepared by the alkaline oxidation of naphthalene.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-735**

발표분야: 유기화학

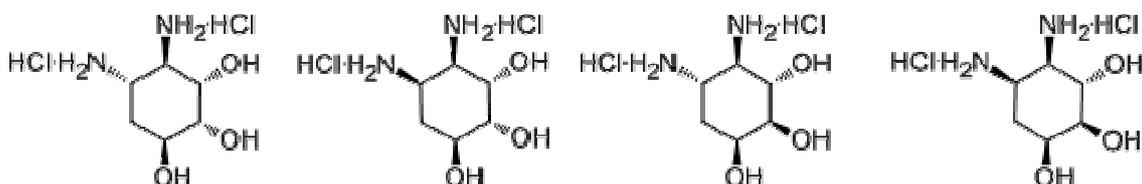
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study toward diaminocyclitols

강한영* 신미리

충북대학교 화학과

Owing to their rich biological activities, aminocyclitols, in particular, vicinal diamino inositol analogs have drawn attention. They have been used in a broad range of medical treatment including infections caused by virus. With anticipation of strong antibiotic activity, several diaminocyclitols, including streptomine and 2-deoxystreptomine have been synthesized. The carba-sugar derivatives have intrigued us for developing sugar-based glycosidase inhibitors. Diaminocyclitols, structures shown below, have been synthetic targets in connection with developing efficient glycosidase inhibitors with containing carba-sugar structures. We imagine that these structures could be synthesized utilizing several key reactions including nucleophilic ring-opening reactions of chiral aziridine derivatives. These reactions have possessed much potential applications in organic synthesis. Combining the ring-opening reactions of aziridines with other key synthetic reactions such as ring-closing metathesis, the carba-sugar derivatives could be efficiently synthesized. Synthetic studies on these diaminocyclitols will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-736**

발표분야: 유기화학

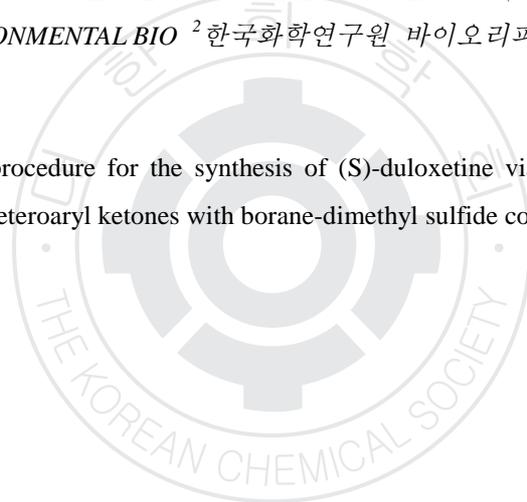
발표종류: 포스터, 발표일시: 수 16:00~19:00

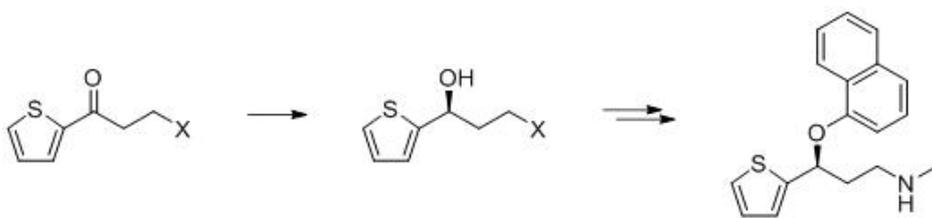
Enantioselective synthesis of (S)-duloxetine via spiroborate ester-catalyzed reduction of α -substituted heteroaryl ketones

이선아 이기인* VENKATA SUBBAIAH SADU¹ A.PITCHAIAH²

한국화학연구원 그린화학연구단 ¹과학기술연합대학원대학교(UST) GREEN CHEM & ENVIRONMENTAL BIO ²한국화학연구원 바이오리파이너리

A practical and efficient procedure for the synthesis of (S)-duloxetine via spiroborate ester-catalyzed reduction of α -substituted heteroaryl ketones with borane-dimethyl sulfide complex is described.





일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-737**

발표분야: 유기화학

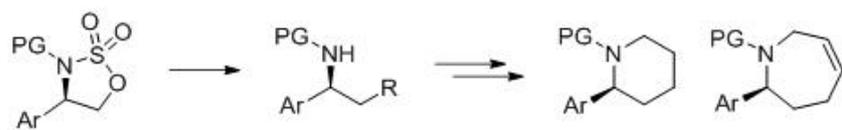
발표종류: 포스터, 발표일시: 수 16:00~19:00

Nickel-Catalyzed ring-opening of cyclic sulfamidates with Grignard reagents; A facile entry to nitrogen-containing heterocycles

이선아 [A.PITCHAI AH](#)¹ VENKATA SUBBAIAH SADU² 김미리³ 이기인*

한국화학연구원 그린화학연구단 ¹한국화학연구원 바이오리파이너리 ²과학기술연합대학원대학교(UST) GREEN CHEM & ENVIRONMENTAL BIO ³과학기술연합대학원대학교(UST) 청정화학
및 생물학

A nickel-catalyzed ring-opening reaction between cyclic 1,2-sulfamidates and Grignard reagents is reported. This protocol is quite useful for enantioselective synthesis of nitrogen-containing heterocycles.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-738**

발표분야: 유기화학

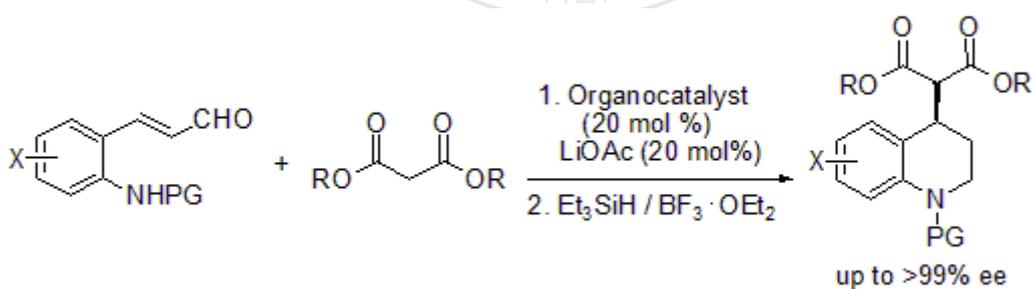
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Enantioselective Conjugate Addition?Cyclization Domino Reactions of *o*-*N*-Protected Aminophenyl α,β -Unsaturated Aldehydes

김신애 허승평 김성곤*

경기대학교 화학과

A highly enantioselective synthesis of biologically useful tetrahydroquinolines has been developed through the asymmetric organocatalytic conjugate addition?cyclization reaction of malonates with *o*-*N*-protected aminophenyl α,β -unsaturated aldehydes using a diphenylprolinol TMS ether as an organocatalyst followed by reductive deoxygenation. This novel protocol allows for the formation of 4-substituted chiral tetrahydroquinolines, which are not easily accessible using other methodologies, in good yields with high enantioselectivities (up to >99% ee).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-739

발표분야: 유기화학

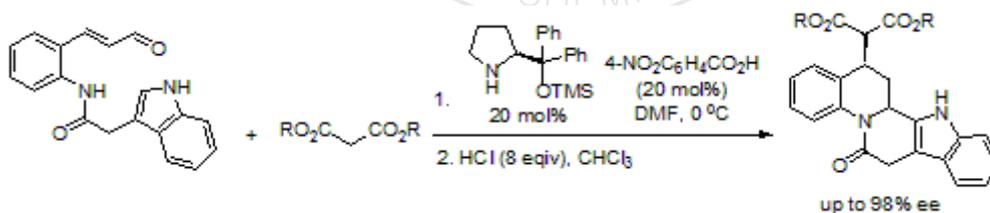
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Construction of Benzindoloquinolizidine: Application of an Organocatalytic Enantioselective Conjugate Addition?Cyclization Cascade Reaction

김철웅 이요나¹ 강기태¹ 김성곤^{1,*}

경기대학교 화학¹ 경기대학교 화학과

The synthetic methodology of enantioenriched benzindoloquinolizidines has been developed based on the organocatalytic enantioselective conjugate addition?cyclization cascade reaction of o-N-(3-indoleacetyl)aminocinnamaldehydes with malonates followed by an acid-catalyzed intramolecular Pictet-Spengler type cyclization. The asymmetric catalytic reactions using diphenylprolinol TMS ether as an organocatalyst have produced the desired products with good to excellent yields and high enantioselectivities (up to 98% ee).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-740**

발표분야: 유기화학

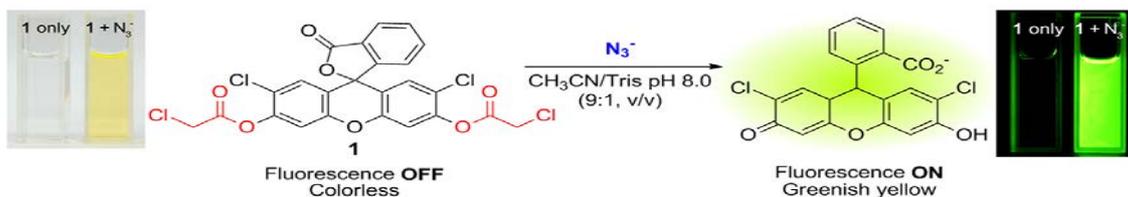
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual Signaling of Hg(II) Ions by Selective Cleavage of Thiophosphinated Rhodol

김홍영 임현규 장석규*

중앙대학교 화학과

A new Hg(II)-selective reaction-based probe based on thiophosphinated *N,N*-diethylrhodol 1 was developed. Probe 1 showed prominent chromogenic and fluorogenic signaling for the Hg(II) ions. Signaling is due to the Hg(II)-assisted hydrolysis of the thiophosphinated group to generate the rhodol fluorophore. An optical signaling with a detection limit of 13 nM, detectable with unaided eyes, was realized in a mixed aqueous environment.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-741

발표분야: 유기화학

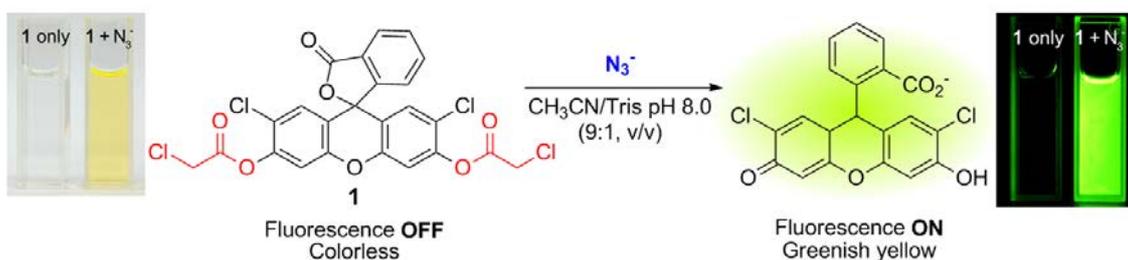
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual Signaling of Azide Ions by Deprotection of a Dichlorofluorescein Chloroacetate

이정우 장석규*

중앙대학교 화학과

We investigated the dual optical signaling of azide ions by the selective cleavage of fluorescein chloroacetates. The chloroacetate derivative of 2',7'-dichlorofluorescein showed prominent colorimetric and fluorogenic signaling behaviors toward azide ions in aqueous acetonitrile solution. The detection of azide ions was not affected by the presence of commonly encountered anions. In particular, significant interference from sulfide ions in the azide-selective signaling of the probe was readily suppressed by using a Hg(II)-*N,N,N',N'*-tetrakis(2-pyridylmethyl)ethylenediamine (TPEN) complex as a masking agent. The detection limit for the determination of azide ions by the chloroacetate of 2',7'-dichlorofluorescein in 10% aqueous acetonitrile was 17 ppb. The signaling of azide ions in real samples using tap water and simulated wastewater was also tested.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-742**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dynamic NMR studies of aryl substituted dibenzylamino-1,3,5-triazines

이은옥 김영준* 송재희¹

충남대학교 화학과 ¹순천대학교 화학과

N2,N2,N4,N4-Tetrabenzyl-6-chloro-1,3,5-triazine-2,4-diamine was used as a starting material and some aromatic groups were introduced to 1,3,5-triazine with Suzuki reaction. The activation of C-N bond rotation of dibenzylamino-1,3,5-triazine in organic solvent was measured by using with variable-temperature ¹H NMR spectroscopy. The ¹H NMR spectra of some dibenzylamino-1,3,5-triazines showed two benzyl signals at room temperature. At elevated temperatures, the two signals coalesced and displayed only one signal. As a result, the free energy (ΔG^\ddagger) of C-N bond rotation of dibenzylamino-1,3,5-triazines was obtained as 16~18 kcal/mol from coalescence temperature and line shape analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-743**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Cyclometalated Platinum(II) β -Diketonates Complexes

이은옥 김영준* 송재희¹

충남대학교 화학과¹ 순천대학교 화학과

Cyclometalated Platinum(II) complexes were prepared and characterized by NMR spectroscopy. These Platinum(II) complexes were synthesized by the reaction of heterocyclic ligands, $[PtMe_2(SMe_2)]_2$, and acetylacetonate (acac) in THF/Methanol at room temperature in the presence of trifluoromethane sulfonic acid (TfOH). A one-pot synthesis of these complexes has some advantages, such as short reaction time at ambient temperature. These Cyclometalated Platinum complexes have been widely explored for use in organic light-emitting diodes (OLEDs) and will be discussed in terms of photochemical properties

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-744**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of the Unsymmetrical Diarylalkynes from Two Different Aryl Bromides and Propiolic Acid by Using Pd(PPh₃)₄ Catalyst

김원영 이선우*

전남대학교 화학과

Unsymmetrical diarylalkynes have attracted much attention, as the molecule structure, having an internal alkyne of two different aromatics, is a core in materials encountered π -conjugated systems. Palladium catalyzed Sonogashira reaction is the most commonly used method for the arylation of terminal alkynes. Instead of the terminal alkynes, the decarboxylative Sonogashira reaction is used from the alkyne carboxylic acids has several advantages, including a depreciable process for the treatment of the carbon dioxide as a reaction waste released after the complete conversion, and is stable for handling and storage. We reported a method for unsymmetrical coupling products from the site selective reaction of propiolic acid with aryl iodides and aryl bromides combinations. Recently, we reported that the Pd(PPh₃)₄ catalyzed a selective Sonogashira reaction with aryl bromides at low temperature. Instead of the advanced reports of the one pot reaction procedures for the synthesis of unsymmetrical diaryl alkynes, we carried out an additional experiment due to the simplicity of the non-sequential addition of aryl bromides and non-column purification. Finally, unsymmetrical coupling of propiolic acid with two different of aryl bromides was carried out with the optimized condition. The optimized condition is that aryl bromide (1.0 and 1.2 equiv), propiolic acid (1.2 equiv), Pd(PPh₃)₄ (5mol%), DBU (2.4 equiv) were reacted in DMSO at 35 °C for 24 h and at 90 °C for 12 h.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-745**

발표분야: 유기화학

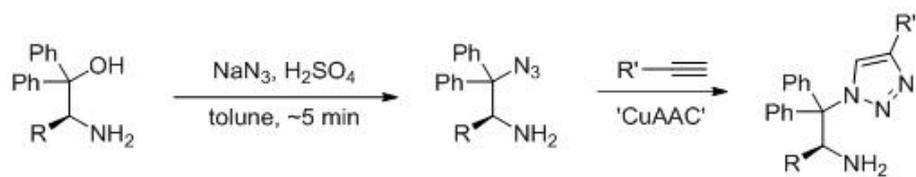
발표종류: 포스터, 발표일시: 수 16:00~19:00

An easy access to highly hindered chiral α -amino triazole ligands via copper-catalyzed azide-alkyne cycloaddition

이선아 VENKATA SUBBAIAH SADU¹ A.PITCHAI AH² 이기인*

한국화학연구원 그린화학연구단 ¹과학기술연합대학원대학교(UST) GREEN CHEM & ENVIRONMENTAL BIO ²한국화학연구원 바이오파이너리

Recent advances in asymmetric organocatalysis employing secondary amine-based molecules have resulted in the development of a large number of asymmetric transformations. Furthermore, pyrrolidine derivatives such as pyrrolidine-pyridine, -imidazole, and -triazole conjugates have been shown to serve as useful asymmetric catalysts for the Michael addition of ketones or aldehydes. In the light of the above, we accomplished a facile entry to α -amino triazole derivatives bearing a gem-diaryl group using click chemistry of alkyne-azide cycloaddition. The highly hindered chiral diamines and α -amino triazoles are currently being investigated as potential molecular catalysts.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-746**

발표분야: 유기화학

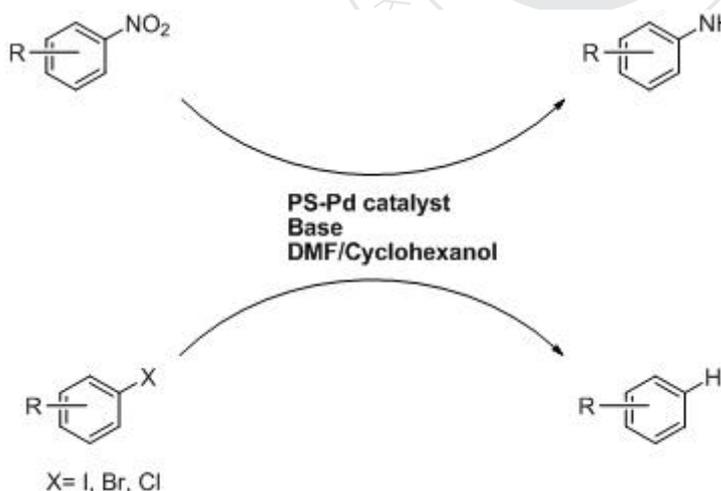
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Reduction of Nitroaromatic Compounds and Aryl Halides

민홍근 이선우*

전남대학교 화학과

The palladium catalyzed reduction of nitroaromatic compounds and aryl halides to produce anilines and non-halogenated benzenes are powerful method. We developed the method of the reduction by using palladium immobilized poly styrene (PS-Pd) as reusable catalyst which is economically efficient. The optimized reaction condition is 10 mol% of PS-Pd, 1.5 equivalent of K_3PO_4 as base, the excess amount of cyclohexanol as the hydrogenation source and DMF as reaction solvent at $150^\circ C$ for 24 hours.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-747**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Diaryl Sulfides by using Palladium-Catalyzed C-S Bond Formation with *N*-Amido Imidazolium Salts as Ligands

변아름 표아영 이선우*

전남대학교 화학과

We developed the method for the synthesis of diaryl sulfide via palladium catalyzed c-s bond cross coupling with *N*-amido imidazolium salts as ligands. The best combination for the coupling with aryl bromides was *N*-amido imidazolium salt 2 and NaHMDS, and that for the coupling with aryl iodides was *N*-amido imidazolium salt 1 and KOtBu. The coupling reactions were conducted in the presence of Pd(OAc)₂ (1 mol%) in DMSO at 80 °C for 12 h.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-748**

발표분야: 유기화학

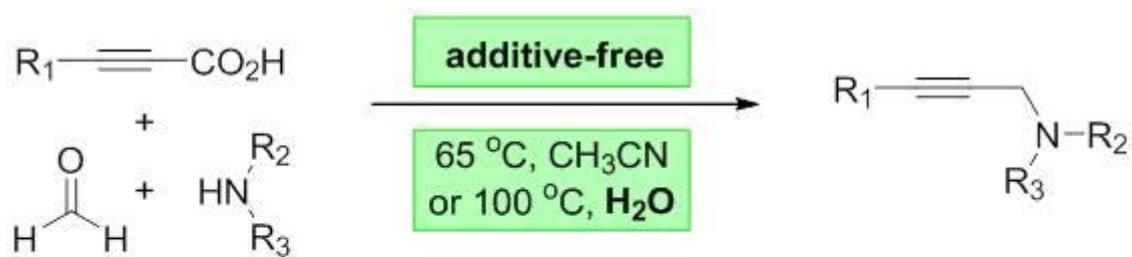
발표종류: 포스터, 발표일시: 수 16:00~19:00

Additive-Free Decarboxylative Three Component Reaction for the Synthesis of Propargylamines from Alkyne Carboxylic Acids

박경호 이선우*

전남대학교 화학과

Propargylamines are the functional group observed in biological active molecules frequently, as well as used for the synthetic intermediate of the heterocyclic compounds bearing nitrogen atom synthesis. The most often used method for the synthesis of propargylamines is the three component reaction of amine, aldehyde and terminal alkyne by using metal catalyst such as copper, gold, silver, iridium, indium, iron and zinc. However, the employment of metal catalyst not only leads to the purification processes of reaction product from the metal impurities which processes are economically burden to industries but also occasionally affords the Glaser homocoupling compound as a byproduct which leads to a decrease in the yield of the product. Moreover, the usage of highly volatile terminal alkynes such as 1-propyne and 1-butyne are difficult. To overcome these limitations, we focused on the development of the additive-free decarboxylative three component reaction from amine, aldehyde, and alkynyl carboxylic acid which is easy to use as non-volatile unlike terminal alkyne. The result of our investigation was that the desired propargylamines was obtained up to 98% yield from the reaction of alkynyl carboxylic acids, paraformaldehyde, and amines in CH_3CN at 65°C for 3 h. The reaction of alkynyl carboxylic acid combined with terminal alkyne showed high selectivity toward alkynyl carboxylic acids. The decarboxylative three component reaction was showed good yield even in water solvent. Reference: K. Park,; Y. Heo,; S. Lee *Org. Lett.* 2013, 15, 3322.



- No metal waste
- No Glaser byproduct
- No column chromatography
- Easy access of alkynes having low b.p.
- Large scale and water solvent are available



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-749

발표분야: 유기화학

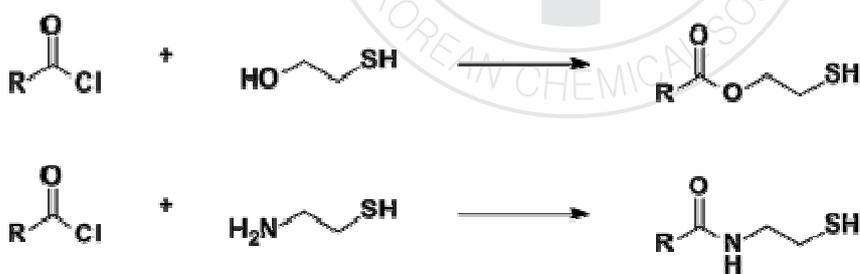
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Investigation of Chemoselective O-Acylation of β -mercaptoalcohol and N-Acylation of β -mercaptoamine with Acid Chloride Derivatives

장지성 김예진 안철진*

창원대학교 화학과

Molecules including free -SH are important to prepare gold nanoparticle(GNP) encapsulating with organic ligand. The selective O-acylation of 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 is reported.



[R = Alkyl, Allyl, Aromatic]

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-750**

발표분야: 유기화학

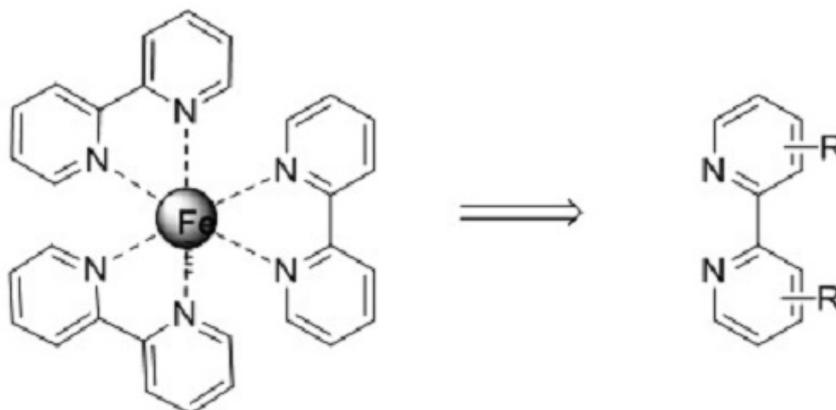
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Bipyridine Ligand Derivatives for Iron: Application for Redox Flow Battery

김기우 안철진* 김은선 진창수¹

창원대학교 화학과 ¹한국에너지기술연구원 에너지저장센터

The iron redox flow battery is a type of rechargeable flow battery that employs iron ions in different oxidation states to store chemical potential energy. To improve the energy density, we try to prepare iron complex including bipyridine ligand. In this paper, we will present the efficient preparation of various bipyridine derivatives.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-751

발표분야: 유기화학

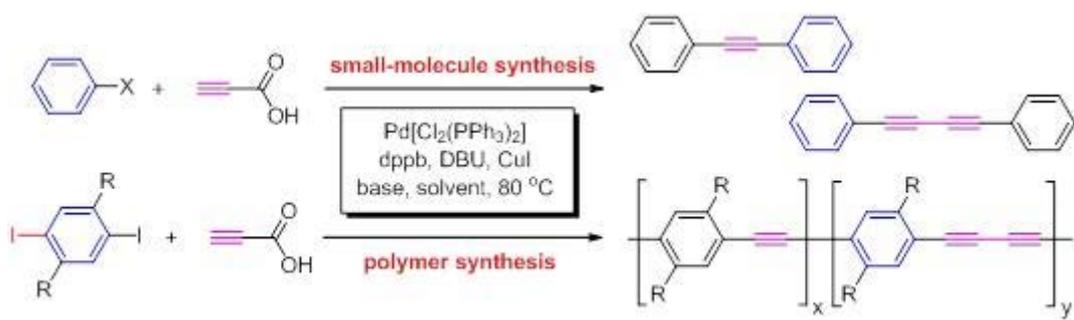
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Step Synthesis of Conjugated Random Co-Polymers via the Decarboxylative Coupling of Propiolic acid with Aryl Iodides

박경호 황진일 이선우*

전남대학교 화학과

Poly-(*p*-phenyleneethynylene)s (PPEs) and poly-(*p*-phenylenebutadiynylene)s (PPBs) are the conjugated polymers (CPs) having diarylalkynes and diaryl diynes as a core, respectively. The most often used method for the synthesis of the CPs is the palladium catalyzed Sonogashira reaction and Hay or Glaser coupling. Although these reactions are applicable to a broad scope of substrates with good reactivity, it is the limitation to produce of reaction waste in each step for the synthesis of CPs whose synthesis typically requires a multi-step. For example, synthesis of CPs typically required conversion of the starting diiodoarenes to diacetylenes prior to polymerization and each step bring out reaction wastes like reagents, solvent and catalysts. To overcome this limitation, we focused on the development of one-step synthetic methods of the diarylalkynes and the diaryl diynes. Recently, we reported palladium catalyzed decarboxylative coupling reaction for the synthesis of diarylalkynes and diaryl diynes from propiolic acids as alkyne source and aryl halides in one-pot. Based on the previous work, we successfully synthesized conjugated random co-polymers containing phenyleneethynylenes and phenylenebutadiynylenes from the palladium/copper-catalyzed decarboxylative coupling reaction of propiolic acid with aryl iodides in one-step. This approach provides a facile route to the CPs. Reference: T. Vokataa,; M. R. Kumara,; K. Park,; J. H. Moon,; S. Lee *Synlett* 2013, 24, 1563.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-752**

발표분야: 유기화학

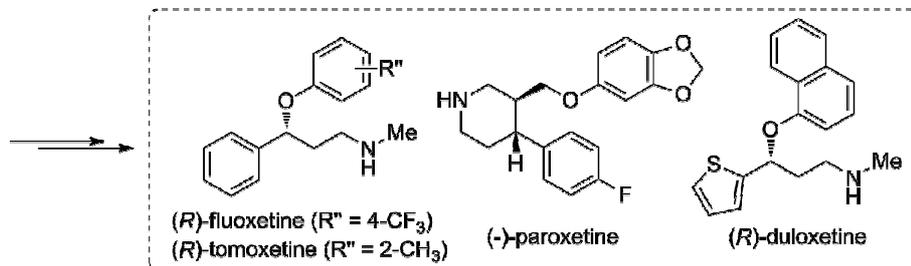
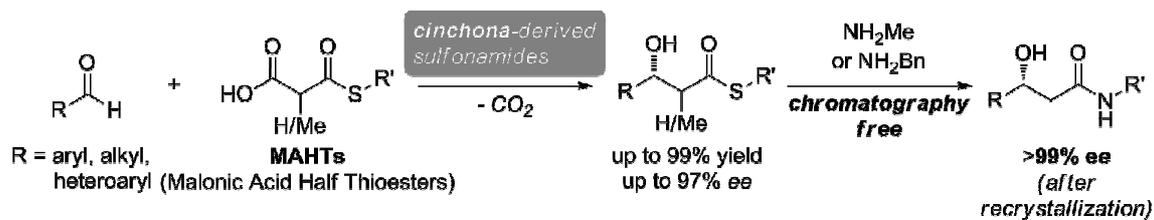
발표종류: 포스터, 발표일시: 수 16:00~19:00

Bio-inspired Organocatalytic Aldol Reaction of Malonic Acid Half Thioesters to Aldehydes

배한용 심재훈 송충의*

성균관대학교 화학과

In the past decade, many efforts have been directed towards introducing enolate nucleophiles with the oxidation state of carboxylic acid derivatives on the basis of catalytic organic synthesis. In the biosynthesis of polyketides and fatty acids, however, nature freely uses the enzymatic activation of malonic acid half thioesters (MAHTs) to generate ester enolates or their equivalents. These undergo the chain elongation step smoothly via decarboxylative Claisen condensation. Inspired by these biocatalytic processes, we discovered that cinchona-derived sulfonamides serve as remarkably effective organocatalysts for enantioselective aldol reaction of MAHTs with a variety of aldehydes to afford chiral beta-hydroxyl thioesters (up to 99% yield and 97% ee). In this presentation, we will cover the developed protocol in detail, focusing on a mechanistic hypothesis. Applications of the developed methods to the formal syntheses of antidepressant drugs such as (R)-fluoxetine, (R)-tomoxetine, (-)-paroxetine and (R)-duloxetine shall also be presented and discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-753**

발표분야: 유기화학

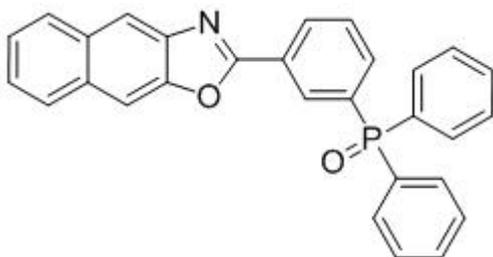
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Electroluminescence Property of 2-(3-(Diphenylphosphoryl)phenyl)naphtho[2,3-d]oxazole (3-PPN) as Blue-Emitting OLED Material

김익환 강은국 이범종^{1,*}

인제대학교 화학과 ¹인제대학교 의생명화학과

In the course of investigation for finding new light-emitting materials based on the phosphino-naphthoxazole structure, 2-(3-(diphenylphosphoryl)phenyl)naphtho[2,3-d]oxazole (3-PPN) was synthesized from 3-amino-2-naphthol and sodium 3-(diphenylphosphino)benzoate in this work. The chemical structure of 3-PPN was determined by ¹H-NMR, ¹³C-NMR, FT-IR, UV-Vis, elementary analysis (EA) and X-ray photoelectron spectroscopy (XPS). 3-PPN shows a strong blue emission under excitation by UV-lamp of 365nm. The physical properties of 3-PPN were determined by thermo gravimetric analysis (TGA), differential scanning calorimetry (DSC), photoluminescence (PL), electroluminescence (EL) and CIE system of color specification.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-754

발표분야: 유기화학

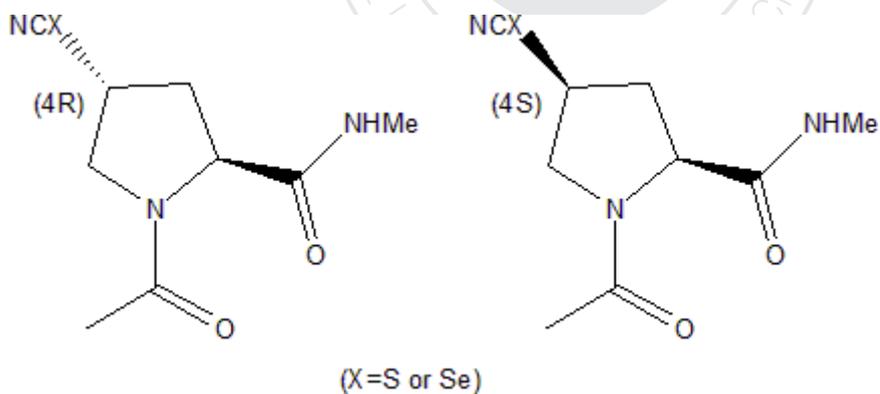
발표종류: 포스터, 발표일시: 수 16:00~19:00

Infrared Probes Based on Nitrile-Derivatized Prolines

박유미 박광희 박성남* 한호규* 조민행*

고려대학교 화학과

The proline residue determines protein structures. Thiocyanate and selenocyanate are nitrile probes that is observed between 2000-2300 cm^{-1} in IR spectroscopy. We have synthesized stereoisomers of thiocyanato- and selenocyanato-derivatized prolines, Pro-SCN and Pro-SeCN and measured their CN stretch lifetimes in D_2O and chloroform with polarization-controlled IR pump-probe spectroscopy. We anticipate that the Pro-SeCN probe can be an excellent site-specific probe of changes in protein local environment.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-755

발표분야: 유기화학

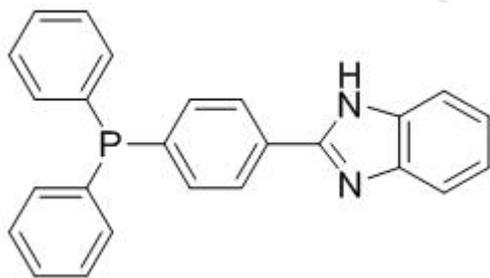
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photoluminescence Property of 2-(4-(Diphenylphosphino)phenyl)-1H-benzo[d]imidazole (4-DPI) as Blue-Emitting OLED Material

강은국 김익환 이범종^{1,*}

인제대학교 화학과 ¹인제대학교 의생명화학과

A novel blue-emitting OLED material based on the phosphino-benzimidazole structure was synthesized from *o*-diaminobenzene and 4-(diphenylphosphino)benzoic acid. The one-pot synthesis of 2-(4-(diphenylphosphino)phenyl)-1H-benzo[d]imidazole (4-DPI) was carried out using polyphosphoric acid (PPA) as solvent and catalyst for the cyclization reaction. The chemical structure of 4-DPI was determined by ¹H-NMR, ¹³C-NMR, FT-IR and UV-Vis. The 4-DPI showed a strong blue emission under excitation by UV-lamp of 365 nm. The photoluminescence (PL) property of 4-DPI will be discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-756**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ruthenium-Catalyzed Reconstitutive Cycloisomerization of *N*-Sulfonyl-*N*-Hydroxylaminoalkynes to Lactams

김성미 김인수 이철범*

서울대학교 화학부

A ruthenium-catalyzed reconstitutive cycloisomerization reaction using *N*-Sulfonyl-*N*-Hydroxylaminoalkynes as a starting material has been developed. In the presence of catalytic amount of $\text{CpRu}(\text{PPh}_3)_2\text{Cl}$, *N*-sulfonyl-*N*-hydroxylaminoalkynes turn to lactams. The catalytic 1,1-gem-difunctionalization is proposed to involve formation of ruthenium vinylidene. We proposed two possible mechanisms.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-757**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ruthenium Catalyzed Redox-Neutral and Single-Step Amide Synthesis from Alcohol and Nitrile with Complete Atom Economy

강병준 홍순혁^{1,*}

서울대학교 화학부 ¹서울대학교 화학과

Atom-economical and environmentally benign amide bond synthesis is one of the top challenges in modern chemistry, especially in pharmaceutical science. To achieve this goal, the avoidance of classical coupling reagents is crucial. Ruthenium catalyzed amide synthesis based on alcohol activation strategy has been under spotlight as a proper alternative of classical method. Here, a completely atom economical and redox-neutral catalytic amide synthesis from an alcohol and a nitrile is realized. The amide C-N bond is efficiently formed between the nitrogen atom of nitrile and the α -carbon of alcohol, with the help of an N-heterocyclic carbene-based ruthenium catalyst, without any single byproduct. Several mechanistic evidences show that the reaction undergoes with unusual N-unsubstituted imine intermediate followed by hydrogen transfer from alcohol to imine and C-N bond formation. A utility of the reaction was demonstrated by synthesizing ¹³C or ¹⁵N labeled amides, which are important materials in protein structure defining process and metabolism study, without involvement of any separate reduction and oxidation step.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-758**

발표분야: 유기화학

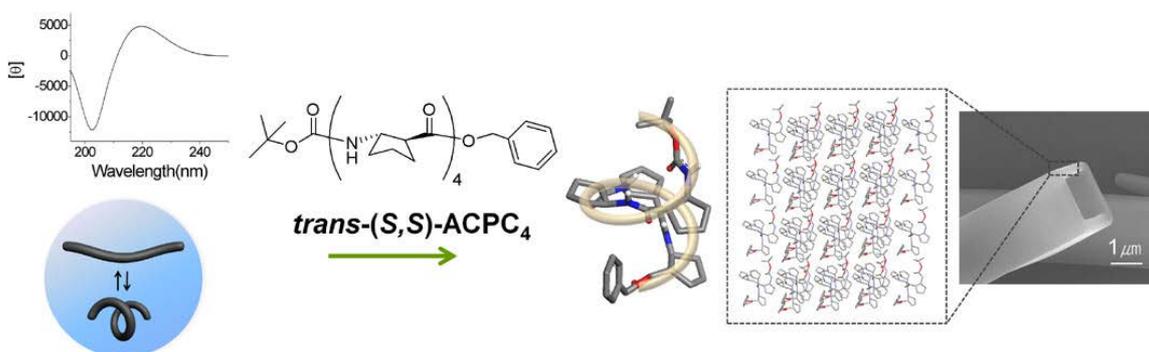
발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation of Rectangular Microtubes by Self-Assembly of a Short β -Peptide Foldamer

권선범 이희승*

한국과학기술원(KAIST) 화학과

In nature, complex and well-defined structures are constructed by the self-assembly of biomolecules. It has been shown that β -peptide foldamers can mimic natural peptides and self-assemble into three-dimensional molecular architectures thanks to their rigid and predictable helical conformation in solution. Using shorter foldamers, which can be prepared more easily than longer ones, to form such architectures is highly desirable, but shorter foldamers have been overlooked due to the seemingly inferior number of intramolecular hydrogen bonds to stabilize a folded state in solution. Here we report that a β -peptide tetramer, although it lacks full helical propensity in solution, does self-assemble to form well-defined microtubes with rectangular cross-section by evaporation-induced self-assembly.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-759**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ruthenium-catalyzed amide bond formation of terminal alkynes using *N*-hydroxyheterocycles

이동길 이철범*

서울대학교 화학부

Herein, we demonstrate an efficient oxygenative amide bond forming reaction of various alkynes and amines. Especially, ruthenium catalysis has been shown to generate α,β -unsaturated amides from propargylic acetates via ruthenium allenylidene formation. This method can be applied to terminal alkyne substrates for the synthesis of various amide bonds in high yields. All reactions without amine counterparts proceed to generate the active ester intermediate, indicating a mechanism involving a reconstitutive rearrangement process.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-760

발표분야: 유기화학

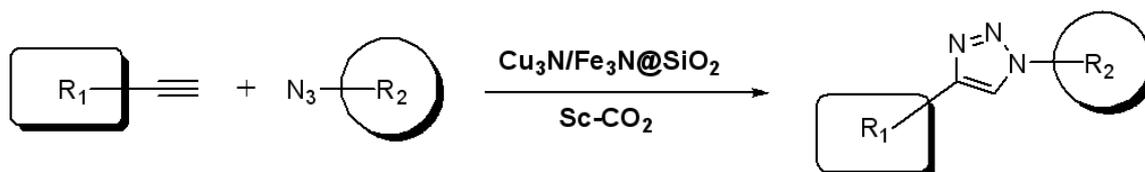
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1,4-disubstituted 1,2,3-triazoles using Mesoporous Silica-supported Copper Nitride Nanoparticle-catalyst in scCO₂

민지은 김학원^{1,*} 이규형² 허남희^{2,*}

경희대학교 화학과 ¹경희대학교 응용화학과 ²서강대학교 화학과

The Huisgen 1,3-dipolar cycloaddition of azides and alkynes, or click reaction is important method for the synthesis of 1,2,3-triazoles. Especially, many Cu(I)-catalyzed Huisgen cycloaddition of terminal alkynes and azides in organic solvent have been studied and reported. Recently, copper nitride nanoparticles supported on a superparamagnetic mesoporous silica microsphere (Cu₃N/Fe₃N@SiO₂) and its use for toxic-free click reaction in an organic solvent have been developed. We have investigated the copper nitride catalyzed click reaction in a supercritical carbon dioxide (scCO₂), considered as a green solvent, in the absence of amine additive. This catalyst showed high catalytic activities in scCO₂, compared with one in organic solvent (hexane, acetonitrile) and other copper catalyst Cu/AIO(OH). Also, Cu₃N/Fe₃N@SiO₂-catalyzed click reactions with various alkynes and azides in scCO₂ will be reported.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-761**

발표분야: 유기화학

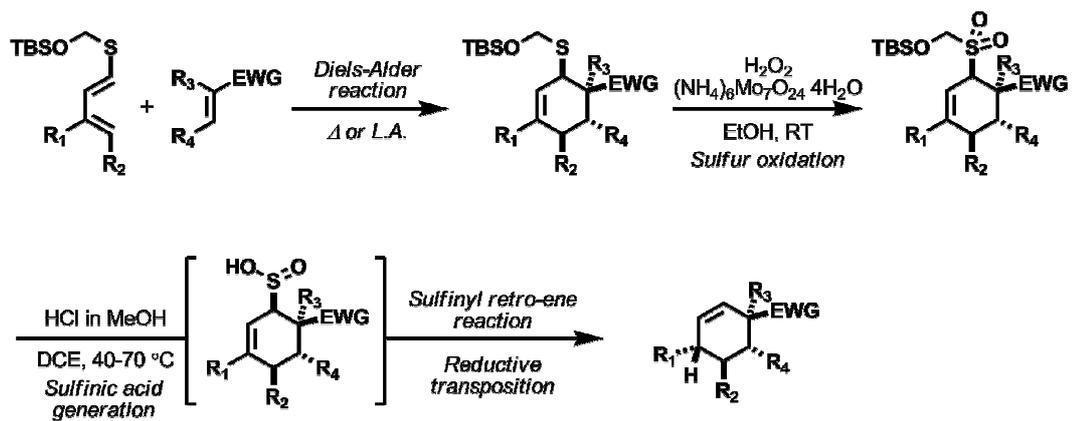
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of non-Diels-Alder Cyclohexenes via Tandem [4+2] Cycloaddition and Sulfinyl Retro-ene Reaction

박호윤 최진 이철범*

서울대학교 화학부

The Diels-Alder reaction has provided the foundation for some of the most impressive achievements in the area of cyclohexene derivative synthesis. Among various categories of the Diels-Alder reaction, the tandem reaction provides additional diversity to the cycloadduct. Our laboratory has been interested in sulfinyl retro-ene reactions that can be performed in tandem with the Diels-Alder reaction. Using this combination of two pericyclic processes, we have developed an efficient protocol for the synthesis of highly substituted cyclohexenes that are inaccessible by the Diels-Alder reaction. The sequence starts with a Diels-Alder reaction of (tert-butyl)dimethylsilyloxymethylsulfidyl group (TBSOCH₂S) substituted dienes in thermal or Lewis acid catalyzed reaction conditions. Subsequently, the Diels-Alder adduct is oxidized and treated with an acidic reagent, whereby a sulfinic acid is generated and undergoes a retro-ene reaction to give a series of cyclohexenes. The reaction described here represents significant expansion of the scope of the Diels-Alder reaction. The details of our studies will be shown in this poster.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-762**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Conjugated Compound for Organic Thin Film Transistors

윤순병 노영리 SHAIK BAJI 이상경*

경상대학교 화학과

Synthesis and physical properties of a novel p-type Organic thin film transistors (OTFTs) materials containing thiophene, benzene, thieno[3,2-b]thiophene and fluorene derivatives were studied. All of the compounds were synthesized under Suzuki and Stille coupling reaction conditions. The obtained monomer was confirmed by FT-IR, ¹H-NMR, ¹³C-NMR spectroscopy and elemental analysis. The synthesized FCTT and FCBT have moderate solubility in common organic solvents such as chloroform, methylene chloride and THF. The thermal properties of these compounds were characterized by thermal gravimetric analysis (TGA) and differential scanning calorimetry(DSC). Optical and electrochemical properties of the compounds were confirmed by UV-vis and cyclic voltammetry.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-763**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of a Novel Material Related with Electron Transfer

노영리 윤순병 SHAIK BAJI 이상경*

경상대학교 화학과

The heterocycle which has eight membered ring was designed and synthesized. The compound was synthesized under Suzuki coupling reaction condition. The obtained material was characterized by ¹H-NMR and ¹³C-NMR. It's optical, thermal and electrochemical properties were measured by thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC) and cyclic voltammetry (CV). In this presentation, we will report for the development of synthetic method, special optical character, and electrochemical properties of the synthesized compound.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-764**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thienothiophene-Fluorene based Organic Thin Film Transistors Compounds; Synthesis and Characterization

SHAIK BAJI 윤순병 노영리 이상경*

경상대학교 화학과

Thienothiophene and fluorene compounds have great potential for use in Organic electronics. Due to their good semiconductor property, ease of preparation, planar structure, and soluble property, thienothiophene and fluorene compounds have been playing major role in organic thin film transistors. Here we synthesized thienothiophene-fluorene compounds. In order to facilitate the intermolecular interactions and supramolecular self assembly and solubility, the alkyl chains introduced. The physical properties like thermal stability, chemical stability, and UV-visible absorption values were measured. The greater absorption in the UV-visible spectra indicates the more conjugation and existence of strong intermolecular π - π interactions. The TGA analysis indicates the compound has good thermal stability. Based on these results we can expect the device prepared by using thienothiophene-fluorene compounds can exhibit high mobility and more on-off ratio.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-765

발표분야: 유기화학

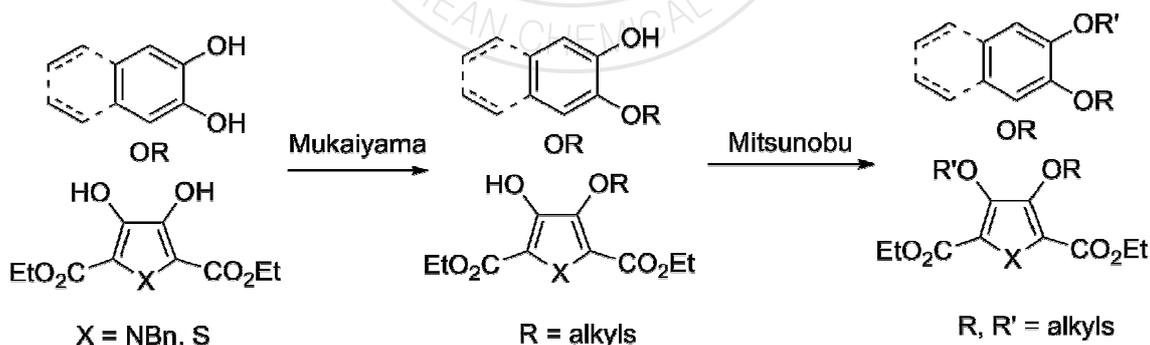
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient asymmetric 1,2-di-O-alkylation of 1,2-dihydroxy aromatic or hetero-aromatic compounds

정규관* 최민정¹

전북대학교 과학교육학부 ¹전북대학교 화학교육과

Asymmetric 1,2-di-O-alkylations of 1,2-Dihydroxy aromatic or hetero-aromatic compounds were successfully achieved via Mukaiyama reaction followed by Mitsunobu reaction. This O-alkylation employed by traditional routes such as Williamson O-alkylation suffered from low yield and harsh reaction condition. Mono-alkylated compounds was then subjected to Mitsunobu reaction that gave asymmetrically 1,2-di-O-alkylated aromatic or hetro-aromatic compounds in high yields. This method allows introduction of different alkyl functional group on the 1,2-dihydroxyaromatics.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-766

발표분야: 유기화학

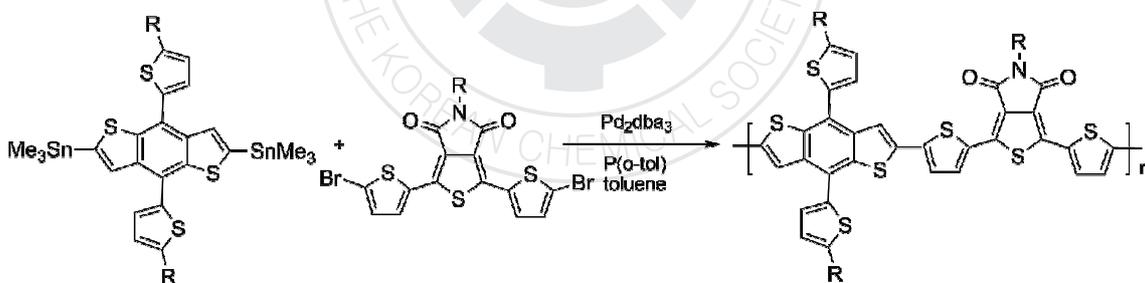
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of conjugated copolymers containing BDT and TPD for polymer solar cells

정규관* 홍남정¹

전북대학교 과학교육학부¹ 전북대학교 사범대학화학교육과

Benzo[1,2-b;4,5-b']dithiophene (BDT) derivatives characterized with two-dimensional structure were synthesized and N-alkylthieno[3,4-c]pyrrolo-4,6-dione derivatives were also synthesized. Conjugated D-A copolymers of BDT as a donor and TPD as an acceptor were synthesized and characterized by NMR, GPC, DSC, and UV-vis.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-767

발표분야: 유기화학

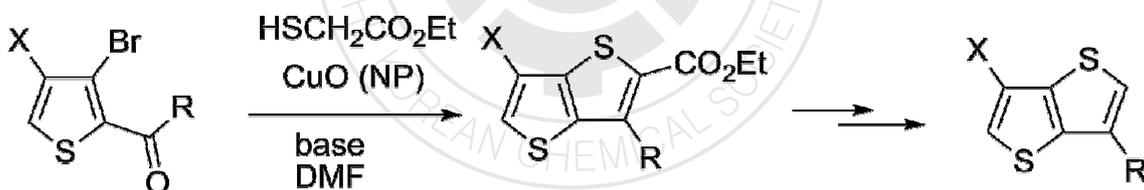
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic studies for alkylthieno[3,2-b]thiophene derivatives

정규관* 이명지¹

전북대학교 과학교육학부 ¹전북대학교 화학교육과

Acylation of 3-bromothiophene or 3,4-dibromothiophene under Lewis acid afforded a variety of 2-acylated thiophene derivatives in good yields. Upon thienylations with ethyl thioglycolate in presence of CuO nanoparticle, these compounds afforded thieno[3,2-b]thiophene derivatives in good yields. A series of manipulations of the compounds gave rise to 3,6-dialkylthieno[3,2-b]thiophene or 3-alkylthieno[3,2-b]thiophene derivatives in good yields.



R = H, alkyls, Aryls
X = H, halogens

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-768**

발표분야: 유기화학

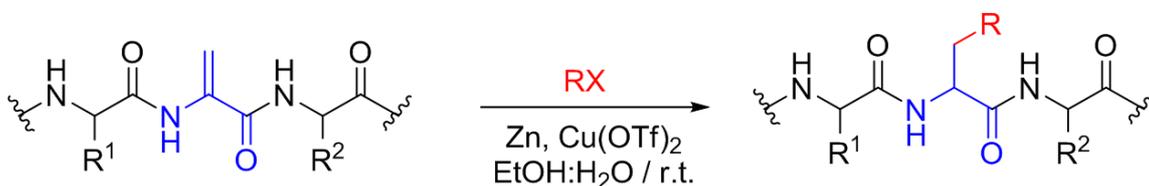
발표종류: 포스터, 발표일시: 수 16:00~19:00

Zinc-mediated carbon radical addition to dehydroalanine in aqueous media

하수라 이희윤*

한국과학기술원(KAIST) 화학과

Chemical post-translational modification of proteins offers incorporation of both natural and unnatural amino acid residues in proteins that are not accessible using standard site-directed mutagenesis. In an effort to introduce natural, unnatural, and modified natural amino acids in proteins, recently, Dehydroalanine (Dha) was synthesized from cysteine or selenocysteine. Dha offers a unique chemical handle for modifications as hetero-atom nucleophiles such as thiolates can undergo 1,4-addition reaction with Dha. As an extension of the repertoire of nucleophiles, we applied the 1,4-addition of alkyl iodides to α,β -unsaturated carbonyl systems in aqueous media to the modification of Dha through C-C bond formation. We have developed a method for generating the radical effectively by using zinc-copper metal in water and subsequent reaction with peptides or proteins containing Dha. The scope of the reaction and the application of the reaction for probing biological phenomena will be discussed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-769**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric C-C and C-N Bonds Formation Reactions Catalyzed by Chiral Anion Generator

권유경 오중석 송충의*

성균관대학교 화학과

Chiral polyethers has shown the unique cation-binding property while generating chiral anions, which are used for various types of asymmetric transformations. By varying functional groups on the catalysts, we observed excellent catalytic activity and enantioselectivity for Mannich reaction and *N,N*-acetal formation reactions. Our catalytic protocol utilizes highly accessible BINOL-derived chiral oligoethylene glycols, which can be prepared in a few synthetic steps from inexpensive starting materials. The mannich reaction combines α -amido sulfones with potassium acetylacetonate to generate the desired products in excellent yield (up to 98%) and enantioselectivity (up to 99% ee). Moreover, various α -amido sulfone substrates (alkyl, aryl and heteroaryl) can also react with phthalimide potassium salt to generate optically enriched *N,N*-acetals, with high yield (up to 99%) and excellent enantioselectivity (up to 97% ee) under mild reaction conditions in the presence of our chiral anion generator.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-770**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Blue-Emitting BODIPY Dyes for Protein Labeling

마동희 안교한*

포항공과대학교 화학과

Since proteins play crucial roles in a variety of cellular events, the study of protein dynamics is critical to understanding of sophisticated living systems. Detection and visualization of protein movements, in particular, has great potential to uncover dynamic protein functions. A number of analytical methods for the detection of proteins have been developed. Especially, methods based on fluorescence spectral responses are more appealing due to the simplicity, high sensitivity and reliability. So far, a number of bio-conjugation fluorescence dyes have been reported but most emission wavelength is over 500 nm and blue-emitting dyes have been rarely explored. BODIPYs are small compounds that have unique photophysical properties: high quantum yields, narrow emission bandwidth, insensitivity to pH and solvent polarity, and low biological toxicity.² BODIPY derivatives have been applied to various research areas including biomolecular labels and chemosensors.³ We have found that known BODIPY 1 can be readily conjugated to a protein, Lysozyme, as confirmed by SDS-PAGE, MALDI-TOF MS analysis. Based on this result, we synthesized new amino-BODIPY derivatives ($\lambda_{em} = 435-470$ nm) starting from 8-thiomethyl BODIPY (1) as protein labeling reagents.⁴ These BODIPY dyes cover the blue region and would be used for protein labeling in complement with the known dyes emitting at longer wavelength. Reference 1. Komatsu, T.; Johnsson, K.; Okuno, H.; Bito, H.; Inoue, T.; Nagano, T.; Urano, Y. *J. Am. Chem. Soc.* 2011, 133, 6745. 2. (a) Boens, N.; Leen, V.; Dehaen, W. *Chem. Soc. Rev.* 2012, 41, 1130. (b) Ulrich, G.; Ziesel, R.; Harriman, A. *Angew. Chem., Int. Ed.* 2008, 47, 1184. (c) Benniston, A. C.; Copley, G. *Phys. Chem. Chem. Phys.* 2009, 11, 4124. 3. Yue, Y.; Guo, Y.; Xu, J.; Shao, S. *New J. Chem.* 2011, 35, 61. 4. Ma, D. H. and Ahn, K. H. to be published.

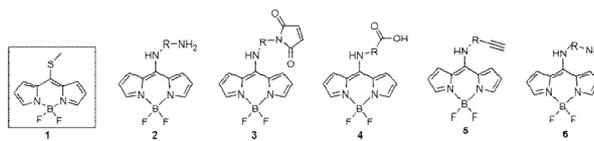


Figure 1. New 8-amino-substituted BODIPY dyes 2–6 and its precursor 1.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-771**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Revised Structure of Panaginsene and Its Total Synthesis

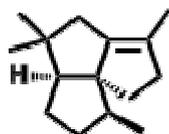
금수정 이희윤*

한국과학기술원(KAIST) 화학과

Panaginsene was recently isolated from the roots of *Panax ginseng* C.A. Meyer (Wilfried A. König and co-workers, 2005) along with panaxene and ginsinsene. These compounds are exceptionally interesting due to ginseng's popularity in Asia for centuries. Panaginsene drew our attention because it possessed the same structural pattern of senoxydene which had been reported as the first angularly fused triquinane from nature, but later was turned out not to possess even the triquinane skeleton. Natural products with triquinane architecture have been extensively studied as a target for development of efficient synthesis because of their unique structure and biological activities. The reported structure of panaginsene **1** was synthesized stereoselectively starting from (+)-citronellal. However, the spectral data of the synthetic compound did not match with those of the natural one, reported by W. A. König group, and that led us to suggest that the actual structure of panaginsene could be the epimer of reported structure at C11 on the basis of the plausible biosynthetic mechanism. Through the total synthesis of epimer structure **2**, we were completely convinced that originally assigned structure of panaginsene should be revised. The first total synthesis of both reported **1** and epimer structure **2** of panaginsene were accomplished through the intramolecular trimethylenemethane (TMM) diyl mediated tandem cycloaddition reaction from a linear substrate with high efficiency and stereoselectivity.



panaginsene
reported structure (**1**)



11-*epi*-panaginsene
epimer structure (**2**)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-772**

발표분야: 유기화학

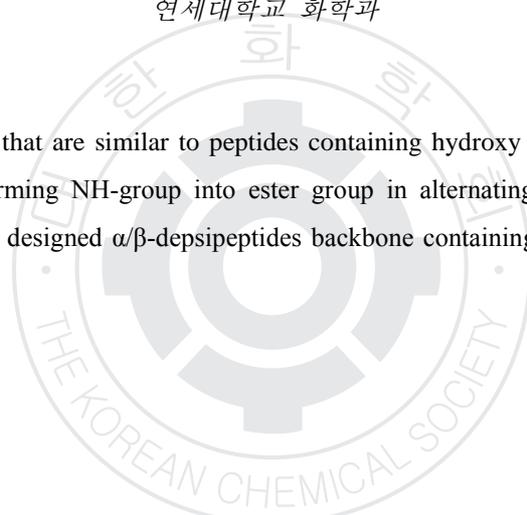
발표종류: 포스터, 발표일시: 수 16:00~19:00

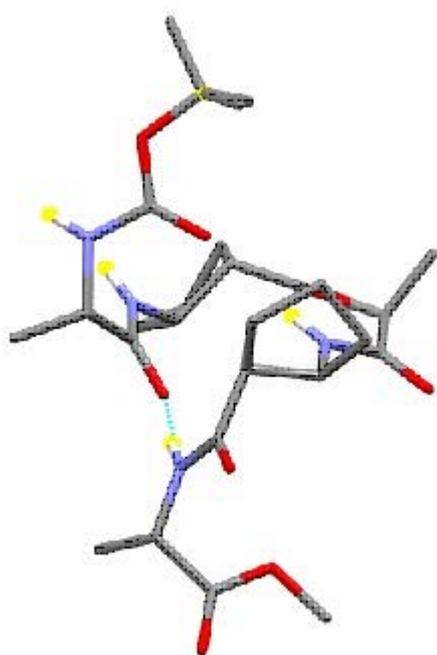
Synthesis And Comformational Study Of Unnatural Peptides Containing Lactic-acid

이재연 장근혁 강필재 최수혁*

연세대학교 화학과

Depsipeptide are oligomer that are similar to peptides containing hydroxy acid residues. We wondered what the effect of transforming NH-group into ester group in alternating 1:1 α/β -peptide containing ACPC would be. Here, we designed α/β -depsipeptides backbone containing Lactic acid to observe new helical pattern.





일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-773**

발표분야: 유기화학

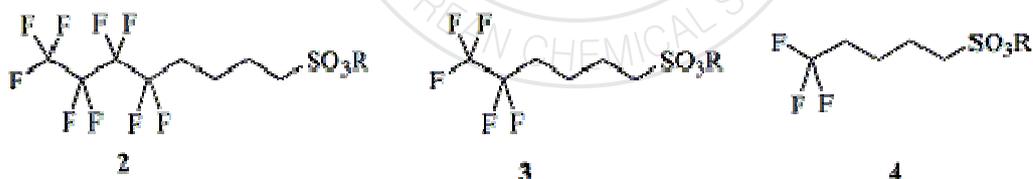
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of new PFOS alternatives in ionic liquid

Vijay kumar 신동수* **B.Prem kumar** 고요한

창원대학교 화학과

Perfluorooctanesulfonic acid (PFOS) 1 and their derivatives are the key ingredients in many stain repellents and also proven to be toxic towards health and environment due to its non-biodegradability. Along with a polar sulfonic acid group, a non-degradable C8-fluorocarbon chain is the reason for its special properties and also hazards. Three partially perfluoroalkyl iodides were simultaneously coupled to phenyl- vinylsulfonate in presence of Zn/CuI in ionic liquid [BMIM]Cl as well as in formamide to obtain phenylperfluoroalkylsulfonate. Various salts of each sulfonic acid series were synthesized from corresponding phenylsulfonates by hydrolysis.



R = Li, Na, K, NH_3 etc.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-774**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of bioluminescence probe for biofunctional molecules detection

남윤석 신인재*

연세대학교 화학과

In recent years, a variety of non-invasive imaging methods have been developed and utilized to study biological processes. Bioluminescence and fluorescence imaging methods are considered to be more advantageous than other imaging methods for their higher sensitivity and ease of handling. In particular, bioluminescence imaging boasts of having almost no background noise in the normal cells as they do not express the enzyme. This point enables the luminescence based probes to have higher sensitivity than fluorescence analysis during imaging. As a part of our group's on-going interest in research of non-invasive imaging probes, we turned our attention to expand the scope and utility of bioluminescence based probes. Current study describes our effort towards the development of two distinct bioluminescence-based probes for detection of ozone and Atg4B enzyme detection, which are thus far unprecedented. Both probe design hinges on installation of functional moiety that gets selectively cleaved in the presence of target analytes (ozone or enzyme activity). Its synthesis and in vitro studies are reported herein.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-775**

발표분야: 유기화학

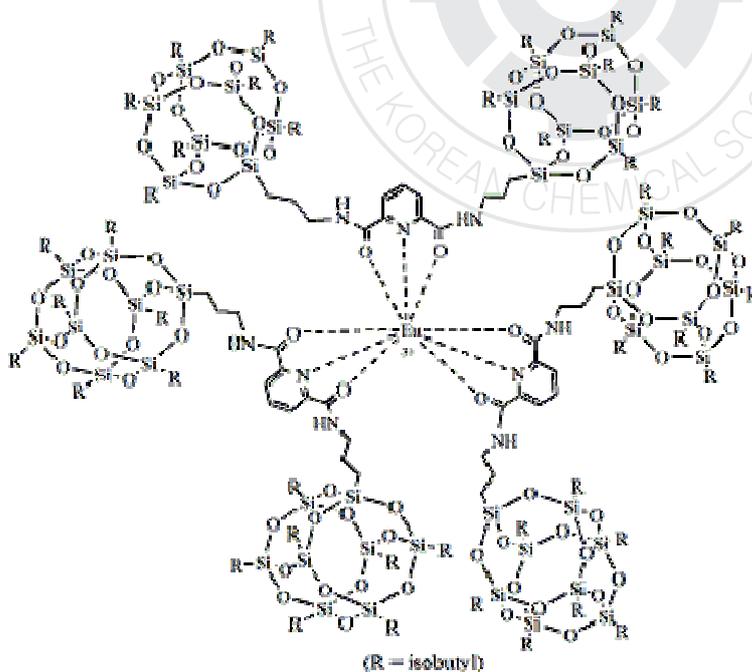
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of PDC-POSS-based hybrid fluorescent material

B.Prem kumar 신동수* **Vijay kumar**

창원대학교 화학과

In this study, we chose the 2,6-pyridinedicarboxylic acid chloride (PDC) as the original ligand to construct bridge molecule with POSS amine, which afterward binded with Eu^{3+} to obtain the binary lanthanide organic-inorganic hybrid material Eu-PDC-POSS. The complex 1 showed efficient fluorescent activity when subjected to different excitation wavelengths like 254 nm, 288nm, 393 nm and 464nm.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-776**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

d9,9-dimethyl-9H-fluorene-2-yl-2-boronic acid와 B-1-naphthalenyl 을

이용한 OLED용 arylamine 합성

송희정 채규윤* 이덕희¹ 김보미 백오현

원광대학교 화학과 ¹원광대학교 바이오나노화학부

OLED 용 Arylamine 은 많은 작용기를 갖고 있다. 본 실험내용은 OLED 용 Arylamine 에 fluorene 과 B-1-naphthalenyl 을 합성하는 방법이다. 이 실험은 Suzuki reaction 반응을 이용한다. Suzuki reaction 은 palladium 촉매를 이용하여 유기할로젠화합물과 유기 붕소화합물을 간단하고 효율적으로 결합시키는 반응을 말한다. 즉, 탄소-탄소 결합하는 예전방식과는 달리 palladium 촉매를 이용해서 탄소 결합과정이 쉬워지는 탄소-탄소 교차 짝지음 반응을 이용하는 실험이다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-777

발표분야: 유기화학

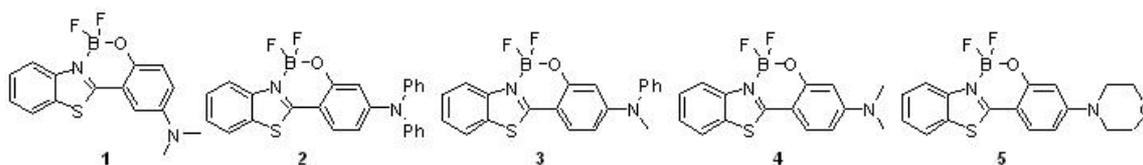
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and Synthesis of Color-Tunable Organoboron Complexes

문현수 안교한*

포항공과대학교 화학과

The highly emissive materials is important for various applications like organic light-emitting diodes, and sensors.¹ Tunable emission wavelength and high quantum yield are two fundamental factors to establish emitting material. Much efforts have been carried out to tune the emission color but there is only a few core structures with flexibility in their synthetic strategies.² Extended π -conjugated molecules such as organoboron complexes received intense interest because they can give desired photophysical properties. Organoboron complexes are promising candidate as light emitting materials for their intense luminescence.³ Moreover, their emission properties can be modulated by altering the substituents on the framework or boron atom. Our group reported on substituent effect of organoboron complexes. Simply by changing the position of N,N-dimethylamino substituents, we could tune emission color from orange to blue in dichloromethane.⁴ Instead of N,N-dimethylamino group, we introduce other amino group. Boron complexes 2, 3, and 5 emit green, yellow, and blue luminescence in dichloromethane, respectively. Boron complexes 2 and 5 show very bright and strong luminescence: 5 shows a fluorescence quantum yield close to unity ($\Phi_F = 0.99$ in cyclohexane). Therefore, boron complex 5 can serve as efficient blue-emitting materials in OLEDs. Reference 1. Jung, B.-J.; Yoon, C.-B.; Shim, H.-K.; Do, L.-M.; Zyung, T. *Adv. Funct. Mater.* 2001, 11, 430. 2. Pohl, R.; Montes, V. A.; Shinar, J.; Anzenbacher Jr, P. J. *Org. Chem.* 2004, 69, 1723. 3. Li, D.; Zhang, H.; Wang, C.; Huang, S.; Guo, J.; Wang, Y. J. *Mater. Chem.* 2012, 22, 4319. 4. Santra, M.; Moon, H.; Park, M.-H.; Lee, T.-W.; Kim, Y. K.; Ahn, K. H. *Chem. Eur. J.* 2012, 18, 9886.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-778**

발표분야: 유기화학

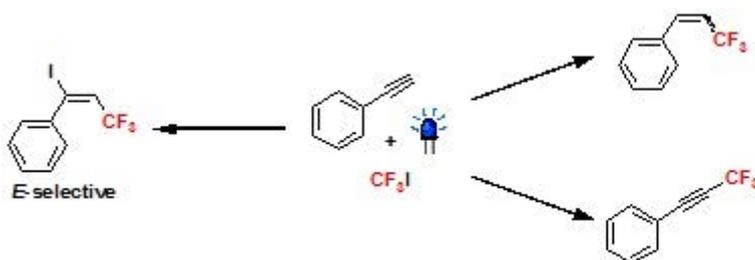
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Trifluoromethylation of Unactivated Alkyne by Photoredox Catalysis

Naeem Iqbal 정재현¹ 박세현¹ 조은진*

한양대학교 응용화학과 ¹한양대학교 바이오테크놀로지학과

Great effort has been made to develop efficient trifluoromethylation methods because of its great interest in many applications such as pharmaceuticals and agrochemicals, since the trifluoromethyl group can dramatically influence the properties of molecules. Three different CF₃-containing compounds, trifluoromethylated-alkenyl iodide, alkene, and alkyne were generated from unactivated alkynes under different catalytic conditions. This product manipulation by mild alteration in the reaction conditions, where the same material converts into various products selectively, is very challenging and attractive in organic synthesis. Trifluoromethyl alkenyl iodide was obtained E-selectively on the other hand, alkenyl-CF₃ compounds was obtained Z-selectively by cascade hydro-trifluoromethylation of alkynes. In addition, trifluoromethylated alkyne was also generated selectively.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-779**

발표분야: 유기화학

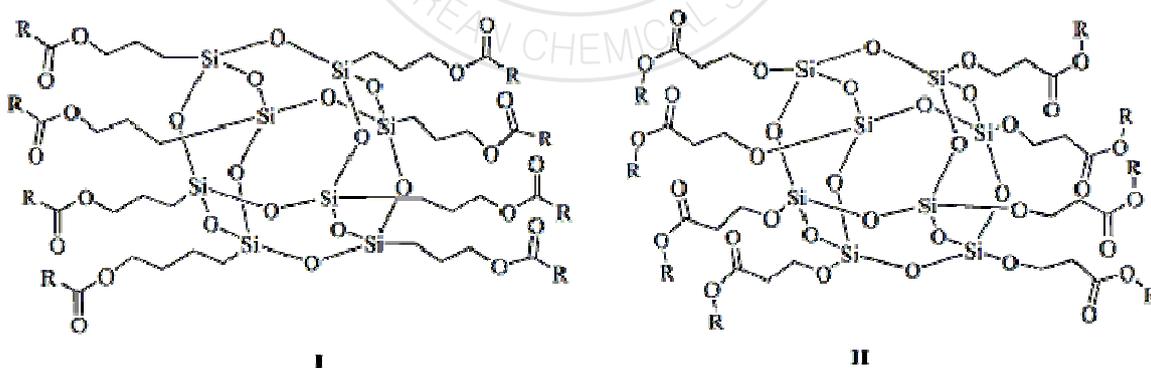
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of POSS derived inorganic/organic hybrid insulating oils

chirumarrysridhar Vijay kumar 신동수* 김영은

창원대학교 화학과

The synthesized transformer or insulating oils make considerable environmental pollution when they spill out. To prevail over this drawback we have come up with the synthesis of biodegradable polyhedraloligomeric silsesquioxane (POSS) based oil additives, which show dramatic influence on the behavior of insulating oils. POSS have a rigid and durable cage structure, is known for its stability even at higher temperatures and expected to show good flow ability at lower temperature when attached to certain ester moieties. Herein, we described the synthesis of esters of octahydroxy-POSS derivative and acyloxysilyl POSS towards the various biodegradable insulating oils.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-780**

발표분야: 유기화학

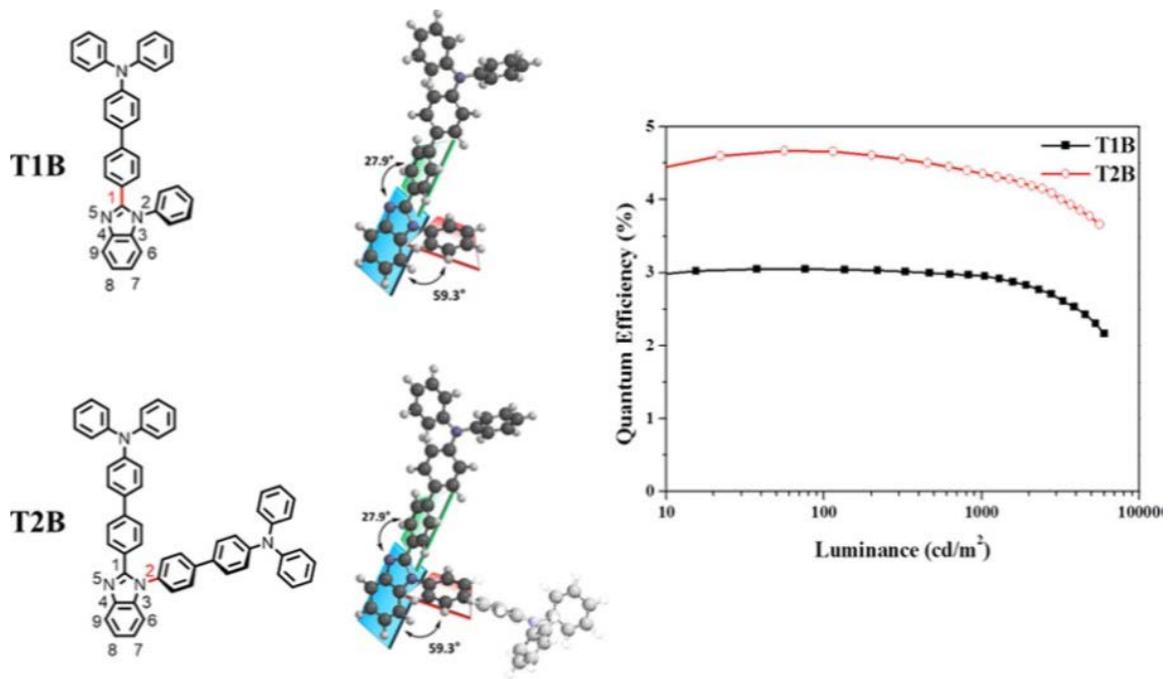
발표종류: 포스터, 발표일시: 수 16:00~19:00

High-performance host free deep-blue emitting imidazole-triphenylamine derivatives for Organic Light-emitting Diodes

정성진 홍종인*

서울대학교 화학부

Deep-blue fluorescent organic light-emitting diodes (FLOLEDs) possessing high efficiency and pure Commission Internationale de l'Éclairage (CIE) chromaticity coordinates are a prerequisite for full-color displays and lighting devices. Nonetheless, because of the wide bandgap of blue emitters, only a few examples of high-performance blue FLOLEDs have been reported, in contrast to red and green FLOLEDs. A nondoped system has an advantage in that it has a simple device structure that employs only a single emitting material without using a complicated host/dopant codeposition process. Two triphenylamine-substituted benzimidazole derivatives were designed and synthesized for use as efficient deep-blue emitters in nondoped FLOLEDs. Nondoped FLOLED devices fabricated using 4',4''-(1H-benzo[d]imidazole-1,2-diyl)bis(N,N-diphenylbiphenyl-4-amine) (T2B) as a blue emitter exhibited an external quantum efficiency of 4.67% with CIE coordinates of (0.15, 0.08).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-781**

발표분야: 유기화학

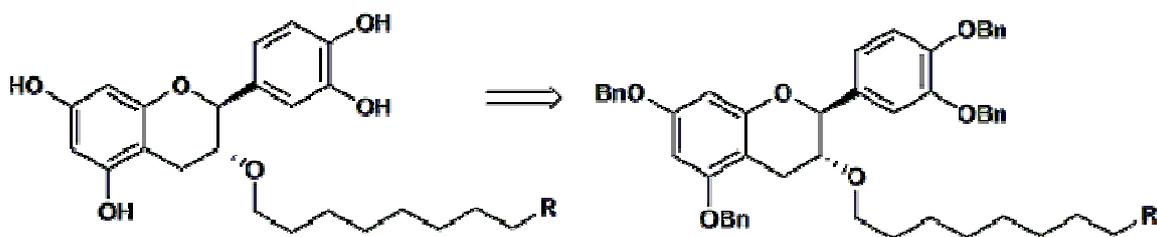
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, Synthesis and antimicrobial activity of (?) -Catechin Analogues

kumar deepak 신동수* **Vijay kumar**

창원대학교 화학과

Recently, much attention has been paid to tea, *camellia sinensis*, for the beneficial biological activities of its compounds, catechins. The catechins are a group of 3-flavanols including (+)-catechin, (-)-catechin, epicatechin, ent-epicatechin and their derivatives. The biological activities of these compounds are very wide ranging, including anti-oxidative, anti-HIV, anticarcinogenic, antiarteriosclerotic and antibacterial. However, the development of flexible strategy that allows regio- and stereoselective construction of multi-substituted catechins with the defined configuration at the C-2 and C-3 positions employing versatile building blocks is highly desirable. The (?) -Catechin analogues were synthesized and evaluated against different strain of bacteria and fungi. Most of the compound shows promising antimicrobial activities.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-782**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric synthesis of (+)-Lentiginosine from a chiral aziridine

윤호중 조경선¹ 심태보*

한국과학기술연구원(KIST) 화학키노믹스연구센터 ¹서강대학교 화학과

Asymmetric synthesis of (+)-Lentiginosine, a indolizidine alkaloid, is described. Key features of the synthesis include the efficient and stereoselective construction of the dihydroxylated pyrrolidine by using Sharpless asymmetric dihydroxylation of aziridine-enoate, which was prepared from commercially available 1-(S)- α -methylbenzylaziridine-2-methanol and subsequent regioselective ring opening-cyclization cascade reaction. A subsequent C-3 Wittig ligation and intramolecular cyclization then produced a precursor, which was converted into (+)-Lentiginosine.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-783

발표분야: 유기화학

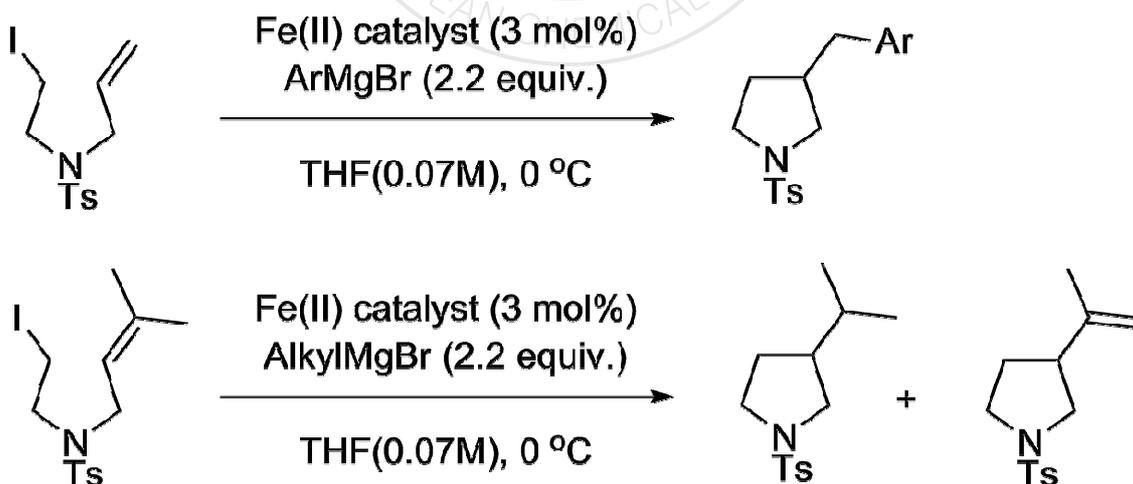
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on the Iron(II)-catalyzed 5-Exo Cyclization Reactions with Grignard Reagents

김재곤 서진원¹ 백종화¹ 강은주^{1,*}

경희대학교 화학과 ¹경희대학교 응용화학과

The radical reactions of alkyl halide have been well-known as carbon-carbon bond formation reactions. In despite of Fe-Grignard complex is one of the most efficient initiator for Fe catalyzed radical reaction, Grignard reagent is used only to activate Fe catalyst. Herein, we reported Fe catalyzed atom-economical tandem reaction of alkene-iodide in the present of equimolar aryl Grignard reagent. Aryl Grignard reagent is used to generate Fe-Grignard complex and the counter aryl anion is used in the further cross-coupling, thereby affording the tandem cyclization/cross-coupling radical reaction.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-784

발표분야: 유기화학

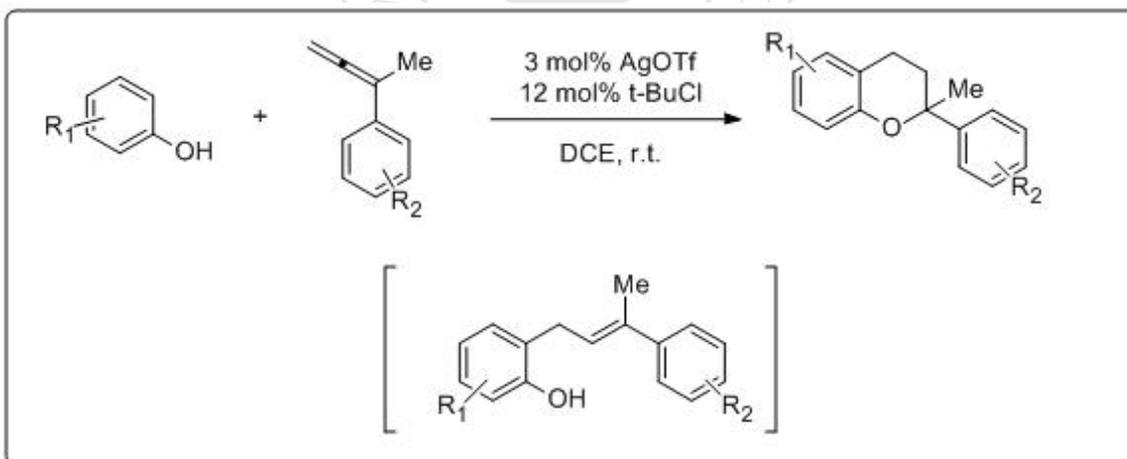
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective One-pot Synthesis of Flavan Derivatives in Hidden Brønsted acid Catalysis

진하정 강은주*

경희대학교 응용화학과

An efficient synthesis of functionalized flavans from commercially available phenols and easily available aryl allene derivatives is reported, which are important skeletons in biological and pharmaceutical fields. The synthesis involves a brønsted acid catalyzed intermolecular hydroarylation and intramolecular hydroalkoxylation reactions. This one-pot synthesis showed a high regioselectivity in both hydroarylation reacting at the terminal position of allenes and hydroalkoxylation forming 6-membered furan derivatives.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-785

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Tandem Reaction for Substituted 3-Pyrroline Synthesis from Terminal Alkyne

신예호 황준영¹ 강은주^{2,*}

경희대학교 화학과 ¹경희대학교 응용과학대학 응용화학과 ²경희대학교 응용화학과

Copper catalysis has recently acquired an increasing importance, in view of the availability, low toxicity and higher environmental compatibility of copper when compared with other transition metal catalysts. As a useful class of compound, allenes not only act as versatile intermediates on organic synthesis, but also exist in many natural products and pharmaceuticals, crabbe reported the CuBr-mediated reaction to form terminal allenes from 1-alkynes and formaldehyde in the presence of diisopropylamine. We have developed a one-step synthesis of 2-substituted 3-pyrrolines and 2,5-disubstituted 3-pyrrolines via corresponding allene-intermediate. The further studies are examined on mechanistic investigation using isolation of allene intermediates, and synthetic application of functionalized pyrroles by DDQ oxidation reactions



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-786**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chlorotrifluoromethylation of Alkenes by Visible Light Photoredox catalysis

오세환 한수봉*

한국화학연구원 신약연구본부

An efficient and versatile method for chlorotrifluoromethylation of alkenes is developed using visible light photoredox catalysis with Ru(Phen)₃Cl₂. Trifluoromethyl sulfonyl chloride is used as the source for trifluoromethyl radical. The mild reaction condition enables the chlorotrifluoromethylation of a range of alkenes that bear various functional groups. The simple and mild reaction condition allows the late stage introduction of trifluoromethyl and chloro groups to natural product. This is the first report of photoredox catalyzed atom transfer radical addition reaction. (ATRA) introducing trifluoromethyl and chloro group to olefins simultaneously. The ease of handling of trifluoromethylsulfonyl chloride compared to earlier employed halotrifluoromethylating reagents in visible light ATRA reactions, gives this method an edge over earlier methods.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-787**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Benzothiadiazole-based planar donor materials for heterojunction solar cells

전용준 홍종인*

서울대학교 화학부

Since the first report of organic solar cells (OSCs) by Tang, the development of OSCs has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene were used as donor materials for heterojunction solar cells due to good charge transport ability. A benzothiadiazole unit was used as low band gap donor materials due to their broad absorption spectra. To improve performance of heterojunction solar cells, we introduced new low bandgap donor materials, consisting of benzothiadiazole, naphthalene, benzothiophene and thiophene. Details of the synthesis, photophysical, electrochemical and theoretical studies and device data will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-788**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot direct conversion of phenols to anilines via Smiles rearrangement

xieyongsheng 신동수* dongwenliang

창원대학교 화학과

A convenient one-pot direct conversion of phenols to anilines has been developed using Smiles rearrangement in presence of a weak base and chloroacetamide. This method can also be useful for the synthesis of aminopyridine from the corresponding hydroxy substrates.



EWG = Electron withdrawing group

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-789**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual-Color Imaging of Cytosolic and Mitochondrial Zinc Ions in Live Tissue With Two-Photon Fluorescent Probes

RATHORE KAILASH 조봉래*

고려대학교 화학과

Zinc ion is an essential trace metal ion that plays important roles in the mammalian cells as catalytic or structural cofactors.¹ A small fraction of the total zinc ion content, exist as cytosolic free Zn^{2+} . Since low nanomolar concentration of free Zn^{2+} can be cytotoxic, it is vital to maintain Zn^{2+} homeostasis. If the $[Zn^{2+}]_c$ level is elevated by the influx of Zn^{2+} , the excess is removed by shuffling Zn^{2+} to subcellular stores such as endoplasmic reticulum and mitochondria and by transferring Zn^{2+} to extracellular space.² To visualize such processes in a live tissue, it is crucial to develop TP probes that can simultaneously detect the Zn^{2+} in different organelles.

Simultaneous detection of Zn^{2+} in the two organelles was not yet possible as the TPEF maxima of the available probes were too close to detect independently. We, therefore, have developed TP probes for cytosolic Zn^{2+} (BZn-Cyto) and mitochondrial Zn^{2+} (FZn-Mito), which emit TPEF at widely-separated wavelength regions upon binding with Zn^{2+} . TP fluorophores used to derive BZn-Cyto and FZn-Mito, exhibited significant TP cross section and emitted TPEF at 469 and 529 nm in aqueous buffer, where as the Zn^{2+} chelators utilized of various K_d values are within the range of expected Zn^{2+} concentration in two organelles. Triphenylphosphonium ion was envisioned as the mitochondrial targeting moiety.³

1. Vinkenborg, Ja. L.; Nicolson, T. J.; Bellomo, E. A.; Koay, M. S.; Rutter, G. A.; Merks, M. *Nat. Meth.* 6, 737-740.
2. Colvin, R. A.; Holmes, W. R.; Fontaine, C. P.; Maret, W. *Metallomic*, 2010, 2, 306-317.
3. Dickinson, B. C.; Chang, C. J. *J. Am. Chem. Soc.* 2008, 130, 9638.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-790

발표분야: 유기화학

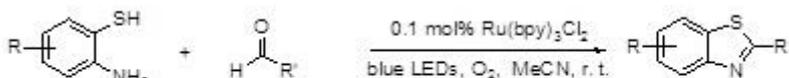
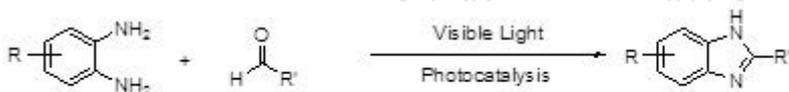
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-Substituted Benzimidazoles and Benzothiazoles by Visible Light-Driven Photoredox Catalysis

정재현 박세현 조은진^{1,*}

한양대학교 바이오나노학과 ¹한양대학교 응용화학과

The benzofused heterocyclic compounds such as benzimidazole and benzothiazole moieties have been of great importance in many applications. Especially, they play important role in pharmaceuticals and agrochemicals or biological interest. A variety of 2-substituted benzimidazoles were generated using *o*-phenylenediamine and a variety of aldehydes as the substrates via visible - light photoredox catalysis. 2-Substituted benzothiazoles were similarly synthesized from 2-aminothiophenol and a variety of aldehydes in the presence of 0.1 mol% [Ru(bpy)₃Cl₂] and O₂ under visible light irradiation.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-791**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence Chemosensor for Fluoride Anion with Coumarine Bypiridine Derivative

윤희상 이환석 남계춘*

전남대학교 화학과

The studies of chemosensors toward F⁻ anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, developments of reliable sensors for fluoride ion are needed for environment and human health care. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition.¹ Especially, coumarine are a particularly elegant basis for ratiometric based optical sensors. Here, we report a novel coumarine bipyridine chemosensor 1 with a specific optical response to fluoride ion. In pursuit of a selective fluoride chemosensor, a coumarine bipyridine derivative 1 was synthesized, and its anion binding properties were investigated by ¹H NMR, uv-vis spectroscopy, color changes, and fluorescence titration analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-792**

발표분야: 유기화학

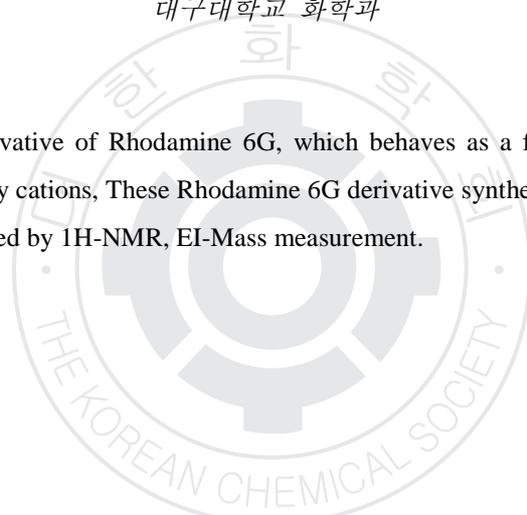
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and fluorescence property of polymer chemosensor with Rhodamine 6G derivative

장우식 장승현*

대구대학교 화학과

The chemosensor is a derivative of Rhodamine 6G, which behaves as a fluorescent and chromogenic sensor toward various heavy cations, These Rhodamine 6G derivative synthesized by polymerization, and the compound was confirmed by ¹H-NMR, EI-Mass measurement.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-793**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis and properties of rhodamine derivative fluorescence sensors

김기백 장승현*

대구대학교 화학과

Rhodamine spirolactam or spirolactone derivatives was non-fluorescent and colorless, whereas ring-opening of the corresponding spirolactam/lactone gives rise to strong fluorescence emission and a pink color. We synthesized rhodamine derivative fluorescent sensors. This compound was synthesized by two-step condensation reaction of rhodamine 6G and ethylenediamine compound, which makes it difficult to develop a turn-on fluorescent sensor and more noteworthy to develop a sensitive one. Ring-closed rhodamine-fluorene derivatives are colorless and non-fluorescent, whereas the ring-open forms were strongly fluorescent and pink in color. Several successful attempts have been made to develop selective fluorescent sensors based on rhodamine-fluorene for Cu^{2+} , Pb^{2+} , Hg^{2+} and Fe^{2+} . And fluorescence properties will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-794**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and fluorescence properties of phenothiazine derivatives

손문수 장승현*

대구대학교 화학과

In this research, we have studied the molecular recognition about various metals and the character of fluorescence including phenothiazine by synthesized new host material. The structures of all reaction products were identified by $^1\text{H-NMR}$, GC-MS, FT-IR. We synthesized new host compounds containing phenothiazine derivate (C1 and C2). Compound1 was synthesized from 4'-Aminobenzo-15-crown-5 and 10-ethyl-10H-phenothiazine-3-carbaldehyde(C1), Compound2 was synthesized from 4'-Aminobenzo-18-crown-6 and 10-ethyl-10H-phenothiazine-3-carbaldehyde(C2). New host compounds were found selectivity for metal cation by fluorescence titration using various metal cation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-795**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Off-On Chemosensor for Fluoride Ion with Pyrene Based on Triphenylphosphine

심남연 윤희상 이환석 남계춘*

전남대학교 화학과

The supramolecular chemistry of anions provides a means to sense and manipulate anions in their many chemical and biological roles. Anions are ubiquitous and they have major roles in the natural world. In particular, the studies of F^- anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, the development of reliable sensors for F^- is needed for environment and human health care. Fluorescent chemosensors can be effectively used as a tool to analyze and classify such roles of charged chemical species in living system as well as to measure the amount of ions from the sources contaminated with them. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. The salt type derivative was obtained successfully by the reaction of triphenylphosphine with pyrene derivative. The binding properties of triphenylphosphine derivative investigated with 1H -NMR and fluorescence titration methods with various anions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-796**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Lysine으로부터 Nylon 6 제조용 caprolactam 합성

고진선

고려대학교 화학

석유자원 고갈로 인한 원료가격 상승과 온실가스 배출에 의한 지구 온난화와 문제 때문에 바이오매스 기반 소재 개발이 활발하다. 본 연구에서는 바이오매스 기반 nylon 6 를 제조하는데 필요한 단량체 caprolactam 을 바이오매스 기반 소재인 lysine 으로부터 합성하였다: Lysine 으로부터 amino-caprolactam 을 먼저 합성하고 이를 다시 reductive deamination 반응을 시켜 caprolactam 을 제조하였다. 반응조건에 따른 caprolactam 수율 변화를 조사하였으며, 대표적 실험인자로는 반응시간, 촉매, 용매 등을 고려하였다. 특히 amino- caprolactam 합성단계에서는 lewis acid 계열인 SiO₂ 촉매와 1,2-propanediol(용매)을 사용하여 96 시간 반응 하였을 때 가장 높은 수율을 얻었다. 이렇게 제조된 화합물의 구조를 1H-NMR, FT-IR 을 통하여 확인하였다. 본 실험에서 제조된 caprolactam 을 개환반응으로 중합하였을때 nylon 6 를 성공적으로 제조할 수 있었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-797**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic Molecular Architectures with Facet Dependent Property by the Controlled Self-Assembly of an Amphiphilic and Helical β Peptide Foldamer

유성현 이희승*

한국과학기술원(KAIST) 화학과

Though various attractive chemical and biological properties of peptide based nano and micro molecular structures were studied intensely these days, facet dependent property, which is well-known for inorganic materials have, was hardly found in the peptidic molecular structure due to its limited shapes on 1D or 2D structures. Here, we show that a well-defined rhombus rod shaped molecular architecture by controlled self-assembly of a helical amphiphilic β peptide foldamer, mimicry of natural peptidic α helix, exhibit facet dependent property in facet-selective Pt nanoparticle adhesion. Molecular arrangement that supports the results above was determined by powder X-ray diffraction analysis combined with global optimization and Rietveld refinement.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-798**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Helical β -Peptide linked to Dithiol Derivative for Novel Foldamer with a High Durability

이양호 이희승*

한국과학기술원(KAIST) 화학과

Nano-micro materials based on peptides, which are biocompatible and bioactive, have been known to be utilized to various biological, chemical applications. 1 Our groups have shown that 3D structures with unprecedented shapes could be synthesized by self-assembly of foldamer, an artificial protein fragment. 2, 3 These molecular structures need to much more physical and chemical stability in order to use in extensive application. We envisioned that dithiol derivatives could increase stability of foldamer through crosslinking. 4 Here, We report synthesis and analysis of helical β - peptide linked to dimercaptobenzoic acid and forms macrocyclic building blocks through thiol oxidation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-799**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphene Oxide-Supported N-Heterocyclic Carbene/Pd as a Recyclable Heterogeneous Catalyst for Suzuki Reaction

박정현 RazaFaizan 전수지 김혜인 김종호^{1*}

한양대학교 융합화학공학과 ¹한양대학교 화학공학과

In order to synthesize an effective heterogeneous catalyst for Suzuki reaction in an aqueous solution, we functionalized graphene oxide (GO) with 3-(3-aminopropyl)-1-methylimidazolium bromide (denoted IMG0), and immobilized Pd(OAc)₂ on IMG0. This catalyst was fully characterized by FT-IR, ICP, and XPS, and it exhibited excellent catalytic activity in Suzuki C-C coupling reaction in an aqueous solution. All aryl bromides and iodides were converted to their corresponding products at high yields within 1 h at 50°C. The catalyst was easily separated from the reaction mixture by simple centrifugation, and it was recycled several times without a loss of its catalytic activity in Suzuki reaction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-800**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

starbust 이용한 OLED 전공수송층 소재 합성

백승지 채규윤* 이덕희¹ 송미선

원광대학교 화학과 ¹원광대학교 바이오테크놀로지화학부

다중 starbust 에 기존의 물성이 좋은 것으로 알려진 spiro 와 fluorene 화합물을 도입시켜 높은 유리전이온도를 갖는 starbust 유도체를 합성한 후 수명이 긴 OLED 전공수송층 소재를 개발하고자 한다. 본 실험에서는 C-C coupling 을 위하여 Suzuki, Heck/Negishi, Kumada 반응을 이용할 것이며, 그 외에도 amination, wittig reaction 을 이용하고자 한다. 구조 확인을 위해서는 FT-IR, FT-NMR, UV, GC-mass 를 이용할 것이다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-801**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of PEG based sucrose and trehalose polymers for biotechnological application

Ashrafuzzaman MD 표정인¹ 정찬성^{1,*}

과학기술연합대학원대학교(UST) Biological Chemistry ¹한국과학기술연구원(KIST) 화학키노믹스 연구센터

Significant research has been conducted over the past decades toward producing safe and effective methods for synthesis of polymers in biomedical and therapeutic application. The use of trehalose and sucrose together with polyethylene glycol (PEG) has gained interest in protein stability, cryobiology, biomedical and pharmaceutical fields. Trehalose has been applied as a cryopreservation agent to a variety of biologicals, including mammalian cells, various tissue, proteins, viruses, bacteria, and yeasts. Besides PEG has wide range uses which can perform as a backbone in various copolymer or polymer conjugate. These applications have led to an increasing demand of well-defined polymers with tailorable properties. Recently, we have synthesized divinyl adipoyltrehalose and divinyl adipoylsucrose molecules by enzymatic processes which were loaded on PEG to receive bilayer polymer. We selected superior enzyme from screening of several enzymes and have immobilized the same enzyme using Sol-Gel method. These polymers will be tested as protein detergent and can also be applied on proteins/cells stability. Such modifications of PEG based sugar polymers are of significance in development of new functional materials in the biomedical and pharmaceutical field with potential application.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-802**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Imidazolium Organic Ionic Plastic Crystals: Thermal Properties of Bis(alkylimidazolium)ethane Salts with branched side-arms

이민재

군산대학교 화학과

After 1,2-bis[N-(N'-alkylimidazolium)]ethane salts were discovered as a new class of organic ionic plastic crystals, we have been investigating the exact structures/motions of each crystalline solid state below the melting temperature. The cationic planar imidazolium ring may be flipping at some solid states, or whole counter anions may move in some distance at other solid states, and both may occur simultaneously. 1,2-Bis[N-(N'-alkylimidazolium)]ethane salts with branched side-arms were also synthesized and their thermal properties were investigated. The ΔS_f of the new imidazolium salts are relatively bigger than the "true" organic plastic crystals, however they also show multiple solid-solid transition on DSC.

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장소: 창원CECO

발표코드: **ORGN.P-803**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and synthesis of borepin derivatives as a fluoride sensor

이혜경 최은정 차인환 송창식*

성균관대학교 화학과

Organoboron molecules are electron deficient due to the empty p-orbital of boron, and thus can be expected unique optical and electronic properties. Among them, borepins are boron-containing, seven-membered conjugated heterocyclic systems that exhibit unusual aromaticity. Here we designed and synthesized the structurally novel electron-deficient molecule, thiophene-fused 1-hydroxyborepin. We measured optical and electrochemical properties by UV-vis spectroscopy, photoluminescence and cyclic voltammetry. To identify the sensing capacity, 1-hydroxyborepin was reacted with various molecules, such as dopamine, catechol, fluoride ion, and so on. Especially, fluorescence quenching of 1-hydroxyborepin was caused by addition of fluoride ion.

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장소: 창원CECO

발표코드: ORGN.P-804

발표분야: 유기화학

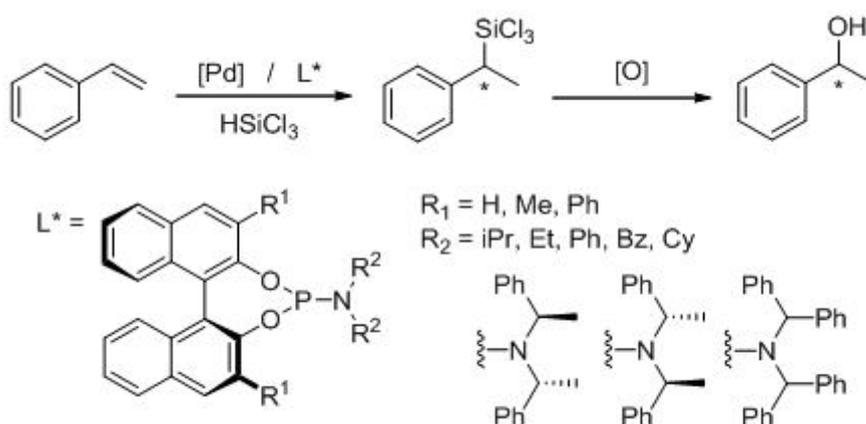
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric palladium-catalyzed hydrosilylation of styrenes using bulky monodentate phosphoramidite ligands

남궁숙 한진옥*

한양대학교 화학과

Pd-catalyzed asymmetric hydrosilylation of alkenes with trichlorosilane is one important example of hydrometallation reactions that display excellent regioselectivities and enantioselectivities for a variety of alkyl-substituted terminal alkenes, styrene derivatives. In this study, asymmetric hydrosilylation of styrenes with trichlorosilane in the presence of palladium complexes of these bulky ligands gave chiral silanes in high yields with excellent reactivities and enantioselectivities.



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장소: 창원CECO

발표코드: **ORGN.P-805**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Domino Meyer-Schuster Rearrangement and Ring Expansion

신선용 안준현 신승훈*

한양대학교 화학과

We recently found that ring expansions of 1-alkynyl cyclobutanol derivatives can be intercepted by Meyer-Schuster rearrangement, followed by ring expansion leading to alpha-hydroxy-alpha-vinyl cyclopentanone derivatives. Enantioselective ring expansion involves differentiation of prochiral faces and thus presents a significant challenge. In this presentation, we present our preliminary efforts toward this goal utilizing chiral monophosphine ligands. Monophosphine ligands provided for a faster conversion compared to bisphosphine ligands with similar selectivity. In addition, a working mechanism will be discussed regarding intermediates in the enantiodiscriminating step.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-806**

발표분야: 유기화학

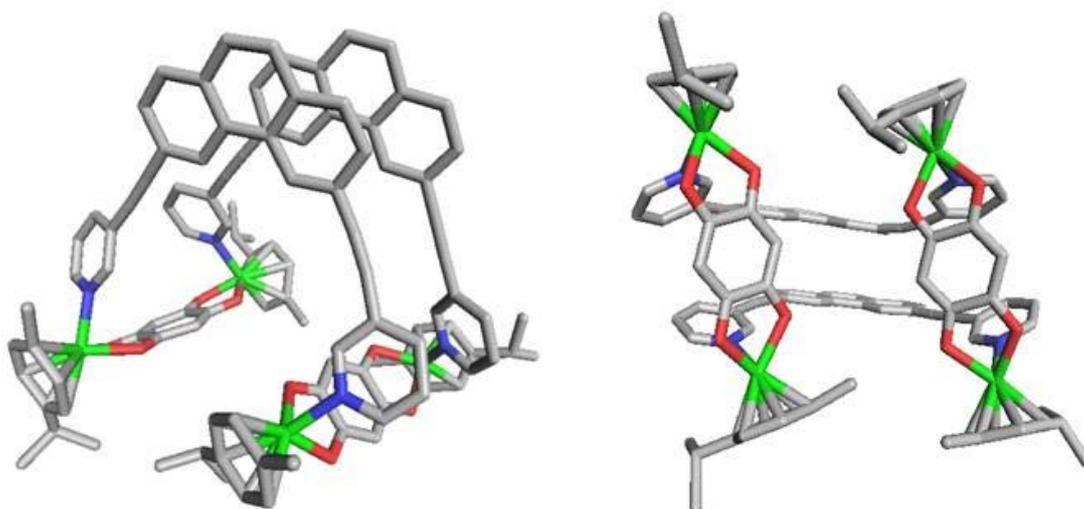
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Assembly between Octahedral Ru-Acceptors and New Dipyridyl Phenanthrene Donor

송영호 민진욱 지기환*

울산대학교 화학과

Self-assembly is a ubiquitous phenomenon in natural systems and is at the heart of many biological processes, including protein synthesis and DNA formation. In the past two decades, coordination-driven self-assembly has emerged as an effective tool for constructing functionalized metalla-supramolecules with the aim of better understanding and mimicking their biological analogues. Arene-ruthenium [2+2] metalla-rectangles have been synthesized by the self-assembly approach using arene-ruthenium acceptors and new dipyridyl ethynyl ligand. All the complexes were characterized by ^1H NMR, ESI-MS, and single crystal X-ray analyses confirm the formation of these newly synthesized rectangles.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-807**

발표분야: 유기화학

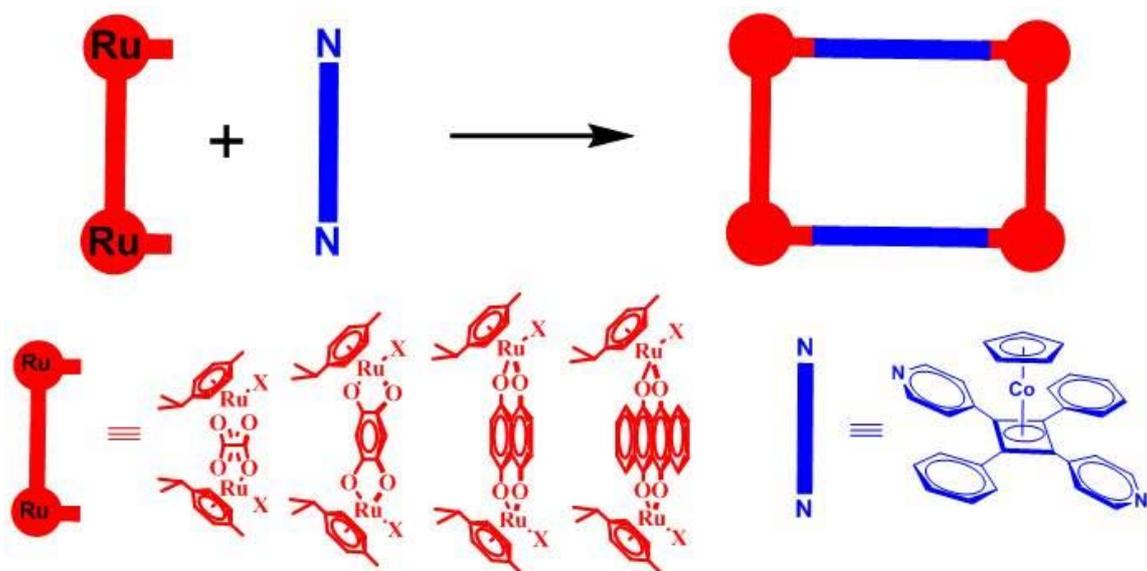
발표종류: 포스터, 발표일시: 수 16:00~19:00

Coordination-Driven Self-Assemblies of Cobalt Sandwich Compound Based N-donor and Half-Sandwich Ruthenium(II) Based Acceptors

SINGH NEM 조재호 이혜우 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 in molecular recognition, separation, catalysis, encapsulation of guests and biological systems. The present work demonstrates the spontaneous formation of metal?ligand bonds in solution, transforming molecular building blocks into 2D metallacycles and 3D metallacages using cobalt sandwich compound based N-donor and different arene?ruthenium acceptors (scheme 1). The resulting supramolecular complexes have well-defined internal cavities to stack planner aromatic guests. These self-assembled metallacycles were also evaluated for biological activities. All the new complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. The poster will address a detail comprehensive account of the mentioned work.



Scheme 1: Synthetic route to the self-assembled metalla-rectangles



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-808**

발표분야: 유기화학

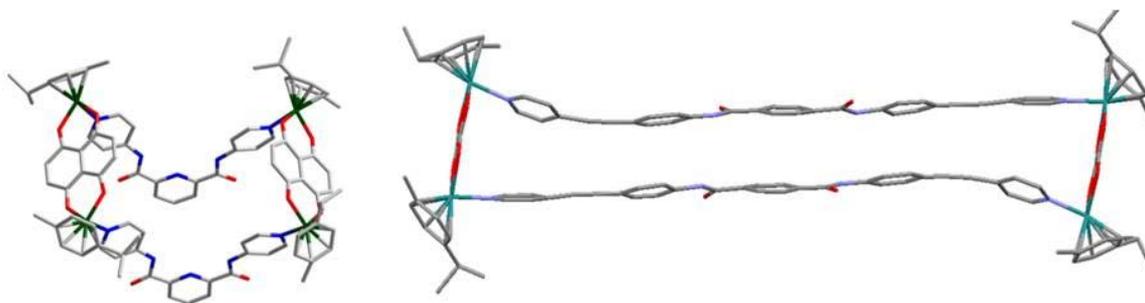
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Assembly and Application of 2D Metallacycles via Amide Ligands and Arene-Ruthenium Acceptors

조재호 ANURAG MISHRA 이승창 지기환*

울산대학교 화학과

The coordination-driven self-assembly of appropriate building units to form discrete supramolecular entities has grown immensely in the past few years. Wide arrays of molecular architectures with various aesthetically pleasing shapes, sizes, and symmetries have been reported. Ligands that incorporate pyridine-N donors are appealing candidates for coordination driven self-assembly because of their ability to interact with metal acceptors to generate interesting assemblies. However, recently organometallic half-sandwich complexes based on Ru fragments are being used as potential building blocks to construct metallacycles and cages due to their stability and interesting electronic as well as structural properties. Such organometallic acceptors have mostly been used with nitrogen based organic linkers. Herein, we apply this strategy to the synthesis of new large molecular metallacycles using N-donor amide ligands with different lengths of arene-ruthenium building blocks. These complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. In additions, we used these new metallacycles for biological activity application.



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장소: 창원CECO

발표코드: **ORGN.P-809**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cyclic dipeptides, plant immunity-activating metabolites from soil-born bacterium *Bacillus vallismortis* EXTN-1

문석식* **Md.Maniruzzaman Manir** V.S.Jamal Ahamed* 박경석^{1,*}

공주대학교 화학과 ¹농촌진흥청 국립농업과학원 농업미생물과

It is well known that plant growth-promoting rhizobacteria help plants to induce resistance against pathogens by secreting biologically active substances. Induced resistance is a state of enhanced defensive capacity developed by a plant itself. This type of resistance is often referred as induced systemic resistance (ISR) and has been demonstrated in many plants species including bean, cucumber, tobacco, and pepper. A soil-born bacterium *Bacillus vallismortis* EXTN-1 itself has been shown to activate plant-immune system to resist against bacterial and fungal plant pathogens. We isolated and characterized active metabolites from the culture broth of the bacterial strain. Here, we report isolation, structure-determination, and biological activities of the metabolites, cyclic dipeptides.

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장소: 창원CECO

발표코드: **ORGN.P-810**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on Control of Physical and Chemical Stability of 3D Foldectures

엄재훈 이희승*

한국과학기술원(KAIST) 화학과

Regardless of scales and constituents, object shape is a subject of fundamental interest for scientists in various fields. In most cases, shapes in biological systems are constructed through precisely controlled self-assembly based on blueprints that are not fully understood. Foldecture is the three dimensional molecular architecture that is derived from the self-association of foldamer in solution. Foldectures are expected as a new kind of nano- and micro materials that can be used for various applications such as template for controlling the nano-structure of inorganics, organic-inorganic complex structure, drug delivery material and biochemical catalyst. To realize the functional molecular architecture, Foldecture must have resistance in wide range of environments such as high temperature, solvent, UV, strong acids and bases. In other words, foldecture need to immobilize through covalent bonding to ensure the stability under a variety of conditions. One of the suggestions for improving the stability of foldecture is inducing cross-linking method which can bind each foldamer of foldecture. So, we modified the previous backbone structure of foldamers as inserting amino acids that include cyclic disulfide group. In this presentation, we report a new example that is controlling physical and chemical stability of 3D Foldectures by cross-linking polymerization.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-811**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold-catalyzed intermolecular coupling involving Sigmatropic Rearrangement

전정호 안준현 신승훈*

한양대학교 화학과

A cooperative polarization of alkynes both by a gold catalyst and a sulfonyl substituent results in an efficient intermolecular reaction. Using this concept, we have recently reported a tandem carboalkoxylation comprising of initial intermolecular alkoxy addition and the following 3,3-sigmatropic rearrangement. In this presentation, alkynes such as propiolic esters and alkynyl sulfones as well as different nucleophilic partners including allyl ethers, allyl amines and benzyl ethers will be presented and their mechanistic differences will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-812**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Regioselective synthesis of new 4-(5-Phenyl-1H-pyrazol-1-yl)thienopyrimidine derivatives using DMFDMA Reagent

이혁주 박재후 송양현^{1,*}

목원대학교 화학과대학원 ¹목원대학교 화학과

Dimethylformamide dimethyl acetal(DMFDMA)와 여러 acetophenone 들과의 반응으로 부터 (E)-3-(dimethylamino)-1-phenylprop-2-en-1-one 유도체를 합성하였고, 이들과 4-hydrazinyl thienopyrimidine 과의 반응으로부터 4-(5-phenyl-1H-pyrazol-1-yl)thieno pyrimidine 유도체를 효과적으로 얻을 수 있었다. 이들 반응은 regioselective 한 과정으로 일어났으며, 이들의 몇몇 화합물은 IL-6(interleukin-6)억제제로서의 활성을 나타내었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-813

발표분야: 유기화학

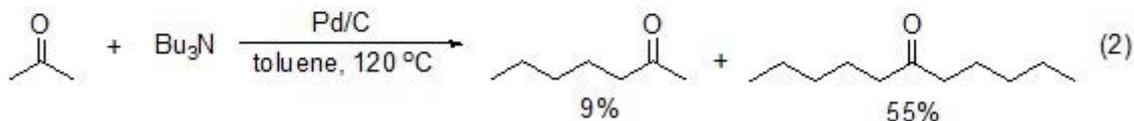
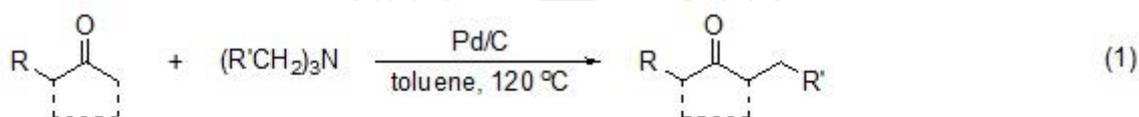
발표종류: 포스터, 발표일시: 수 16:00~19:00

α -Alkylation of Ketones by Trialkylamines under Pd/C Catalysis

조찬식* 윤일철

경북대학교 응용화학과

Treatment of methyl(alkyl), methyl(aryl), and cyclic ketones with an equimolar amount of trialkylamines in toluene in the presence of a catalytic amount of Pd/C (10 mol%) at 120 °C for 40 h afforded α -alkylated ketones in good yields, and in the case of unsymmetrical ketones the reaction takes place regioselectively at the less hindered α -position (eq 1). Similar treatment of acetone with two equiv. of tributylamine in the presence of Pd/C (20 mol%) under the employed conditions afforded 2-heptanone and 6-undecanone in 9% and 55% yields, respectively (eq 2).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-814**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Expedient Synthesis of 2-Aminoquinoxalines via One-Pot Cyanide-Based Multicomponent Reaction

김경희 조연호 천철홍*

고려대학교 화학과

Quinoxalines have been known as common building blocks of biologically and pharmaceutically important compounds, antibiotics, and materials. Consequently, significant efforts have been made to develop efficient methods for the synthesis of quinoxalines and their derivatives. Among the quinoxaline derivatives developed, 2-aminoquinoxalines are considered one of the most important quinoxaline derivatives due to their unique biological activities and potential applications in multicomponent reactions. We recently developed highly efficient aerobic oxidative cyclization methods for the synthesis of benzoxazoles and benzothiazoles in the presence of NaCN as a nucleophile. During the extension of this protocol to the synthesis of benzimidazoles, we unexpectedly found that 2-aminoquinoxalines were formed rather than benzimidazoles under these conditions. Herein, we present highly efficient and expedient synthesis of 2-aminoquinoxalines via cyanide-based multicomponent reactions. A variety of substrates from aromatic aldehydes to aliphatic aldehydes bearing acidic α -protons, are applicable to this protocol and afforded the desired 2-aminoquinoxalines in high yields.

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장소: 창원CECO

발표코드: **ORGN.P-815**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chloride catalyzed synthesis of benzimidazoles via aerobic oxidation

이예솔 조연호 천철홍*

고려대학교 화학과

Benzimidazoles are common building blocks in biologically and therapeutically active compounds. One of the conventional methods for these syntheses of benzimidazoles is oxidative cyclization of imines from aldehydes and o-phenylenediamines in the presence of strong oxidants. Unlike these conventional methods, we developed the one-pot synthesis of benzimidazoles with o-phenylenediamine and aldehydes via aerobic oxidation using potassium chloride as a catalyst. The desired benzimidazoles were obtained from high yields with broad substrate scope. Moreover, this protocol could be extended to aldehydes bearing functional groups sensitive to oxidative conditions.

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장소: 창원CECO

발표코드: **ORGN.P-816**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

General Methods for Synthesis of ortho- and para-Phenol MIDA Boronates

안수진 이춘영 천철홍*

고려대학교 화학과

Boronic acids are one of the most useful intermediate due to their low toxicity, ready availability. Although some boronic acids, particularly heteroaromatic boronic acids, are known to unstable, it is generally accepted that aryl boronic acids are stable. Very recently, we found that ortho- and para-phenol boronic acids readily underwent metal-free thermal protodeboronation in DMSO, which renders it difficult to store these important boronic acids. In order to resolve this limitation of ortho- and para-phenol boronic acids, we developed a range of N-methyliminodiacetic acid (MIDA) boronates of ortho- and para-phenol boronic acids from their parent boronic acids. In addition, we developed an alternative, but more efficient method for the synthesis of MIDA boronates from protected phenol boronic acids followed by deprotection.

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장소: 창원CECO

발표코드: **ORGN.P-817**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Beyond Benzoin Reaction: Unusual Trimerization of Aldehydes in the Presence of NaCN

김유진 천철홍*

고려대학교 화학과

A new, highly efficient and mild synthesis of trimers from aromatic aldehydes was developed. The trimerization of aldehydes proceeds in presence of sodium cyanide at room temperature via aerobic oxidation through a benzoin intermediate. The reaction highly depends on the choice of solvent and steric effect of aromatic aldehydes. Interestingly, the presence of water significant effect on the efficiency of this transformation; the presence of water significantly accelerated oxidation of aldehydes to afford the corresponding carboxylic acids. This transformation displayed broad substrate scope; the trimerization could be applied to wide substrate scope from many kinds of substituted benzaldehydes derivatives to hetero aromatic aldehydes.

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장소: 창원CECO

발표코드: **ORGN.P-818**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of fluorescent probes based on desferrioxamine B and their characterization

김현석 최성지 송운영 선미진 김학중*

고려대학교 화학과

Siderophores are iron(III) chelators produced and utilized by the majority of bacteria including deadly human pathogens. Recently, there are numerous efforts to exploit siderophores for discovery of novel antibiotics, potentially effective in treating problematic drug-resistant bacterial infections. Among them, one approach is to design and construct conjugate molecules between siderophores and antibiotic drugs, where siderophores function as active intracellular delivery vectors. This is often called “Trojan horse” strategy, since it involves intracellular penetration of drugs through endogenous receptors by disguising their xenobiotic nature. Although there are several dozens of examples in this direction, success has been rather scarce. Upon careful scrutiny of literatures, we reasoned that the failures are in part due to the lack of the information on the cellular uptake efficiency of the conjugates tested. In this consideration, we have designed unique fluorescence-based probes capable of monitoring the intracellular delivery of the siderophore-drug conjugates in quantitative manner. In this poster, our current progresses in synthesis, physicochemical characterization, and cellular uptake experiments of fluorescent probes based on desferrioxamine B will be presented, and the power of our approach leading to successful development of novel antibiotic concept will be discussed as well.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-819**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Spectroscopic Properties of Rhodamine-Spiropyran Dyad

신은주* 허대영

순천대학교 화학과

Nonpolar, colorless, UV-absorbing spiropyran(SP) is well-known photochromic compound accomplishing reversible molecular structural change to polar, colored, VIS-absorbing merocyanine(MC) by the photochemical ring opening on UV irradiation. In turn, MC is reversed to SP by ring closure thermally or on irradiation of visible light. Reversible photochromic SP-MC transformation is one of subjects of active research on switch, sensor and optical memory. Rhodamine(Rh)-based dyes have been extensively studied because of their large absorption coefficient, absorption and emission at a long wavelength, high fluorescence quantum yield. In presence of specific metal ions, the colorless and nonfluorescent rhodamine spirolactam structure would be converted into the colored and highly fluorescent ring-opened amide form, which provides not only excellent enhancement in absorption and fluorescence intensity, but also naked eye detection. Incorporating Rh into SP might lead to excellent light-controlled ion sensing system. In this study, Rh-SP dyad was prepared and their spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-820**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Photochromic Reaction of Spiropyran-Pyrene Dyad

신은주* 정소나

순천대학교 화학과

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 pyrene(Py) moiety is one of the most useful fluorophores in the construction of fluorogenic chemosensors for a variety of important chemical species. Pyrene is widely employed as ratiometric fluorescent chemosensors, due to its wellknown photophysical properties in monomer/excimer emission switching. Incorporating SP into Py might should lead to a variety of photoresponsive systems, the properties of which can be manipulated by light. In this study, SP-Py dyad was prepared and their spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-821

발표분야: 유기화학

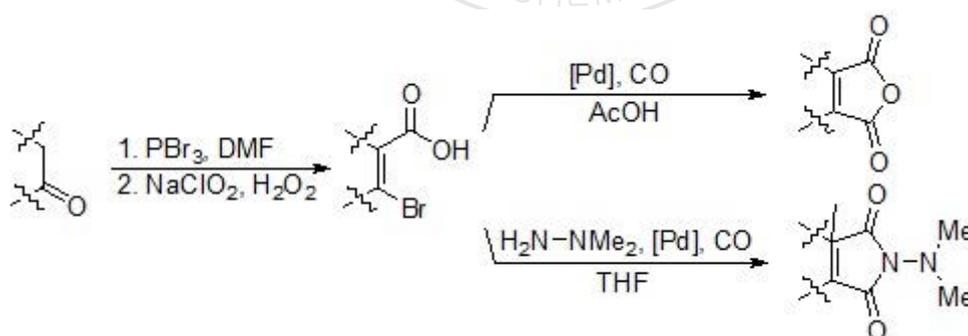
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Carbonylative Cyclization of β -Bromo- α,β -unsaturated Carboxylic Acids: Synthesis of Maleic Anhydrides and 1-(Dimethylamino)-1H-pyrrole-2,5-diones

조찬식* 배연규¹

경북대학교 응용화학과¹ 경북대학교 응용화학학부

β -Bromo- α,β -unsaturated carboxylic acids are carbonylatively cyclized under carbon monoxide pressure in acetic acid in the presence of a catalytic amount of a palladium catalyst along with a base to give the corresponding maleic anhydrides in high yields. β -Bromo- α,β -unsaturated carboxylic acids are also carbonylatively cyclized with 2,2-dimethylhydrazine under carbon monoxide pressure in THF in the presence of a catalytic amount of a palladium catalyst along with a base to give 1-(dimethylamino)-1H-pyrrole-2,5-diones.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-822**

발표분야: 유기화학

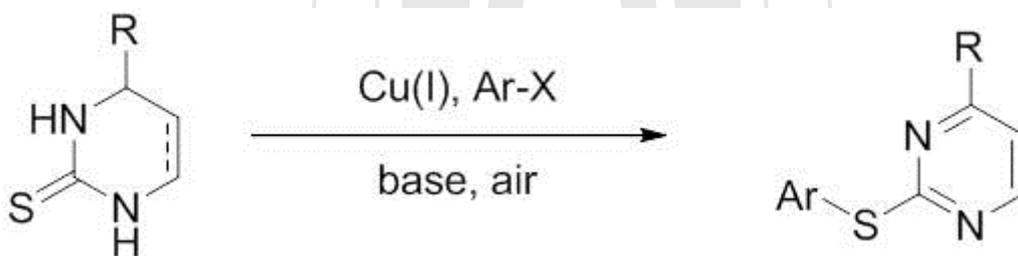
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Aerobic Oxidative C-S Cross-Coupling of Cyclic Thiourea with Aryl Halides

이옥숙 손정훈*

충남대학교 화학과

A new method for copper-catalyzed tandem C-S bond formation/oxidation through reaction of cyclic thioureas with aryl halides under air to produce pyrimidine derivatives is described



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-823

발표분야: 유기화학

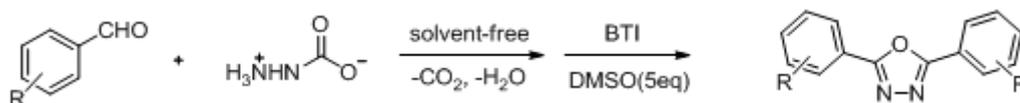
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot synthesis of 2,5-disubstituted-1,3,4-oxadiazole from aldehyde

이강우 김학원^{1,*}

경희대학교 화학과 ¹경희대학교 응용화학과

Recently, there has been growing research interest associated with the solvent-free synthesis of organic compounds. In this report, a mild, general, convenient and efficient one-pot synthesis of 2,5-disubstituted-1,3,4-oxadiazoles from aldehyde is described. Several aldehydes were efficiently grinded with hydraziniumcarboxylate to give the corresponding azine intermediates. Resulting azines underwent a smooth BTI(bis(trifluoroacetoxy)iodobenzene)-mediated cyclization reaction in the absence of solvent to afford 2,5-substituted-1,3,4-oxadiazoles in good yields.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-824**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anion Binding Study of Phosphonium Derivatives Receptors

이환석 윤희상 남계춘*

전남대학교 화학과

Anions play an important role in a wide range of chemical and biological processes, and considerable attention has been focused on the design of host molecules that are able to selectively recognize and sense anion species. Color changes that can be detected by the naked eye are widely used as signals for events owing to the inexpensive equipment required or no equipment at all. This color variation can be related to either structural or conformational changes in the receptor structure when a complex is formed or the formation of a charge transfer complex. Among the biologically important anions, fluoride is of particular interest due to its established role in preventing dental caries. Anion can be recognized by either positively charged or neutral artificial receptors. Positive charges within receptor can be provided by phosphonium ion, which offer a binding site to electrostatic force of the envisaged anion. We synthesized two new positively charged anion receptors and investigated their binding properties with ^1H NMR, UV-Vis and color changes with various anions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-825**

발표분야: 유기화학

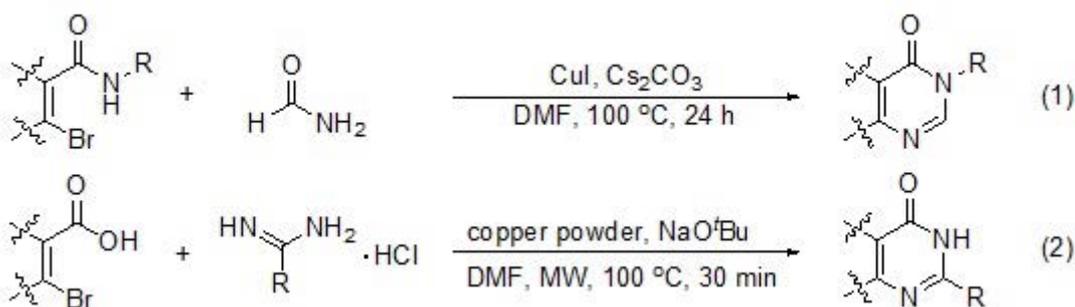
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Coupling and Cyclization of β -Bromo- α,β -unsaturated Amides and Carboxylic Acids with Formamide and Amidines Leading to Pyrimidinones

조찬식* HOSONLONG

경북대학교 응용화학과

β -Bromo- α,β -unsaturated amides are coupled and cyclized with formamide in DMF at 100 °C in the presence of a catalytic amount of a copper(I) salt along with a base to give the corresponding pyrimidinones in good yields (eq 1). β -Bromo- α,β -unsaturated carboxylic acids are coupled and cyclized with amidines under microwave irradiation conditions in the presence of a catalytic amount of copper powder along with a base to give pyrimidinones in high yields (eq 2).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-826**

발표분야: 유기화학

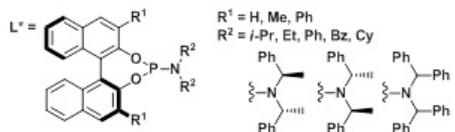
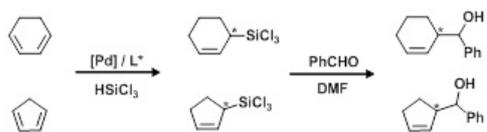
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed asymmetric hydrosilylation of cyclic 1,3-dienes with bulky phosphoramidite ligands

신혜미 박희건 한진욱*

한양대학교 화학과

Optically active allylsilanes are useful intermediates in stereoselective organic synthesis, and increasing attention has been paid to their preparation by asymmetric catalysis. It has been reported that the optically active allylsilanes are accessible by asymmetric hydrosilylation of 1,3-dienes. The palladium-catalyzed hydrosilylation with chiral monophosphine ligand is a well-established procedure which shows high catalytic activities and enantioselectivities for carbon-carbon double bonds. Moreover, the palladium-catalyzed asymmetric hydrosilylation of olefins is a very atom economical reaction in the sense that it is an addition reaction and it usually proceeds without any solvent.¹ Chiral phosphoramidites, which are readily available from chiral diols and amines, have been reported to be effective as ligands for various catalytic asymmetric reactions. Chiral phosphoramidites have already been utilized in the palladium-catalyzed asymmetric hydrosilylation of cyclohexa-1,3-diene giving excellent enantioselectivities and catalytic activities. Herein we report that a chiral phosphoramidite ligand derived from 3,3'-substituted (S)-binaphthol and a secondary amine showed a higher enantioselectivity in the palladium-catalyzed asymmetric hydrosilylation of cyclic 1,3-dienes. References 1.(a) Han, J. W.; Hayashi, T. *Tetrahedron: Asymmetry* 2010, 21, 2193. (b) Park, H. S.; Han, J. W.; Shintani, R.; Hayashi, T. *Tetrahedron: Asymmetry* 2013, 24, 418.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-827

발표분야: 유기화학

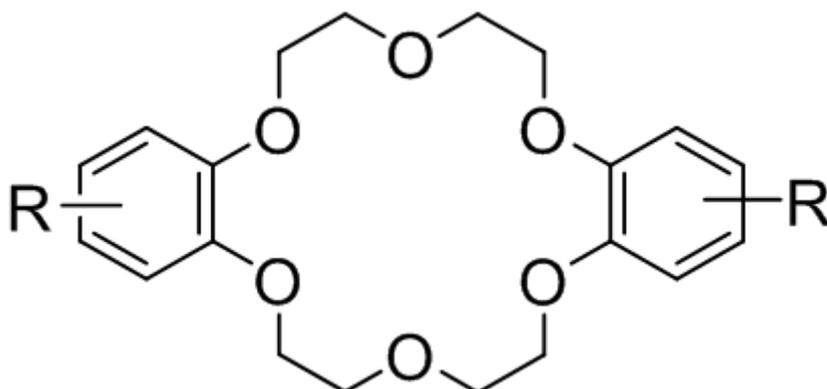
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and CO₂-Solubility of Bisbenzo-18-Crown-6 ethers as a CO₂-Philic Chelating Ligand for Metal Extraction into scCO₂

노경탁 김학원^{1,*} 민지은 이현진¹

경희대학교 화학과 ¹경희대학교 응용화학과

Supercritical carbon dioxide (scCO₂) has been suggested as an attractive, environmentally benign, green solvent for heavy metal ion extraction. However, direct extraction of metal ions by scCO₂ is inefficient because of the charge neutralization requirement and weak solute-solvent interactions. In order to overcome these drawbacks, the use of highly CO₂-soluble chelating ligands has been suggested to make the CO₂-insoluble metal ions CO₂-soluble and extractable through the in situ formation of CO₂-soluble metal complexes. To meet these goals, we designed and synthesized novel CO₂-philic chelating ligands containing metal binding segments, such as bisbenzo-18-crown-6 ether moiety. Solubilities of newly synthesized various bisbenzo-18-crown-6 ether derivatives and the metal extraction efficiencies for various metal ions in scCO₂ were tested.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-828**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic Sensitizers Based on 3,6-Disubstituted Carbazole and Quinacridone for Highly Efficient Dye-sensitized Solar Cells

양동욱

서울대학교 화학부

Solar energy is expected to be the most renewable alternative energy source. Dye-sensitized Solar Cells (DSCs) are attracting attention because of their relatively low cost of manufacturing, easy fabrication and comparatively high power conversion efficiency than other kinds of solar cells. As a key factor in highly efficient DSCs, dyes should possess several properties: Optimum absorption overlap with the solar spectrum for efficient light harvesting, appropriate HOMO and LUMO energy levels for efficient electron injection and regeneration, and hydrophobicity for minimizing charge recombination. In this respect, we have developed bulky organic dyes of a D-D-?-A structure to reduce the molecular aggregation and enhance the blocking effect, thereby improving the Voc[1]. In this presentation, we report several organic dyes based on a 3,6-disubstituted carbazole moiety as an electron donating unit and a quinacridone ?-spacer as an electron transferring unit for efficient DSCs. Quinacridone, an electron-deficient unit employed as the ?-spacer, is not commonly used in DSCs but exhibited outstanding long-term stability when used with ionic-liquid electrolytes.[2] Not only photophysical and electrochemical properties of the dyes but photovoltaic performance of the DSC devices were systematically investigated. Details will be discussed in the presentation. Reference[1] Chem. Asian. J., 2012, 7, 343.[2] J. Mater. Chem., 2012, 22, 24356.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-829**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Study of Donor-Acceptor Dyads Containing Monoimides, Diimides, and Aryl Moiety

김성식* Mamoru Fujitsuka¹ Tetsuro Majima¹

전북대학교 화학과 ¹Osaka University

Synthetic study of some donor-acceptor dyads containing monoimides, diimides, and aryl spacers is reported. Two types of monoanhydride intermediates were prepared to get three target molecules. The effect of substituents upon the chemical yields of the final step were investigated. It was observed that solvents, catalysts, reaction temperature, and other reaction conditions are also important factors in these reactions. The final compounds were characterized by some spectral data.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-830**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Glyco-Ferritin Nanoparticles for the Development of Lectin Targeted Delivery

양현지 홍성유*

울산과학기술대학교(UNIST) 나노생명화학공학부

Every organism presents specialized lectins on its cell surface. Lectin recognizes and binds to specific glycan structures and individual carbohydrate-lectin interactions are involved in biological events including cell signaling and immune response. In this study, we developed surface glycosylated protein cage nanoparticles. Maleimido-derivatives from mannose and galactose were synthesized in order to link to thiol groups on the surface of the cage proteins. Synthesized organic compounds were checked by NMR, ESI-Mass. Bioconjugated human ferritins (HFns) were investigated by SEC, TEM, Mass spectrometry. The specific binding between carbohydrate-conjugated HFns and lectins were confirmed by SPR. Moreover, to investigate the potential application of human ferritins (HFns) as specific delivery nanoplatfoms, lectin targeted cell binding tests were carried out.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-831

발표분야: 유기화학

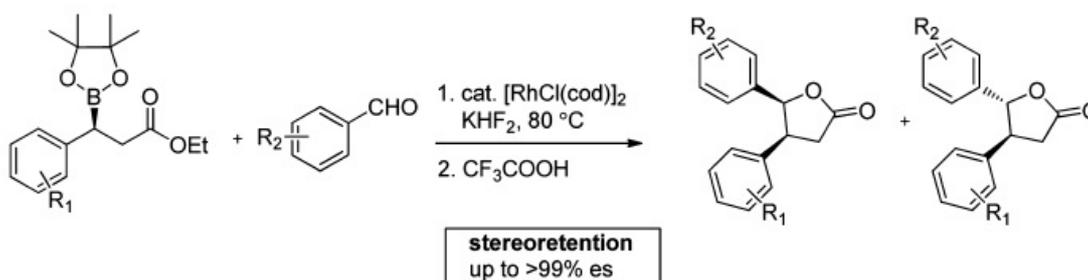
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on Chirality Transfer in the Rh-Catalyzed Addition of Alkylboron Derivatives to Aldehydes

이수민 이우림 윤재숙*

성균관대학교 화학과

The Rh-catalyzed 1,2-addition and 1,4-addition of sp^2 -carbon boron derivatives to aldehydes, enones and imines have been extensively studied. In comparison, sp^3 -carbon boron derivatives have been rarely studied. Recently, Aggarwal and co-workers reported Rh-catalyzed 1,2-addition of secondary and tertiary alkyl trifluoroborate salts to aldehydes in good yield and with stereoretention. So, we investigated Rh-catalyzed 1,2-addition of chiral secondary alkyl pinacolboronates to aldehydes in the presence of KHF_2 and obtained lactone products in good yield and with stereoretention. We were able to use this method to synthesize enantioenriched γ -butyrolactones with high enantiospecificity.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-832**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-free synthesis of oxindole derivatives through C-H activation in air

손세인 강필준¹ 이원구^{1,*}

서강대학교 화학¹ 서강대학교 화학과

Derivatives of oxindole and 1,3-disubstituted-2H-pyrrolo[2,3-b]pyridine 2-ones can be used for a wide range of application including traditional herbal medicine like Horsfiline¹, radical carboaminoxylation and olefination reactions², anti-inflammatory agents and molecular probes for pharmacological research.³⁻⁵ Therefore, much efforts have been made to develop efficient methods to prepare above molecules.⁶⁻¹⁰ Here, we would like to describe the synthesis of 3,3-disubstituted oxindole derivatives without organic solvent in air by C-H and Ar-H coupling reaction. The required oxidant in this methodology is oxygen in air and this reaction does not require inert atmosphere. Also, this method is appropriate for the preparation of pyridine derivatives which are rarely prepared through a C-H activation as well as benzene derivatives. Overall, this methodology is environmentally friendly and can adapt for the preparation of a variety of oxindole derivatives.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-833**

발표분야: 유기화학

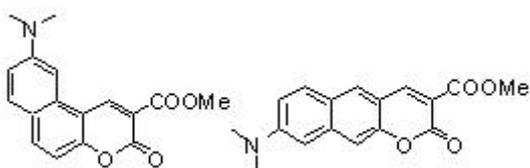
발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Shape Dependent Luminescent Behaviour of π -Extended Coumarins

PHAMXUANQUI 안교한*

포항공과대학교 화학과

Luminescent molecules continue to attract attention for their potential application to various fields including optoelectronic materials, bio-sensing and imaging tools. To develop such luminescent materials, it is prerequisite to have better understanding on the structure and photophysical relationship. Solid state photophysical properties of luminescent molecules are highly dependent on their aggregation patterns.¹ In the course of our study on π -extended coumarin derivatives, we observed the shape dependent luminescence behaviour: bent and linear shape coumarins show opposite luminescent behaviour in solution and solid states. The linear coumarin shows strong fluorescence in solution, even in polar solvent,² but it shows no fluorescence in the solid state. On the contrary, the bent one shows strong fluorescence in the solid state but non-fluorescent in polar solvent.³ Analysis of the crystal structures and packing patterns reveal that both coumarins show stacking patterns of H-aggregation. Theoretical calculation shows that orbital interactions between stacked molecules are different. In case of the linear coumarin, significant HOMO and LUMO orbital interactions in the aggregated state seem to quench the fluorescence, whereas the bent one shows poor interactions between stacked molecules and thus fluoresces in the solid state. This study demonstrates the potential of shape control toward the development of solid state luminescent materials. Reference1. Lydon, J. et al. J. Mater. Chem. 2010, 20, 10071.2. Kim, I.; Kim, D.; Sambasivan, S.; Ahn, K. H. Asian. J. Org. Chem. 2012, 1, 60.3. Qui, P. X.; Kim, D.; Moon, H.; Kim, Y.; Kim, Y. K.; Ahn, K. H. to be published.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-834**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Selective Fluorescent Sensor Based on Pyrene Ligand for Homocysteine and cysteine

박선희 윤주영^{1,*} 이혜연²

*이화여자대학교 화학나노과학과*¹ *이화여자대학교 화학·나노과학과*² *이화여자대학교 화학나노과학*

Biothiols, such as cysteine(Cys), homocysteine(Hcy) and glutathione(GSH), play important roles in maintaining biological systems. Abnormal levels of biothiols have been shown to be associated with human diseases such as slow growth, liver damage and skin lesions. Although the structures of Cys, Hcy and GSH are similar, they play different important biological roles associated with different diseases. Therefore, It is necessary to develop fluorescent sensors that could discriminate the three thiols. We developed a new Hcy and Cys sensor based on pyrene derivative.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-835**

발표분야: 유기화학

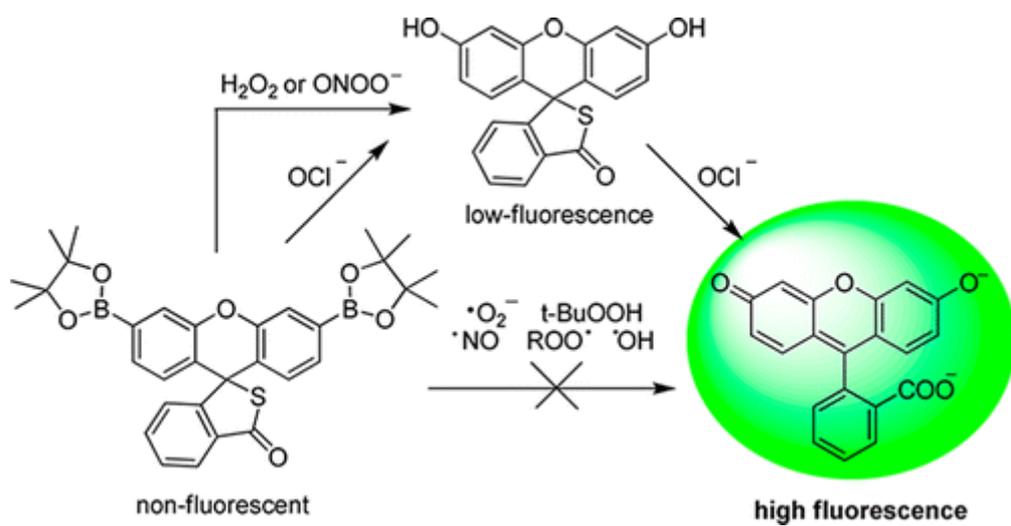
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Specific Fluorescent Probe for Hypochlorous Acid and Its Application in Imaging Microbe-Induced HOCl Production

이송이 윤주영^{1,*}

이화여자대학교 화학·나노과학과 ¹이화여자대학교 화학·나노과학과

Oxidative stress induced by reactive oxygen species (ROS) plays crucial roles in a wide range of physiological processes and is also implicated in various diseases, including cancer, chronic inflammatory diseases, and neurodegenerative disorders. Among the various ROS, hypochlorous acid (HOCl) plays as a powerful microbicidal agent in the innate immune system. The regulated production of microbicidal HOCl is required for the host to control the invading microbes. However, as a result of the highly reactive and diffusible nature of HOCl, its uncontrolled production may lead to an adverse effect on host physiology. Because of its biological importance, many efforts have been focused on developing selective fluorescent probes to image ROS. However, it is still challenging to design a fluorescent probe with exclusive selectivity toward a particular member of ROS. In the current work, we designed FBS as a new fluorescent HOCl probe which has high selectivity, sensitivity, and short response time in a broad range of pH. Compared with other sensors, the “dual-lock” structure of FBS has an advantage of eliminating interferences from other ROS/RNS. Importantly, we further showed that our HOCl probe could be applied for the in vivo imaging of physiological HOCl production in the mucosa of live animals. This probe provides a promising tool for the study of HOCl production.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-836

발표분야: 유기화학

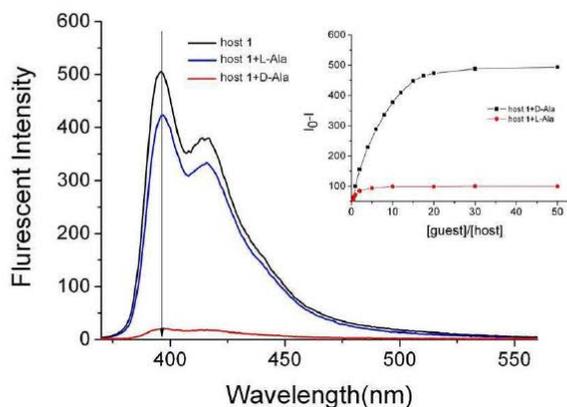
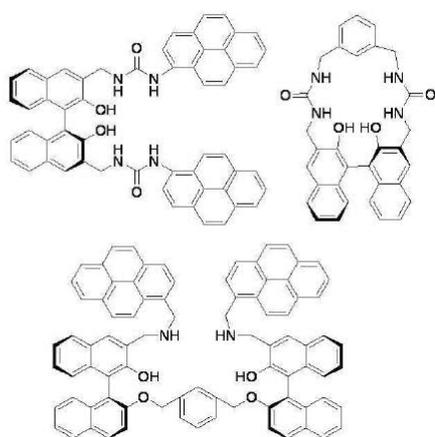
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Binaphthyl-Based Chiral Receptors for Colorimetric and Fluorescent Recognition of Amino Acids

김다빈¹ Hu Ying¹ 김관목^{2,*} 윤주영^{3,*}

이화여자대학교 화학·나노과학과¹ 이화여자대학교 화학·나노과학과² 이화여자대학교 화학
과³ 이화여자대학교 화학·나노과학과

We describe the design and synthesis of three representative BINOL derivatives. These receptor were examined for their chiral recognitions with D- and L-t-Boc-amino acid anions: an open system 1, which bears two urea groups and two pyrene groups; a closed ring system 2, which bears two urea groups with a closed ring system; and a dimeric system 3, which bears two benzylic amine groups and two pyrene groups. Dimeric system 3 displayed a $\Delta ID/\Delta IL$ of 12.95 for t-Boc-alanine.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-837**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Naphthoimidazolium-based Fluorescence Chemosensor for Phytate

조선정 이민지¹ 윤주영^{2,*}

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과학과

Inositol 1,4,5-trisphosphate (IP_3) is known as the important second messengers in intracellular signal transduction process. On the other hand, myo-inositol hexakisphosphate (IP_6) known as phytate is a fully phosphorylated form of inositol, which are found in blood, urine, and intracellular fluids. IP_6 is known as an antinutrient due to its ability to chelate essential trace minerals. Various beneficial properties of IP_6 have been reported recently, which include blood-glucose-lowering and lipid-lowering effects, antioxidative properties and anticancer activities. There have been some efforts to sense IP_3 and IP_6 via fluorescent changes. But these methods were based on a ligand exchange in which metal ions are removed from metal complexes by IP_6 . And these systems cannot be easily applied to image IP_6 in the cell. In the current study, we synthesized a new tetranaphthoimidazolium receptor 1, as a first example of non-metal ion based fluorescent chemosensor for IP_6 . In 100% aqueous solution at pH 7.4, chemosensor 1 showed a selective fluorescence enhancement for IP_6 over simple anions, phosphate, pyrophosphate, AMP, ADP and ATP. We further showed successful in vivo imaging of IP_6 in the cell. By using this relatively simple receptor, we could obtain reasonable selectivity for IP_6 in 100 % aqueous solution at pH 7.4.

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장소: 창원CECO

발표코드: **ORGN.P-838**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric and Fluorescence Probes for Cationic Surfactants based on Polydiacetylene Including Boronic Acid

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A new polydiacetylene oxyphenylboronic acid (PDAOPBA-1) bearing group was synthesized and showed diverse colorimetric changes, such as yellow, orange, and red, upon the addition of cationic surfactants at pH 7.4. On the other hand, anionic surfactants and simple ammonium salts did not show any color change. Specifically, color changes to yellow for cetyl trimethylammonium chloride (CTAC), red for dodecyl trimethylammonium bromide (DTAB), orange for benzylcetyldimethylammonium chloride (BCDA), and dark orange for hexadecylpyridium bromide (HDPB) are observed, respectively. Different head groups and alkyl chain lengths of cationic surfactants can be intelligently distinguished via a unique penetration process.

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장소: 창원CECO

발표코드: **ORGN.P-839**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The cyanine based near-infrared flurescent sensors

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이화여자대학교 화학·나노과학과 ¹이화여자대학교 화학·나노과학과 ²이화여자대학교 화학·나노과학과

Light in the near-infrared (NIR) region (650-900 nm) is relatively poorly absorbed by biomolecules and can penetrate deeply into tissues. There is also less autofluorescence in this region. Thus, much higher signal-to-noise ratios can be obtained, and probes that absorb and emit in the NIR are expected to be suitable for in vivo imaging. The rising interest in small animal optical in vivo imaging has accentuated the need for novel NIR fluorescent dyes that exhibit good photostability properties. Amongst NIR dyes, the tricarbocyanine scaffold is synthetically accessible and displays enhanced fluorescent properties over other cyanine structures.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-840**

발표분야: 유기화학

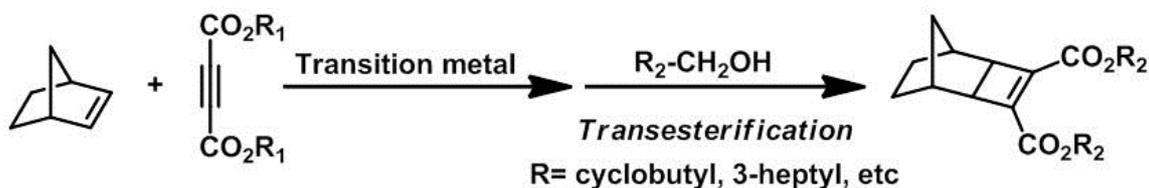
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Non-Polar Energetic Plasticizers with Ring-Strained Skeletal Moieties

박은경 전철호*

연세대학교 화학과

For the last several years, there have been many efforts to develop energetic plasticizers due to their potential additives for highly advanced propellants or explosives. Most researches have been focused on the development of polar energetic plasticizers bearing highly energetic functional group such as nitro group. Since their polar physical properties are problematic for mixing with explosive ingredients, we have tried to find new type of nonpolar energetic plasticizers bearing strained carbon skeletal moieties. Finally cyclic strained molecules bearing cyclobutene ring moieties are prepared by transitionmetal catalyzed [2+2] cycloaddition reaction of norbornylene and acetylene dicarboxylate. The physical properties of these compounds were analyzed and compared with DOP and DOA, which are common plasticizers.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-841**

발표분야: 유기화학

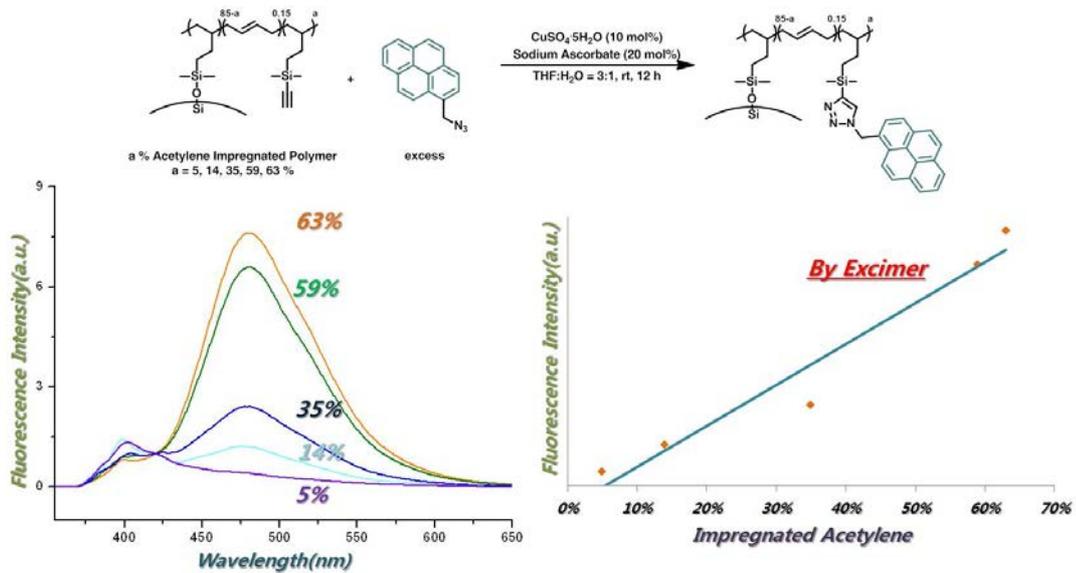
발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantitative Analysis of Polymer-Immobilized Functional Group on Inorganic Solid Surface by Fluorescence Determination

김민석 전철호*

연세대학교 화학과

Fabrication of highly robust organic-inorganic hybrid material is important for reproducible and reusable chemo-sensors. However, its heterogeneous nature shows limitations on the quantitative analysis. To improve this limitation, we designed new method to analyze how much functional group was impregnated onto inorganic solid surface using fluorescence determination. To impregnate fluorescence substrate onto immobilized polymer, the reaction of azido methyl pyrene and polybutadiene bearing acetylenyl group as a side chain was carried out by [2+3] cycloaddition reaction conditions (Click chemistry). By Click chemistry, various amount of pyrenyl group-impregnated polymer was prepared, and these were catalytically immobilized onto solid surface. Amount of pyrenyl group onto solid surface was determined by fluorescence determination. After making calibration curve of fluorescence intensity with amount of pyrenyl group immobilization, grafting efficiency onto solid surface of unknown sample was measured.



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장소: 창원CECO

발표코드: **ORGN.P-842**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the conformational behavior of depsipeptides containing unnatural residues

장근혁 이재연 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.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-843

발표분야: 유기화학

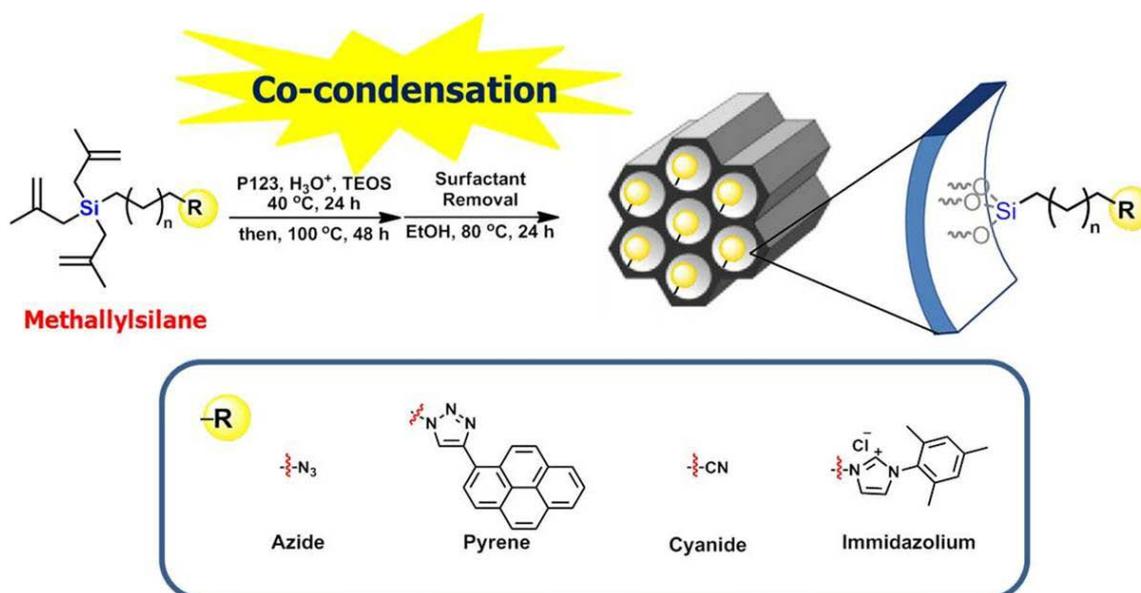
발표종류: 포스터, 발표일시: 수 16:00~19:00

Manufacturing mesoporous SBA-15 with various functional group by co-condensation method using methallylsilane derivatives

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One step co-condensation method was used to manufacture SBA-15 mesoporous silica material. In an acidic condition, trimethallylsilane derivatives were utilized as an organosilane precursor to synthesize functional group-modified SBA-15. In this process P123 was used for structure inducing reagent. Stable methallylsilanes with various functional group were prepared and purified by column chromatography. These were applied for preparing various functional group modified SBA-15. Azido, pyrenyl, cyanide and imidazolium group modified SBA-15 were synthesized successfully. The structure of SBA-15 was confirmed by FT-IR, fluorescence, TEM etc. Different chain length between functional group and silica showed different reactivities in organic transformation.



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장소: 창원CECO

발표코드: **ORGN.P-844**

발표분야: 유기화학

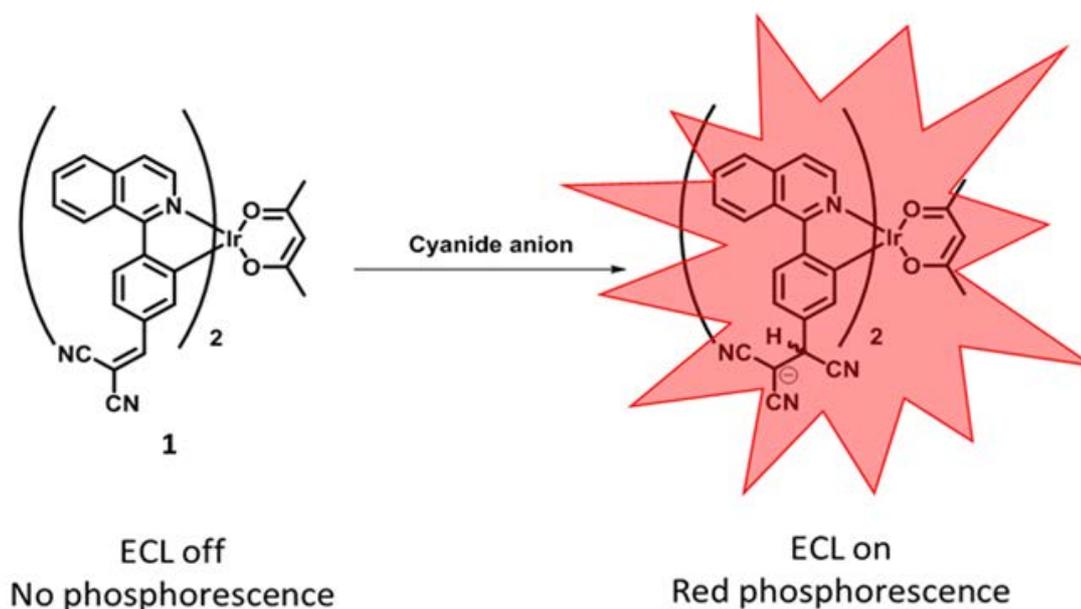
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly selective and sensitive detection of cyanide anion by electrogenerated chemiluminescence

김훈준 홍종인*

서울대학교 화학부

Cyanide anion is a highly dangerous material that damages through lungs, gastrointestinal track, and skin. It can kill mammals upon binding to a heme unit. Humans may be exposed to cyanides from dietary, industrial and environmental sources. Therefore, quantitative detection of cyanide anion in environmental samples is the one of the important issues. Recently, the use of electrogenerated chemiluminescence (ECL) has attracted increasing interests due to their advantages such as high sensitivity, wide linear response range, good reproducibility and easy operation. Herein, we present ECL-based probe for cyanide anion based on cyclometalated Ir(III) complex. Details of synthesis and photophysical studies will be presented.



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장소: 창원CECO

발표코드: ORGN.P-845

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on stereochemical control of 2,5-disubstitute tetrahydrofuran ring by Oxa-michael reactions

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고려대학교 화학과

The synthetic utility of the oxa-Michael reaction based on the conjugate addition of a hydroxyl group as the nucleophile has been underappreciated compared to the carbon nucleophile-based Michael reaction. It is in part due to the paucity of the information regarding its enantio- and diastereoselectivity. Yet, considering that the plethora of biologically active natural products possesses the products of oxa-Michael reactions, tetrahydrofuran or tetrahydropyran rings, within their structures, their potential in synthesis of complex molecules seems worth exploiting. In that regard, our laboratory has been investigating the stereochemical control in the construction of 2,5-disubstitute tetrahydrofuran rings by examining a number of different reaction conditions, i.e., the use of acids, bases, and chiral catalysts. In addition, the effects of different functional groups and chirality of various electron acceptors have been also systematically analyzed. We are assured that our study will not only disclose the relationship between reaction conditions and stereochemical outcomes, but also provide a useful reference point for future application of oxa-Michael reactions in total synthesis of a variety of natural products bearing oxacyclic rings.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-846**

발표분야: 유기화학

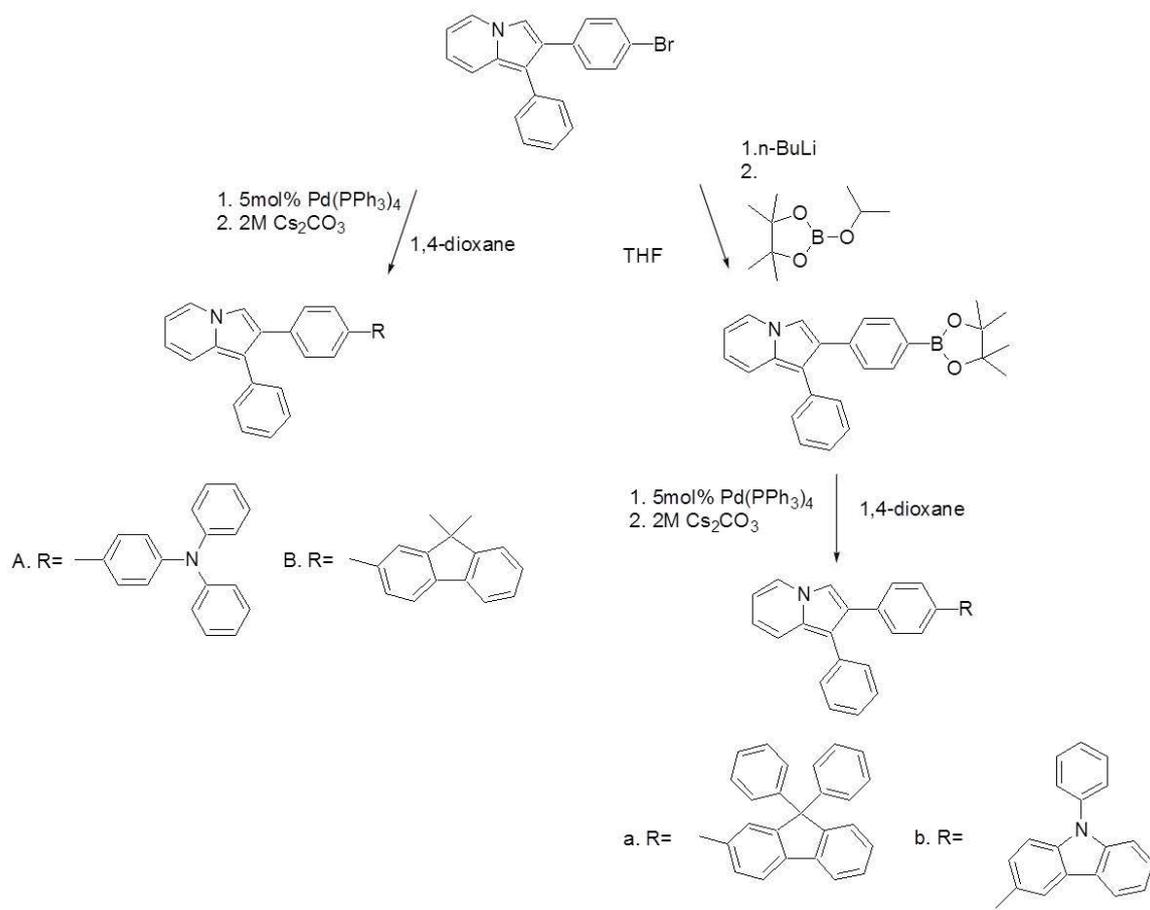
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photoluminescent Properties of Indolizine-derived Molecules for Fluorescent Blue OLEDs

송영란 임춘우^{1,*} 김태우^{1,*}

경희대학교 동서의과학과 ¹경희대학교 동서의학대학원

Organic light-emitting diodes (OLEDs) are attracting great scientific and industrial interests related to their promising applications in large-area, full color, flexible display. Although the performance of green and red emitting materials for OLED is already satisfactory for industrial applications in terms of the device efficiency and lifetime. However the blue emitting materials is still unsatisfactory and demanded for device efficiency, lifetime and color coordinate. Therefore, to accelerate the commercialization of OLEDs, improving blue-emission efficiency is necessary. In this study, we have designed and synthesized a new blue emitting materials. The optical properties, thermal properties and the device performance will be investigated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-847**

발표분야: 유기화학

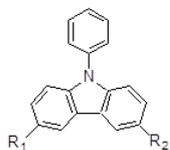
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and photophysical study of 1,3,5-triazine derivatives for phosphorescent green host material in OLEDs

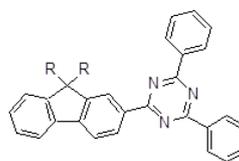
송정은 임춘우^{1,*} 김태우^{1,*}

경희대학교 동서의과학과 ¹경희대학교 동서의학대학원

Organic light-emitting devices (OLEDs) have attracted great attention because they can be applied to full-color flat-panel displays. Phosphorescent organic light-emitting materials are potential for high efficiency and reduced power consumption and phosphorescent Green and red materials are currently used in flat-panel displays. However, device performance, power consumption and lifetime in phosphorescent Organic light-emitting devices (OLEDs) still need to be improved for the application of large flat-panel displays. Development of bipolar host materials is one of the promising approaches for improving device performance in phosphorescent Organic light-emitting devices (OLEDs) technology. In our work, host materials which are composed of 1, 3, 5-triazine derivatives, are designed and synthesized. The optical properties (UV, PL), thermal properties (DSC, TGA) and molecule modeling will be presented.



PCT1: onyl R₁ = 2,6-diphenyl -1,3,5-triazine
PCT2: R₁, R₂ = 2,6-diphenyl -1,3,5-triazine



PFT: R = Phenyl
MPT: R = Methyl



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-848**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reduction of benzylic alcohols in micro tube system by hydriodic acid in a biphasic reaction medium

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Reduction of benzylic alcohols has been studied for a long time and applied to various studies of organic chemistry, a aqueous hydriodic acid (HI) was widely acceptable catalyst for the reduction. However, the reduction was suffered from long reaction time and harsh reaction condition, because they were only accomplished at limited interface of aqueous-organic mediums. We expected that droplet form with maximized contact area of non-miscible mediums can overcome such drawback; we designed droplet microchemical system for the hydriodic acid catalysed reduction. The droplet system increase the mass transfer of aqueous hydriodic acid into reagents resolved in organic solvent. Organic phase and aqueous phase are injected separately, T-junction micro-tube system forms small droplet(less than 1 mm diameter) continuously. The reduction of 2-phenyl 2-propanol is conducted high reaction temperature, the reaction parameters including temperature, solvent, reaction time, and reagents is regulated. The results are analysed with NMR and GS/MSD.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-849**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characteristics and performance of 2,2-bithiophene-3,3-dicarboximide based copolymers for OPVs

김남희 송수희 서홍석*

부산대학교 화학과

A new acceptor unit, 4H-dithieno[3,2-c:2',3'-e]azepine-4,6(5H)-dione, was prepared and to synthesize the conjugated polymers containing electron donor-acceptor pair for OPVs. The dithienoazepinedione and bithiophene imide (BTI) group, is an attractive electron deficient unit since it has strong electron-withdrawing ability, planarity and has good solubility. The polymer with linear dodecyl-BTI unit and benzodithiophene unit substituted with bulky 2-octyldodecyl side chain was synthesized by Stille reaction to generate P1. New polymer P2, was also synthesized by Suzuki reaction with carbazole, thiophene and octyl BTI unit to increase conjugation length. The best device with P1:PC71BM in ODCB with 2% DIO showed a Voc of 0.97V, a Jsc of 3.06 mA/cm², and a FF of 0.49, which yielded PCE of 1.49%. The highest PCE of P2:PC71BM (1:2) reached to 0.76% with 0.84V Voc, Jsc was 2.48 mA/cm², and the FF was 0.36.

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장소: 창원CECO

발표코드: **ORGN.P-850**

발표분야: 유기화학

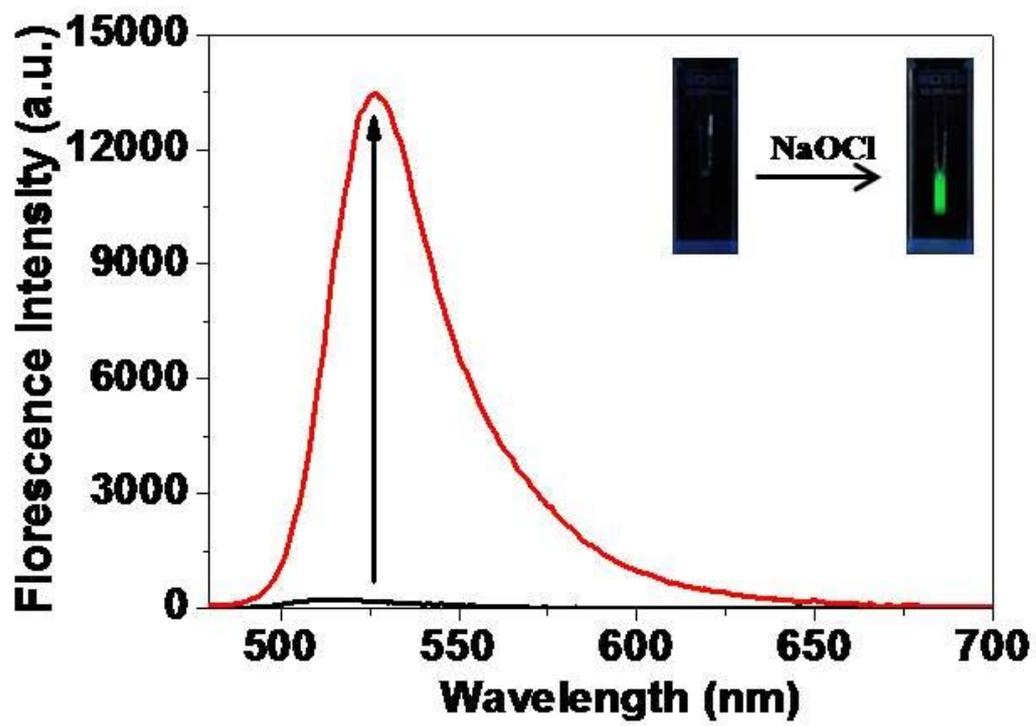
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Water-Soluble BODIPY-Based Probe for the Selective Detection of Hypochlorous Acid

김지영 김영미*

단국대학교 화학과

Reactive oxygen species (ROS) such as hypochlorous acid (HOCl) are essential for a wide range of biological and pathological events, and play important roles in the human immune-defense system. The overproduction of hypochlorous acid in living organism is associated with many human disease such as cancer, cardiovascular diseases, rheumatoid arthritis, and Alzheimer's disease. Therefore, the detection of hypochlorous acid is important. We present BODIPY-based probe for the detection of hypochlorous acid in aqueous media. Probe showed a fluorescent turn-on response to hypochlorous acid with high sensitivity and selectivity.



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장소: 창원CECO

발표코드: **ORGN.P-851**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymer Based on Alkoxy-substituted-MBI for High Performance Bulk-heterojunction Organic Solar Cell

신경아 송수희 서홍석*

부산대학교 화학과

Solution-processed organic solar cells (OSCs) are promising candidates for renewable energy sources for their advantages of low cost, light weight, and large-area fabrication on flexible substrates. Power conversion efficiency (PCE) of single junction PSCs have already exceeded 9% in several recently reported devices. In most cases, fullerene derivatives, such as [6,6]-phenyl-C61-butyric acid methyl ester (PC61BM) or [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM), are used as acceptors, and conjugated polymers are used as donors. Because most of the solar energy is harvested by donor polymers, extensive research efforts have been devoted to developing small band gap conjugated polymers for PSCs. To achieve high efficiency, polymer donors should have a good solubility and miscibility with the fullerene acceptor, a relatively low energy levels of the highest occupied molecular orbital (HOMO) for a high open circuit voltage (V_{oc}), and a low band gap to efficiently absorb more photons in the near infrared region of the solar radiation. We design and synthesize three D/A alternating copolymers with thiophene and bithiophene as the donor unit and 4,7-dibromo-5,6-dioctyloxy-2,2-dimethyl-2H-indene as the acceptor unit. The above result demonstrates that the absorption and electrochemical properties can be improved by fine-tuning the conjugated polymer structure. The best solar cell performance obtained has a layered structure of ITO / PEDOT:PSS / PTDOMBI:PC71BM(1:4) / Al. Under white light illumination (AM 1.5 G, 100 mW/cm²), the obtained J_{sc} is 4.03 mA/cm², V_{oc} is 0.58 V, FF is 32%, and PCE is 0.76%. Study to improve the solar cell architecture and PCE is underway.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-852

발표분야: 유기화학

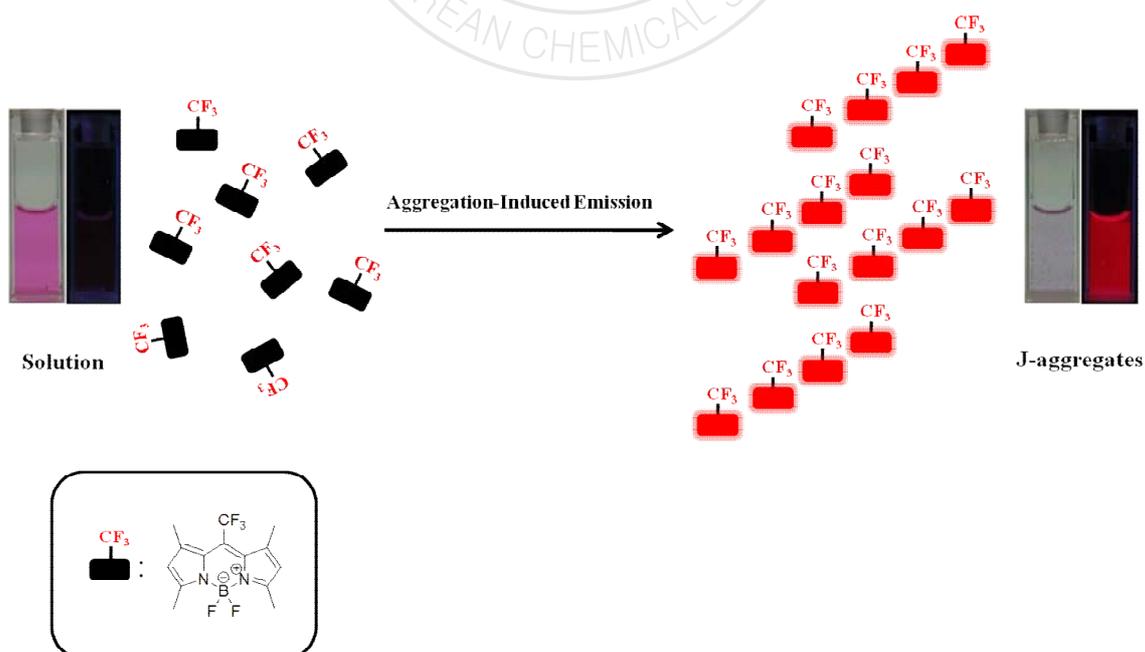
발표종류: 포스터, 발표일시: 수 16:00~19:00

Aggregation-induced Emission Enhancement of CF₃-BODIPY via J-aggregation

최소희 김영미*

단국대학교 화학과

In recent years, J-aggregates have been studied both experimentally and theoretically, and utilized for biosensing applications. Although J-aggregates of a broad variety of dyes such as cyanines, porphyrins, phthalocyanines, and perylene bisimides have been widely studied, there has not been to this date an unambiguous report of J-aggregates of BODIPY. We present the structurally characterized emissive J-aggregates of CF₃-BODIPY, which show a narrow absorption band that is bathochromically shifted relative to the monomer band and high fluorescence intensity with small Stokes shift.



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장소: 창원CECO

발표코드: **ORGN.P-853**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of BTI Derivatives as Acceptor Building Block for Organic Solar Cells

신경아 송수희 서홍석*

부산대학교 화학과

Bulk-heterojunction organic solar cells (BHJ OSCs) have substantially potential because of their high internal quantum efficiency and large-scale printing technique. Although polymers have been widely used to BHJ OSCs and achieved impressive progress of power conversion efficiencies (PCEs) over 8%, the interest in solution-processable small molecular p-conjugated organic donors has been accelerating for BHJ photovoltaic applications in recent years, owing to the advantages of definite structure, facile purification, high purity and good photovoltaic performance reproduction. To develop innovative materials, novel computationally aided design strategy was made through the development of a new class of electron-transporting polymers by incorporating highly tailorable solubilizing groups into an electron-deficient core based upon the N-alkyl-2,2'-bithiophene-3,3'-dicarboximide unit (BTI). In comparison to other acceptor units, BTI units have the advantage of decreased steric encumbrance achieved by placing the imide group at the center of BTI unit, and this should enable BTI copolymerization with a variety of comonomers to realize extended conjugation. The low HOMO energies and relatively small band gaps, combined with good solubilities, favorable geometries, and promising charge transport properties, raise the intriguing question of whether BTI-based polymers might be effective donor components of BHJ solar cells.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-854

발표분야: 유기화학

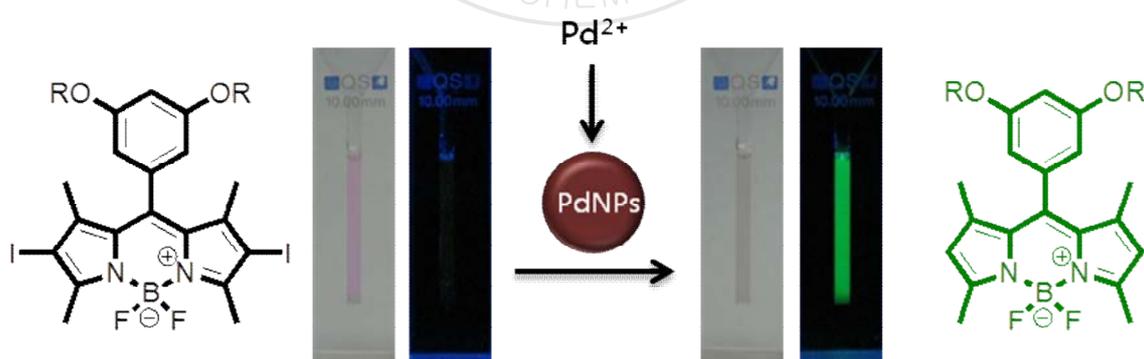
발표종류: 포스터, 발표일시: 수 16:00~19:00

A BODIPY-Based Probe for Detection of Palladium Species by C-I Bond Cleavage

금동호 김영미*

단국대학교 화학과

Palladium species have been extensively employed as one of the most indispensable catalysts in various chemical transfer materials. However, even after purification, residual palladium species remain often in the final product, which may cause deleterious effects on humans and environment. For example palladium ions can bind to thiol-containing amino acids, proteins, DNA, hence, disturbing a variety of cellular processes. Therefore, the detection of palladium species is an important issue. We present a sensitive and selective fluorescent probe based on C-I bond cleavage reaction under mild conditions by in-situ generated PdNPs from palladium ion in ethanol-water mixture.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-855**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Phenanthrothiadiazole Derivatives for High Performance Solar Cells

신경아 송수희 서홍석*

부산대학교 화학과

Polymer solar cells afforded a capable way to utilize the solar energy power conversion efficiently (PCE) while maintaining low cost. Design and synthesis of π -conjugated polymers used as electron-donor materials for bulk heterojunction of organic solar cells have fascinated remarkable attention during the past decade. New low-band gap polymer solar cells incorporating phenanthrothiadiazole(PT) as an electron-accepting unit have designed and synthesized in solar cells with benzodithiophene as the electron-donating unit. The DBDTPT was synthesized by stille reaction in OPVs. In conclusion, DBDTPT shows absorption band with maximum peak at about 361 nm in solution. The HOMO and LUMO levels of DBDTPT were exhibited at -5.46 eV and -3.65 eV, respectively. The small molecule has good thermal stability. The HOMO?LUMO energy band-gap of this material shows 1.81 eV for DBDTPT.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-856**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of copolymer based pyrrolo[3,2-b]pyrrol with low-Bandgap for OPVs

김남희 송수희 서홍석*

부산대학교 화학과

A new acceptor unit, pyrrolo[3,2-b]pyrrole-2,5-dione, was organized and utilized for the synthesis of the new low-band gap conjugated polymer containing D^πA pair for OPVs. Pyrrolo[3,2-b]pyrrole-2,5-dione unit, regioisomer of the branded pyrrolo[3,4-c]pyrrole-1,4-dione, is originated beginning the structure of rigid synthetic pigment. The low-band gap conjugated polymer with pyrrolo[3,2-b]pyrrole-2,5-dione, thiophene and carbazole was synthesized by Suzuki polymerization to construct Polymer. The solid film of Polymer shows absorption band through maximum peaks at 374 and 548 nm, and the absorption onset at 679 nm, matching to band gap of 1.83 eV. The hole mobility of Polymer is 2.2×10^{-5} cm²/Vs. The device based on the polymer:PCBM (1:2) blend without thermal performance showed VOC of 0.82 V, JSC of 6.28 mA/cm², and FF of 0.39, giving a PCE of 2.00%.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-857**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pyrrolo[3,2-b]pyrrole based small molecules as donor unit for organic photovoltaic devices

김남희 송수희 서홍석*

부산대학교 화학과

Recently a novel acceptor unit, pyrrolo[3,2-b]pyrrole-2,5-dione, is attractive material for the electron-deficient moiety of the conjugated donor-acceptor copolymer for organic photovoltaic cells (OPVs). Pyrrolo-[3,2-b]pyrrole-2,5-dione unit, the regioisomer of known pyrrolo[3,4-c]pyrrole-1,4-dione, derived from the structure of a stable synthetic pigment. The low bandgap molecules containing pyrrolo-[3,2-b]pyrrole-2,5-dione, thiophene and triphenylamine units were synthesized by the Suzuki coupling reaction to generate SM-B, SM-M and SM-H. The UV-vis absorption spectra of SM-B in a thin film showed two absorption bands with maximum peaks at 356 and 517 nm and the absorption onset was at 667 nm. The optical band gap of this molecular is 1.86 eV. The device blended SM-B and PC71BM (1:4) showed the following photovoltaic performances, a VOC of 0.79 V, a JSC of 6.04 mA/cm², and a FF of 0.33, a power conversion efficiency of 1.56%.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-858**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A mass production of epoxy alcohols in a microchemical system

임효진 박찬이 박찬필*

충남대학교 분석과학기술대학원

The enormous potential of epoxy alcohols as key building block for valuable materials has led to intensive research; the practical preparation for the epoxy alcohols was metal-catalyzed epoxidation of allylic alcohols that can be generated from a photooxygenation of various alkenes. However, the traditional photooxygenation in a batch system was suffered from tedious reaction time and low selectivity, which was the bottleneck in mass production of the epoxy alcohols. Herein we report a facile and efficient continuous flow process consisted of microchemical photo-oxygenation and microchemical epoxidation, which shows an improved selectivity and shorten reaction time than reported batch reactions. The microchemical photooxygenation was connected into the mass production of epoxy alcohols without delayed synthesis of peroxide intermediate. The combination of methylene blue as photosensitizer and $\text{Ti}(\text{O}-i\text{-Pr})_4$ as epoxidation catalyst was perfect, alkenes were directly converted into epoxy alcohols with excellent yield and good selectivity. Asymmetric synthesis of a chiral epoxy alcohol was studied, a diethyl tartrate (L-(+)-DET) as a chiral auxiliary gave good enantioselectivity. As such, the microchemical synthesis would be invaluable not only for the mass production of epoxy alcohols but also for asymmetric synthesis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-859**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Suzuki-Miyaura coupling reaction in the microreactor wall-coated with Pd-catalyst

김미진 박정현 박찬필^{1,*}

충남대학교 분석과학기술대학원 분석과학기술학과 ¹충남대학교 분석과학기술대학원

The palladium-catalyzed Suzuki-Miyaura coupling reaction is one of the most powerful and convenient methods for the preparation of biaryl and alkene derivatives that are structural components of natural products, agrochemicals, pharmaceuticals, and polymers. Batch reaction and microchemical reaction can have several differentias. Some catalyst used in traditional batch systems should be modified in microchemical reactions. Even though Pd/C catalyst with advantages of its availability, reusability, and easy handling showed excellent results in broad batch reactions, the application in some microchemical reaction was restricted due to the reactor channel clogged with solid catalyst. Herein, we report a microchemical system wall-coated with Pd catalyst, which has the advantages of thermal, chemical stability, and cost-effectiveness. No limitation compared with traditional Pd/C catalyst is showed, excellent yield and selectivity is observed. A ligand is firstly introduced on inner wall of commercially available silica tube, which binds a palladium catalyst for repeated application in Suzuki-Miyaura coupling reaction. We could simply get the various biaryl compounds with easy handling of reaction parameters including temperature, solvent, and reaction time.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-860

발표분야: 유기화학

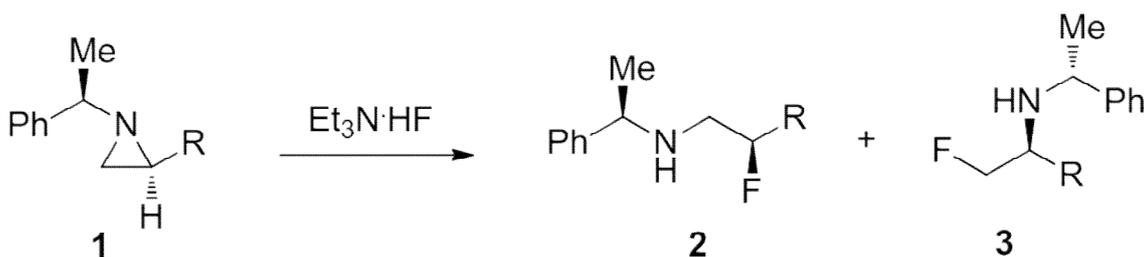
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of Fluoroamines from Chiral Aziridines

박현정 하현준^{1,*} 이원구^{2,*}

한국외국어대학교 화학¹ 한국외국어대학교 화학과² 서강대학교 화학과

The fluorinated organic molecules have attracted great attentions from synthetic and medicinal chemists with wide use of various agrochemicals and pharmaceuticals. Their uniqueness is originated from its electronic characteristics and the small size without altering the molecular conformations of non-fluorinated compounds. The fluorine is the second most widely used atom in the commercial drugs following the amine. Thereby, the elaboration of fluoroamines bearing two most widely used atoms in drugs is one of the most challenging problems in drug synthesis and its development. Herein, we described an efficient preparation of fluoroamines by the ring opening reactions of chiral aziridines with Et₃N·HF. Most cases both regioisomers were obtained from the ring openings either at C2 and C3 depending to the substituents at C2 of the substrates.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-861

발표분야: 유기화학

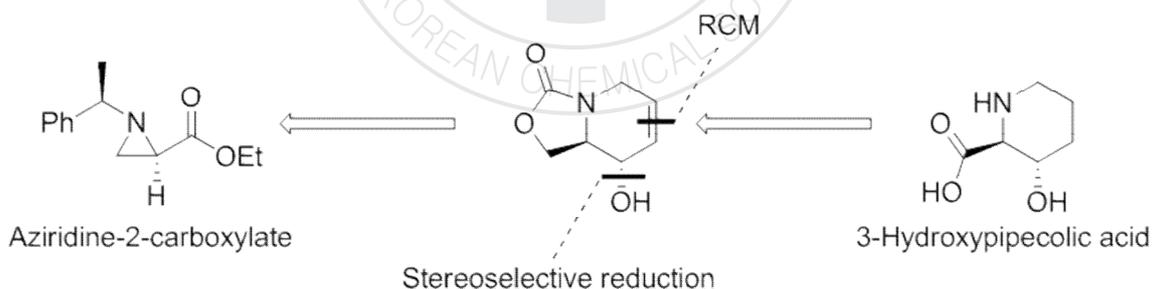
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of 3-Hydroxypipercolic Acid from Chiral Aziridines

최지은 하현준* 이원구^{1,*}

한국의국어대학교 화학과 ¹서강대학교 화학과

Functionalized chiral, non-racemic piperidines are common structural units found in many biologically and medicinally important natural and non-natural products. 3-hydroxypipercolic acid is six-membered cyclic-amino-hydroxy acid and has shown potent and specific α -D-mannosidase inhibitory activity. We synthesized 3-hydroxypipercolic acids and its analogues through bicyclic intermediate prepared from chiral aziridine-2-carboxylate via stereoselective reduction of 2-acylaziridine as a key step.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-862**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Double Asymmetric Alkylation Reactions Using symmetric Benzene Based 2-imidazolidinone Chiral Auxiliaries

강병선* 김택현¹

전남대학교 신화학소재공학과 ¹전남대학교 응용화학공학부 광바이오사업단

Asymmetric alkylations using chiral auxiliaries are now important and general methods for asymmetric carbon-carbon bond formation. To develop more effective chiral auxiliaries, bifunctional symmetric auxiliaries were investigated, allowing for two diastereoselective reactions to occur with the same sense of asymmetric induction on a single substrate molecule. In this study, double asymmetric alkylation reactions using the symmetric benzene based 2-imidazolidinone Chiral Auxiliaries will be introduced with high diastereoselectivity and yields. In addition, the good recycling of our chiral auxiliaries will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-863**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Improved tripod amphiphiles for Membrane Protein Manipulation

조경호 채필석*

한양대학교 생명나노공학과

Integral membrane proteins (IMPs) play critical roles in controlling material transfer and signal transduction across lipid barriers within individual cells as well as multicellular organisms. Our understanding of membrane protein structure and function, however, is significantly limited mainly due to the difficulties associated with handling these bio-macromolecules. Amphipathic agents serve as convenient tools for membrane protein manipulation. Here we introduce new tripod amphiphiles designed specifically for membrane protein structure determination. This class of agents displays favorable behaviors toward membrane protein solubilization and stabilization over the conventional detergents and previously-designed tripod amphiphiles.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-864**

발표분야: 유기화학

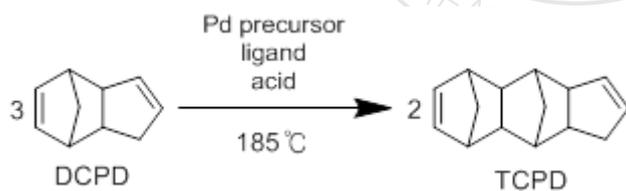
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient and Selective Synthesis of Tricyclopentadiene by Palladium/Acid Catalysts

우정오 박종은 한정식¹ 손경선*

충남대학교 화학과 ¹국방과학연구소 1기술본부 5부

Efficient synthetic strategies for tricyclopentadiene (TCPD) were investigated to improve the yield and the selectivity. Using a catalytic system comprising a palladium complex and a carboxylic acid, TCPD was prepared up to 78% conversion from dicyclopentadiene (DCPD 98%). The catalytic system produced the [2+2] TCPD isomers with high selectivity, whereas the trimeization of DCPD with no catalyst generated a mixture of isomers. The effects of Pd precursors, ligands, acids, and starting materials on the productivity and the selectivity of TCPD synthesis were evaluated.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-865**

발표분야: 유기화학

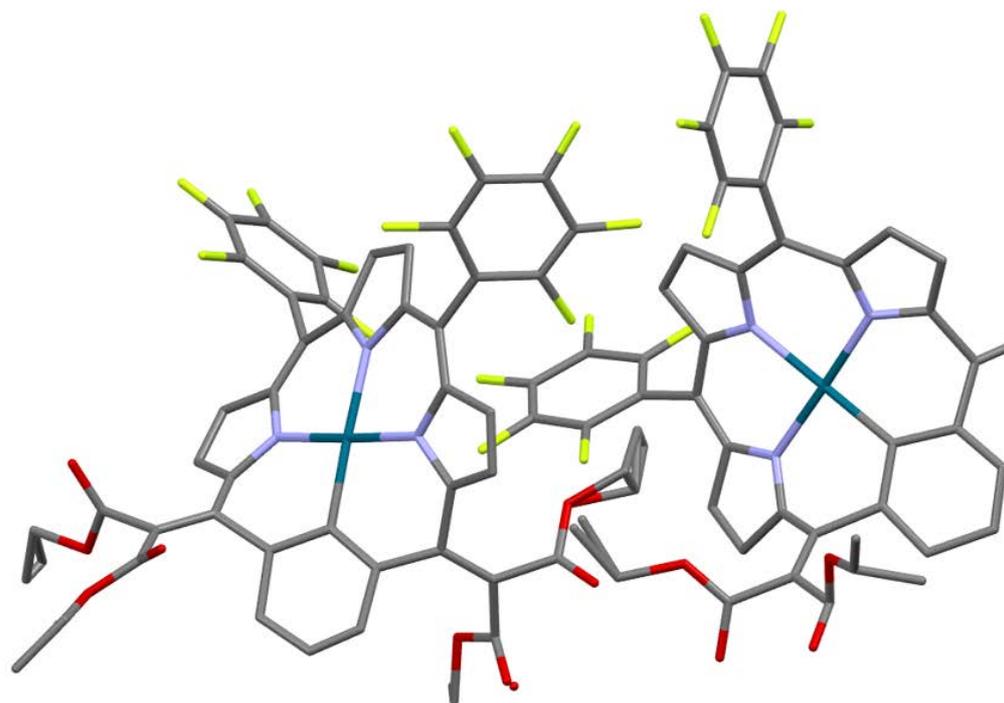
발표종류: 포스터, 발표일시: 수 16:00~19:00

meso-Alkylidenyl porphyrins and their metal complexes: Structures and Properties

이창희* 박도우 최나영

강원대학교 화학과

Since the Pd(II)-complexes of meso-alkylidene-(m-benzi)-porphyrin show promising catalytic activity toward C-C bond forming reactions such as Sonogashira coupling, we extend the metallation chemistry of meso-alkylidene-(m-benzi)-porphyrin to other transition metal ions. The reaction is straight forward and column chromatographic separation usually results in pure metal complexes. Pd(II), Cu(II) and Ni(II) form stable complexes. However, the Ag(I) need axial ligands to stabilize the metal complex. The inner aromatic sp²-carbon participates in the coordination with metal ion in the case of Pd(II) and Ni(II), however, in the case of Cu(II), only three core nitrogens participate in the coordination. All adducts were characterized by spectroscopic means. The current metal complexes can be used as catalysts in the various C-C bond forming reactions as well as C-H activations.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-866**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Unprecedented Dibenzo-hexaphyrin Analogs Carrying Four Exocyclic Double Bonds at meso-Positions

이창희* 박도우 황선아

강원대학교 화학과

We have previously reported that the meso-alkylidene porphyrins are non-aromatic and display interesting properties such as site-selective protonation and the dependency of the protonation selectivity on the number of core-hydrogens. For instance, the porphyrins with no core hydrogen are protonated at core nitrogen first. However, the porphyrins containing one or more core-hydrogens are protonated at meso- (α)-position. The protonated porphyrins displayed large hypsochromic shift of the absorption spectra. As continuing efforts for the construction of the new expanded version of these porphyrin analogues, we have synthesized expanded meso-alkylidenyl porphyrins and fully characterized by spectroscopic means. The synthesis was accomplished by a typical '3+1' type of the mixed-condensation and the products contain multiple exocyclic carbon-carbon double bonds at meso-positions. The single crystal x-ray structure analysis of the compounds revealed asymmetric nature of the compound.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-867**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dimensional probes of aryl-picket calix[4]pyrroles for the anion affinity

이창희* 김진주 이정태¹ 김주연²

강원대학교 화학과 ¹한림대학교 화학과 ²한림대학교 화학

Series of calix[4]pyrroles containing aromatic pickets at crossing meso-positions have been synthesized and characterized. The guest binding pocket created by the two crossing meso-aryl groups and four pyrrole N-Hs is expected to exhibit different affinity and selectivity depending on the substituents on the aryl group as well as the distance between aryl group and carbon at meso-position. Anion binding studies confirmed that the synthesized receptors form stable complex with various anions in organic media. The binding affinities are directly related with the distance between aryl group and the meso-carbon. Cooperative nature of the hydrogen bonding and anion- π interaction seems to play a key role on the enhanced binding affinity. Due to the limited dimension of the binding pocket, The compounds synthesized here would be good model systems for dimensional probes for the role of the aromatic picket to the binding affinity and the contribution of anion- π interaction can be quantitatively assessed, .

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-868**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Calix[4]pyrrole fused with tetrahydrothiophene as a cation-selective ion-pair receptor

이창희* 유소은 김보람

강원대학교 화학과

Calix[4]pyrroles which are fused with tetrahydrothiophene have been synthesized and characterized. The ion binding study of the synthesized hosts displayed very interesting properties. The deep cavity, cation binding pocket which was created by anion binding shows different selectivity depending on the nature of applied cations. For example, the cone conformation resulting upon the pre-complexation with fluoride anion, forms stable ion-pair complex with cesium cation. The cesium cation is thought to be bound to the deep inside the cavity by cation- π interaction. On the other hand, the Hg(II) ion form stable donor-acceptor complex with the sulfur atom. The ion binding studies confirmed that the synthesized receptors form stable complexes with various metal salts in organic media. The binding affinities and spectroscopic changes upon ion binding will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-869**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pi-extended meso-alkylidene porphyrins by 1,3-Dipolar Cycloaddition and the effect of the redox state for the product formation

이창희* 박도우 지혜수¹

강원대학교 화학과 ¹강원대학교 자연과학대학 화학과

1,3-Dipolar cycloaddition reaction of porphyrinoids using in-situ generated azomethine ylide has been well documented. The reaction usually ends up to the pi-extended of the mother macrocycles. We adopted these reactions to the pi-extended and chemical modification of meso-alkylidene porphyrins which we have synthesized recently. The reaction of in-situ generated azomethine ylide (generated from the reaction of N-methyl glycine with formaldehyde) with alkylidene-(m-benzy)porphyrin or its expanded analogue resulted in a mixture of the cyclized adducts. The reaction took place regioselectively on the pyrrole adjacent to the alkylidene double bond in the case of porphyrinoids. However, the expanded analogues resulted different regiochemical adducts. All adducts were characterized by spectroscopic means. The regioselectivity was thought to be originated from the combination of strong dipolarophile and electron rich pyrrole ring. The current synthetic methods can be applied to the construction of the reduced porphyrins which are useful in various porphyrin-related applications.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-870**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold nanoparticle decorated with functionalized, reduced porphyrins as a photosensitizer for PDT application

이창희* 이가원

강원대학교 화학과

Gold nanoparticles decorated with a single-armed chlorins were prepared and characterized. The chlorin?nanoparticle conjugate was characterized by various spectroscopic means including. Transmission electron microscopy imaging revealed that the average diameter of the particles was approximately 4.3 nm both before and after attachment of the receptor to the surface. The chlorin-functionalized nanoparticles exhibited similar absorption spectral properties as monomeric congeners without losing any fluorescence intensity. The photosensitizer?nanoparticle conjugate showed no aggregation in solution which is ideal for PDT application. Oxidation resistant bacteriochlorins and 15-halogen substituted chlorins were also synthesized and characterized. Full characterization of the gold-chlorin nano-hybrid will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-871

발표분야: 유기화학

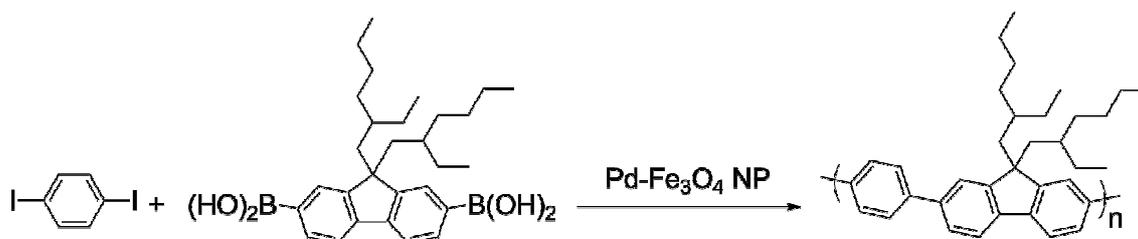
발표종류: 포스터, 발표일시: 수 16:00~19:00

Recyclable Pd-Fe₃O₄ Heterodimeric Nanocrystals for the Synthesis of Conjugated Polymers

배일학 변상문 최태림* 김병문*

서울대학교 화학부

Conjugated polymers have attracted much interest in industrial and academic fields due to their electrical and optoelectronic properties. Most of Conjugated Polymer have been synthesized via metal-catalyzed reactions in homogeneous system such as Pd-catalyzed Suzuki, Stille, Heck reactions, Ni-catalyzed Negishi, Kumada reactions, Ru-catalyzed olefin metathesis reactions (ROMP, ADMET), and Cu-catalyzed Sonogashira reaction. However, these homogeneous systems are mostly limited in that catalysts always remain within the polymer as metal and ligands after the reaction. These residual catalysts could reduce the electrical performance of Conjugated Polymer because those residual catalysts could act as a trap site of a hole or an electron. We report on the utilization of Pd-Fe₃O₄ heterodimer nanocrystals as a magnetically recyclable and effective catalyst for the repetitive synthesis of CP via Suzuki cross-coupling reactions. After optimization of various reaction conditions of the polymerization, it was found that Pd-Fe₃O₄ heterodimer nanocrystal exhibit good catalytic activity for the synthesis of CP's, can minimize the Pd content in the product CP, was magnetically recoverable through external magnet, and finally was reusable for the polymerization eleven times.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-872**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly efficient green synthesis of 2-amino-3-cyano-4*H*-chromen-4-yl phosphonates catalyzed by tetramethylguanidine

kallareddimohannaidu 김일*

부산대학교 고분자공학과

A highly efficient, rapid, and green synthesis of 2-amino-4*H*-chromen-4-yl phosphonates and 2-amino-4*H*-chromenes has been accomplished via Knoevenagel/Pinner/Phospha-michael reaction of salicylaldehyde, malononitrile, and dialkyl/aryl phosphites catalyzed by 1,1,3,3-tetramethylguanidine (TMG) under neat conditions at room temperature. The mild reaction conditions, simple work-up procedure, and use of TMG as an inexpensive catalyst provides an economical protocol for the preparation of important phosphorus-containing compounds.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-873**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Continuous flow synthesis of triols in a tube-in-tube microreactor

박찬이 박찬필* 임효진

충남대학교 분석과학기술대학원

Triols involving three hydroxy group (-OH) are very important building block in the synthesis of various materials, each hydroxy group can be further transformed into other functional groups including ketone, aldehyde, halide, amine, and so on. Photo-oxygenation conducted with only light and O₂ gas is one of the most useful green chemical processes, which can be used in production of valuable fragrances, pharmaceuticals, and fine chemicals. However, the reaction integrated with another chemical process was rarely studied. In previous reports, microfluidic systems performing photooxygenation easily solved the problems related with short lifetime of singlet oxygen in organic solvents. Herein we report a continuous flow synthesis consisted of photooxygenation and TfOH catalyzed reaction. Singlet oxygen produced by O₂ gas and photosensitizer (Methylene Blue) yields allyl hydroperoxide regioselectively in a mono-channel microreactor with segmented flow of O₂ gas bubbles and liquid slugs, the hydroperoxide was efficiently converted to the triols in the following TfOH catalyzed reaction in batch or continuous flow manner. We newly designed and tested another microreactor with inner membrane tube (AF-2400) and outer transparent tube, the O₂ gas injected in inner tube was continuously diffused into solution occupied in outer tube through gas permeable AF-2400 tube. The microreactor of tube-in-tube type enhanced the contact efficiency between light (LED lamp), oxygen gas, and liquid including reagent and photosensitizer. More importantly, the microreactor was excellent in terms of productivity that is one of the most important issues in microchemical society. We carried out the syntheses of rose oxide and ascaridole from alpha-terpinene and (-)-beta-citronellol. The photooxygenation of hexamethylbenzene was tested, the product ratio of mono- and dual-reaction was perfectly controlled under exact reaction time and temperature as another example.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-874**

발표분야: 유기화학

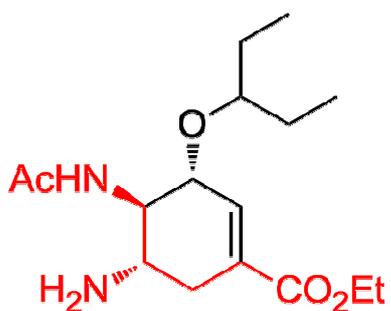
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of γ , δ -Diiminoesters as versatile chiral building block

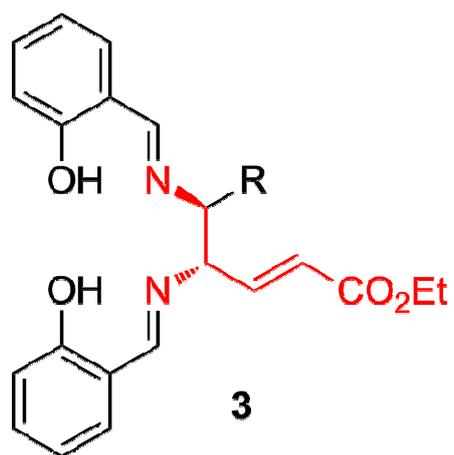
권순호 Jik Chin^{1,*} 김병문*

서울대학교 화학부 ¹Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6

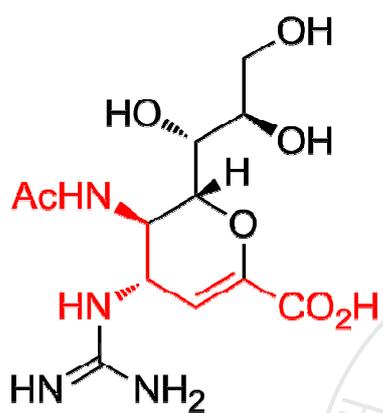
Antiviral agents such as oseltamivir (1) and zanamivir (2) contain γ , δ -diaminoacid structural motifs. They have also been reported to be useful as intermediates for the preparation of other therapeutic agents. The synthetic challenge of oseltamivir-type antivirals has attracted considerable interest in developing efficient synthetic methods. Here we report on a one-pot reaction for the synthesis of γ , δ -diiminoesters (3) with two adjacent chiral centers in enantiomerically pure form. Diaza-Cope rearrangement (DCR) of diimines formed from 1,2-bis(2-hydroxyphenyl)-1,2-diaminoethane (hpen) and aldehydes were used to synthesize a variety of γ , δ -diiminoesters. DFT computation provides valuable insights into the stereospecific rearrangement reaction. The crystal structure of the product diimine (3d) formed from the reaction of (R,R)-hpen and 2,6-dichlorobenzaldehyde and the DCR reaction gives the product diimine in S,S configuration as expected from the chair-like six-membered ring transition state with all equatorial substituents.



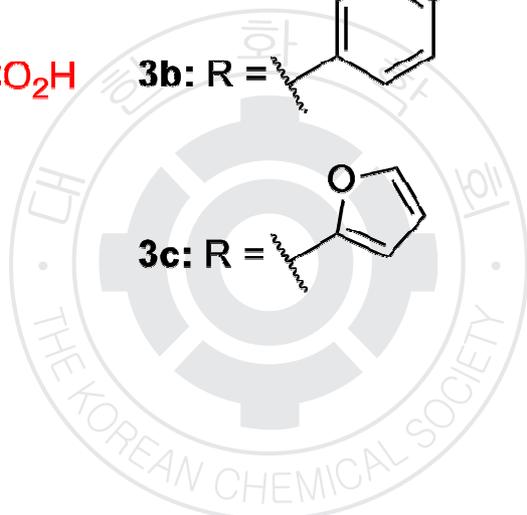
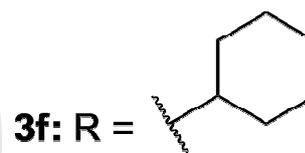
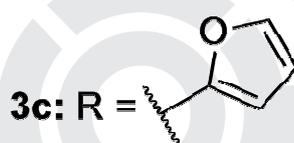
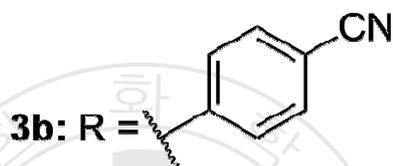
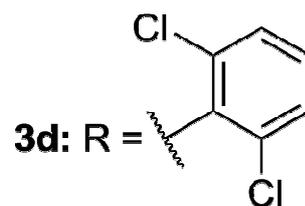
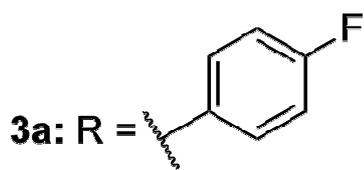
1



3



2



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-875

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of vicinal quaternary carbon center via diaza-Cope rearrangement

권순호 Jik Chin^{1,*} 김병문*

서울대학교 화학부 ¹Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6

About a decade ago, resonance assisted hydrogen bond (RAHB) directed diaza-Cope rearrangement (DCR) was shown to be useful for stereospecific synthesis of a chiral vicinal diamine. Since then this method has been used for the preparation of a variety of vicinal chiral diamines including C₂ symmetric aryl and alkyl substituted diamines as well as nonsymmetrical diamines. Herein we describe that the reaction between 1,2-bis(2-hydroxyphenyl)-ethylenediamine (hpen) and methyl pyruvate gives the DCR product with good yield and excellent stereoselectivity. The product containing two chiral quaternary carbon centers was characterized with chiral high performance liquid chromatography and X-ray crystallography. DFT computation provides insight into why the diaza-Cope rearrangement takes place readily with methyl pyruvate but not with other ketones such as acetone and substituted acetophenones.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-876

발표분야: 유기화학

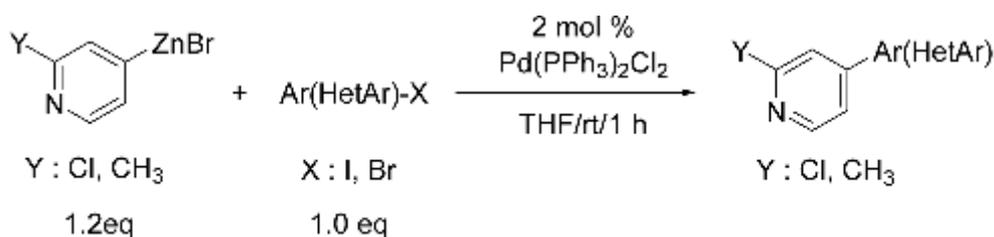
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation 2-Substituted-4-pyridylzinc Bromides via Direct Insertion of Active Zinc and Their Coupling Reactions

조경환 김승희*

단국대학교 화학과

Heterocyclic compounds which contain a pyridine moiety have played a very significant role in a wide range of organic compounds, such as pharmaceuticals, agrochemicals, medicinal chemistry, and material chemistry. For example, bipyridine groups were found to be a key element in antibiotics, and pyridylpyrimidines were used as fungicides as well as tyrosine kinase inhibitors. In addition, pyridinecontaining oligomers are frequently found in liquid crystals. More specific examples utilizing 4-pyridyl moiety are also found in a wide spread of fields in chemistry. Consequently, new practical synthetic approaches for introducing a pyridine ring into complex organic molecules are of high value. To this end, transition-metal-catalyzed cross-coupling reactions of pyridylmetallic reagents have been frequently utilized. However, the preparation of electron-deficient pyridyl organometallic reagents has been a challenging subject mainly because of some difficulties such as instability and formation of by-products. In addition to those difficulties, the regiochemistry should be considered when the corresponding pyridylmetallic reagents were prepared because, unlike benzene, pyridine ring has unevenly distributed electrons.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-877

발표분야: 유기화학

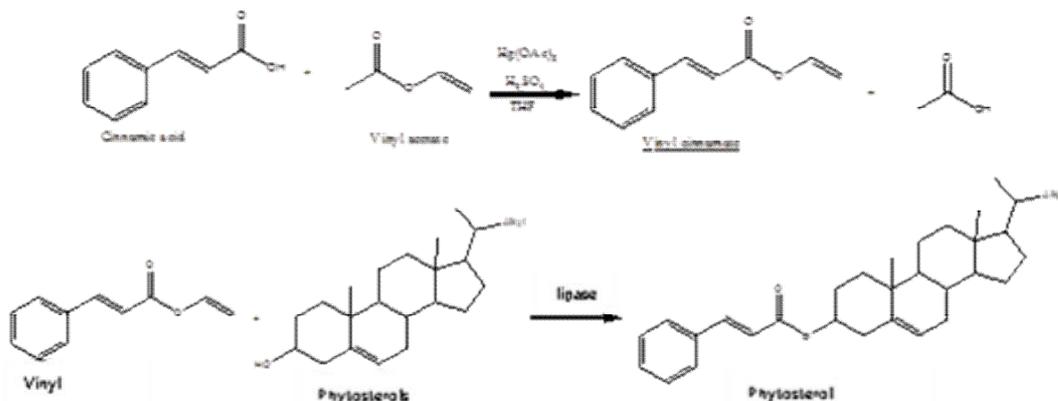
발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemoenzymatic Synthesis of Phytosteryl Cinnamate

임순성

한림대학교 식품영양학과

Particular attention has been paid to phytosterols and their derivatives (phytosteryl esters) because of their health benefits in humans, especially their capability to lower serum cholesterol levels. However, there are only few reports on phytosteryl phenolates. In this study, phytosteryl cinnamate was successfully synthesized via a two-step chemoenzymatic route. The intermediate vinyl cinnamate was first chemically produced and subsequently esterified. Five commercial lipases were tested and the lipase from *Candida antarctica* was the most active one. Furthermore, 20 solvents were screened with regard to the conversion rate and the highest yield was achieved in a binary organic solvent system consisting of hexane and 2-butanone at a ratio of 8:2. A high conversion yield was obtained at 65°C, a phytosterol to cinnamic acid ratio of 1:1, and an enzyme concentration of 300 U. Keywords: Phytosterol; Cinnamic acid; Lipase; Phytosteryl cinnamate



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-878**

발표분야: 유기화학

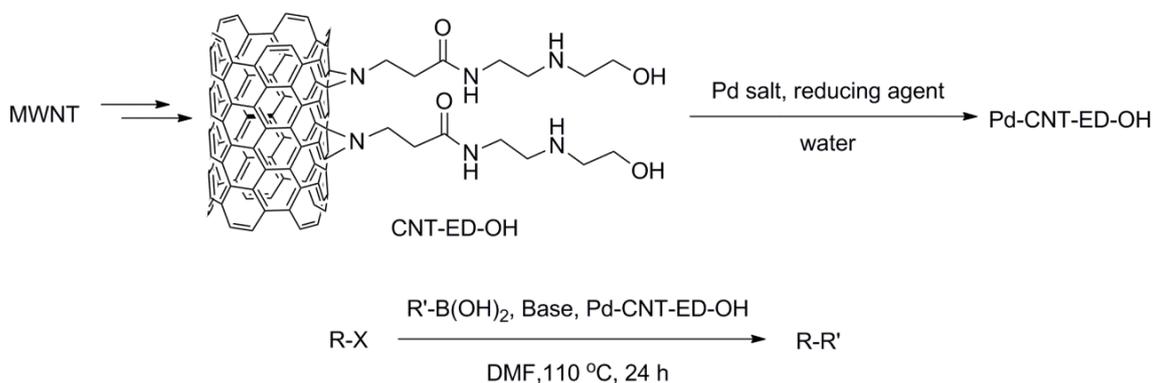
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on the functionalization of MWNTs and C-C bond Coupling Reactions Using Heterogeneous Pd-MWNTs

김은석 김병문^{1,*}

서울대학교 화학과 ¹서울대학교 화학부

Modified carbon nanotubes (CNTs) have attracted much attention due to their high specific surface areas, chemical stability, and electrical conductivities. Functionalization of multi-walled carbon nanotubes (MWNTs) was studied using nitrene chemistry as a functionalization method. Using this method, we have synthesized multi-walled carbon nanotubes modified by surface functionalization using nitrene chemistry. Using this method, carboxylate functionalized carbon nanotubes were prepared, and transition metals were incorporated on the linker-MWNT via reductive methods. For the reduction methods we have studied various ways to effectively immobilize Pd on the MWNT surfaces and found that use of hydrazine hydrate was the best condition. After immobilization of Pd on MWNT, its role as a catalyst for the Suzuki reaction as a representative C-C bond forming reaction was examined. The functionalized MWNT-Pd catalyst showed good reactivity in Suzuki-coupling reactions. The catalysts could be retrieved upon completion of the reaction by filtration; the recycled catalyst could then be used in further reactions up to seven times before any loss in catalytic activity was observed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-879**

발표분야: 유기화학

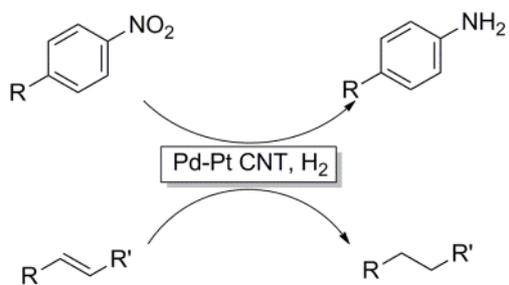
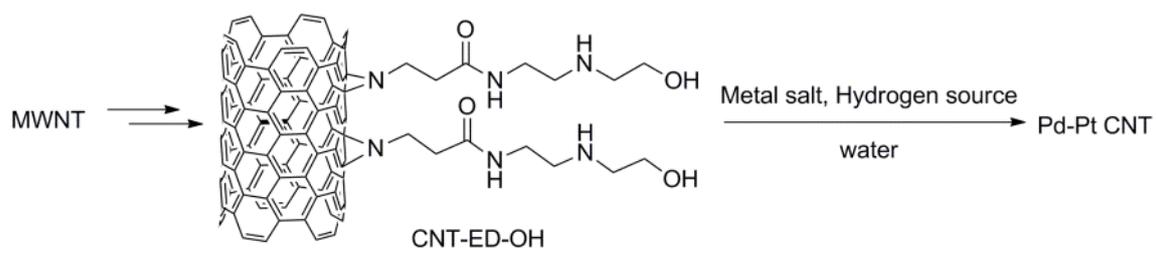
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-Pt bimetallic nanoparticles on multi-wall-nanotubes catalyzed efficient, chemoselective reduction of nitro compounds and olefins

김은석 김병문^{1,*}

서울대학교 화학과 ¹서울대학교 화학부

Metal nanoparticles are a new class of heterogeneous catalysts. Recently, bimetallic nanoparticle catalysts have attracted much attention as potential catalysts. Carbon nanotubes used as suitable supports for metal nanoparticle redox catalyst systems, cause they have many-electron systems and sufficient surface area. Therefore, we have synthesized Pd-Pt bimetallic nanoparticle catalysts using functionalized multi-wall-carbon nanotubes (MWNTs).³ Efficient reductions of nitro-compounds and olefins could be achieved using hydrogen gas in the presence of Pd-Pt bimetallic nanoparticle MWNT catalysts at ambient temperature. Moreover the bimetallic nanoparticle system showed improved activity in reduction reactions, compared to mono metal-supported catalysts. Under the optimized conditions, various nitro compounds and alkenes were cleanly reduced at ambient temperature. Furthermore, this catalytic system had excellent activity and high chemoselectivity for nitro compounds and alkenes. After the reaction, the used catalysts could be collected through filtration, and the recycled catalysts could then be used in further reactions up to 10 times without any loss in catalytic activity was observed.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-880**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Magnetic recyclable Pd-Fe₃O₄ nanocrystal catalyst for Heck and Sonogashira Reactions

정주영 변상문 현택환¹ 김병문*

서울대학교 화학부 ¹서울대학교 화학생물공학부

Palladium-catalyzed carbon-carbon coupling reactions have become essential methods in organic synthesis, owing to their versatility in the convergent synthesis of a range of substrates. We have developed a very convenient Pd-Fe₃O₄ nanocrystal catalyst system for Heck and Sonogashira coupling reactions. It is of particular note that in both reactions the heterobimetallic nanocrystal-catalyzed reactions proceeded smoothly without requiring any transition metal additives. This catalyst system offers robust reaction conditions that are environment-friendly and atom efficient for both Heck and Sonogashira reactions. Furthermore the nanocrystal catalyst could be easily recovered by an external magnet and recycled 6 times without losing the catalytic activity. This eco-friendly and highly efficient Pd-Fe₃O₄ nanocrystal catalyst system is expected to be potentially useful for the development of large-scale processes. Further research in the development of efficient heterobimetallic nanocrystal catalyst systems and their application is in progress

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-881

발표분야: 유기화학

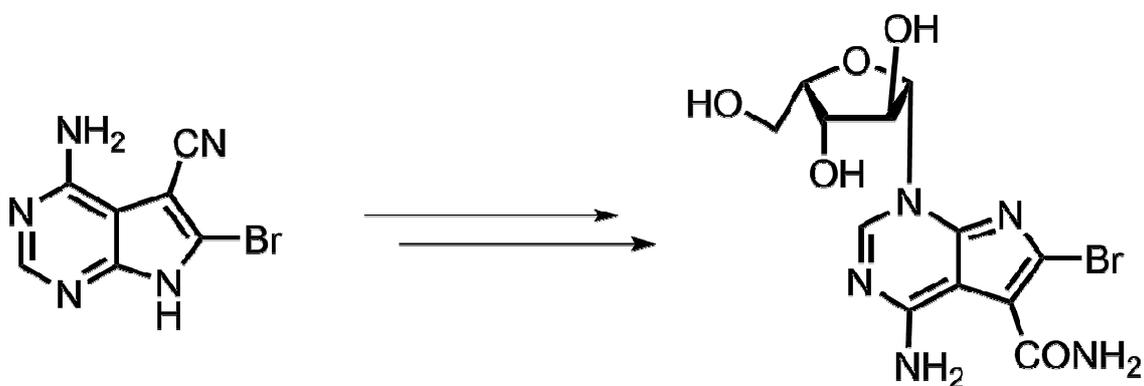
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of a Potent Cyclin-Dependent Kinase Inhibitor, BMK-Y101

송명중 권순호 김병문*

서울대학교 화학부

BMK-Y101 is a novel pyrrolo[2,3-d]pyrimidine-based potent cyclin-dependent kinase (Cdk) 7 and 9 inhibitor, which is characterized by an intriguing structural feature of N-1 nucleoside, the structure of which departs from previously reported N-7 nucleoside Cdk inhibitor, xylocyidine. Although N-1 nucleosides have appeared in the literature, they have often been considered as kinetic products and thus intermediates of N-7 glycosylation. In the course of the synthetic studies of xylocyidine derivatives, we have developed a highly regioselective method to obtain the N-1 nucleoside. The origin of the selectivity is apparently based on the reactivity of the silylated nucleobase and the unexpected kinetic stability of the resulting N-1 nucleoside. The choice of BSA as a silylating agent was critical in securing the N-1 nucleoside, BMK-Y101. On the other hand, proper selection of reaction conditions promoting transglycosylation provides an efficient route to N-7 nucleosides.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-882**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Microwave-assisted Fast and Facile Synthesis of Functional Unsymmetrical Methylenebisarenols

김충식 Takuya Oguma¹ Tsutomu Katsuki^{2,*}

International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University ¹*International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University and Department of Chemistry, Graduate School of Science Kyushu University* ²*International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University, Institute for Advanced Study, Kyushu University, and JST-ACT-C*

Ortho-substituted methylenebisarenols are important organic compounds of being able to serve as antioxidants and stabilizers for polymers, petroleum products, rubber, and food. Because of this increasing industrial demand, a number of approaches to these compounds have been developed. Herein, we report that an efficient synthetic method to prepare unsymmetrical methylenebisarenols from C3-substituted 2-naphtols and salicyl alcohol derivatives via microwave-assisted reaction, affording good yields (up to 80%) of desired products at the short reaction time. Addition of potassium carbonate as an additive is the key for this unsymmetric methylenebisarenol synthesis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-883**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Isocoumarins and Pthalides from 2-Iodobenzoic Acids and Alkynes by Regioselective Cyclisations via Temperature Control

IRUDAYANATHANFRANCISMARIARAJ 이선우*

전남대학교 화학과

The copper-catalyzed coupling reactions of 2-iodobenzoic acids and alkynes such as terminal acetylene, alkynyl carboxylic acids, and trimethylsilyl acetylenes selectively afforded isocoumarins and phthalides in the presence of Cs_2CO_3 and DMSO. At 100 °C, the 6-endo-dig product, isocoumarin, was formed and at 25 °C the 5-exo-dig product, phthalide, was formed as a major product. A variety of alkynes produced the corresponding isocoumarins and phthalides in good yields. The usage of alkynyl carboxylic acids holds advantage over using low volatile terminal alkynes for synthesizing isocoumarins. A mechanism is suggested in which the formation of 2-alkynyl benzoic acid as an intermediate via Sonogashira-type coupling was ruled out in the reaction pathway.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-884

발표분야: 유기화학

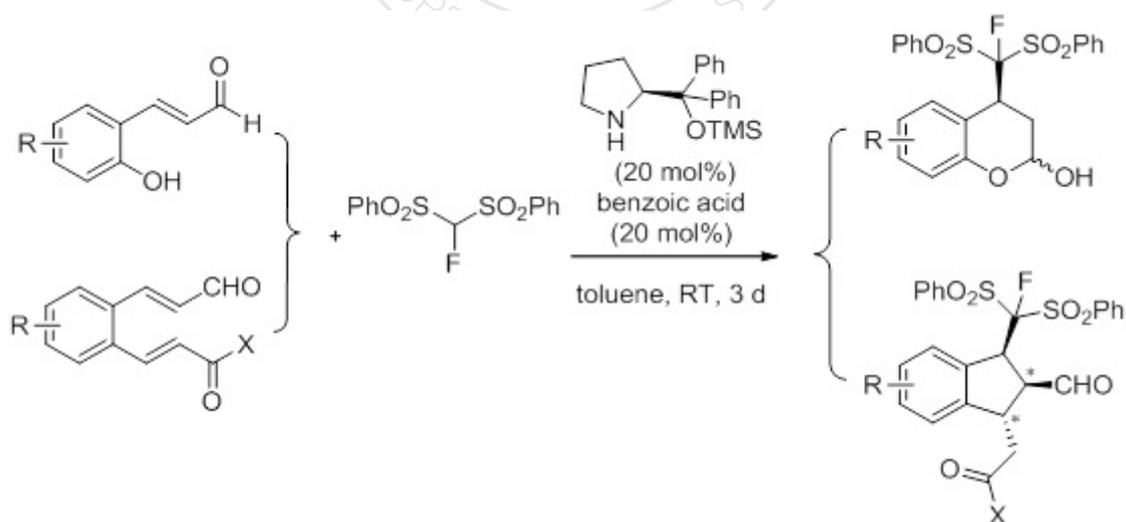
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Organocatalytic Cascade Reactions of Fluorobis(phenylsulfonyl)methane with Enals

김영석 김선민 양정운*

성균관대학교 에너지과학과

Cascade reactions are powerful tools in synthetic chemistry. The most attractive features of cascade reaction is the formation of desired target molecules in a single flask without the isolation of intermediates. We have developed highly enantioselective cascade reactions for the synthesis of fluoroindanes and chromanols derivatives. The cascade reactions consist of either a double Michael reaction or Michael-hemiacetal formation via the addition of fluorobis(phenylsulfonyl)methane to enals. The final products are obtained in good yields with excellent stereoselectivities.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-885**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Tau and β -Amyloid Fluorescence Imaging Agents

LIHUA 강순방 금교창^{1,*}

한국과학기술연구원(KIST) 뇌의약연구단 ¹한국과학기술연구원(KIST) 케모인포메틱스연구센터

Alzheimer disease is a progressive neurodegenerative disorder characterized by the gradual onset of dementia. The pathologic hallmarks of the disease are beta-amyloid (A β) plaques, neurofibrillary tangles (NFTs), and reactive gliosis (see the Fig 1 and Fig 2 images and slideshows below). Tau is a highly soluble microtubule-binding protein. Mutations in tau have not yet been linked to AD, although tau mutations cause frontotemporal dementia with Parkinsonism linked to chromosome 17. Hyperphosphorylation of tau, particularly that mediated by MARK, CDK5 and GSK3 β , destabilizes microtubules, causing impairments in axonal transport and neuronal dysfunction. Self-assembly of hyperphosphorylated tau results in the formation of NFTs. However, soluble tau species might also exert potent pathological effects. Targeting the tau pathology might help to attenuate the cognitive decline that occurs in AD. Current diagnosis of Alzheimer disease is made by clinical, neuropsychological, and neuroimaging assessments. Routine structural neuroimaging evaluation is based on nonspecific features, such as atrophy, which is a late feature in the progression of the disease. Therefore, developing new approaches for early and specific recognition of Alzheimer disease at the prodromal stages is of crucial importance. Effective therapies to halt or slow disease progression and an appropriate cure are still lacking. A number of in vivo neuroimaging techniques, which can be used to reliably and noninvasively assess aspects of neuroanatomy, chemistry, physiology, and pathology, hold promise. With time and improvements in technology, these imaging techniques might yield acceptable neuroimaging biomarkers of Alzheimer disease.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-886

발표분야: 유기화학

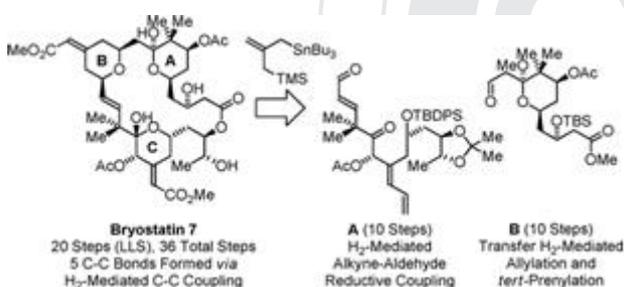
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Bryostatin 7 via C-C Bond Forming Hydrogenation

우상국* 민진욱

울산대학교 화학과

The marine macrolide bryostatin 7 is prepared in 20 steps (longest linear sequence) and 36 total steps with five C-C bonds formed using hydrogenative methods. This approach represents the most concise synthesis of any bryostatin reported, to date.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-887

발표분야: 유기화학

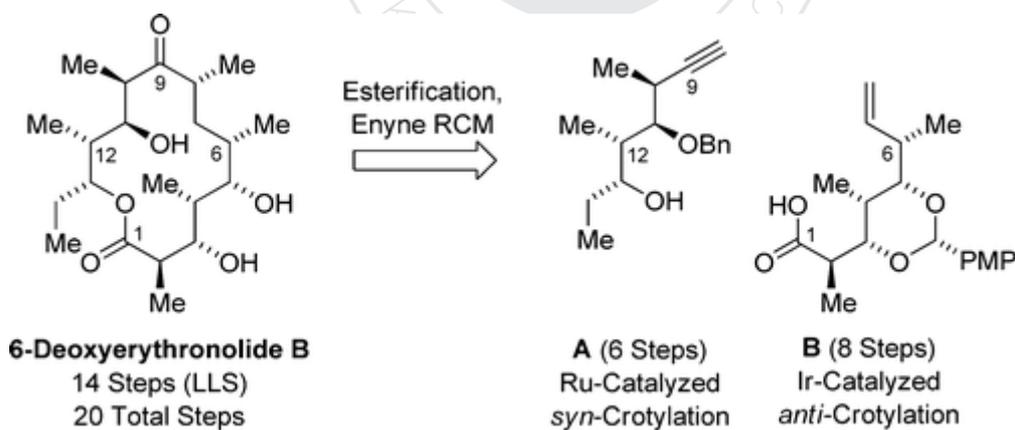
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of 6-Deoxyerythronolide B via C-C Bond-Forming Transfer Hydrogenation

우상국* 이승창

울산대학교 화학과

The 14-membered macrolide 6-deoxyerythronolide B is prepared in 14 steps (longest linear sequence) and 20 total steps. Two different methods for alcohol CH-crotylation via transfer hydrogenation are deployed for the first time in target-oriented synthesis. Enyne metathesis is used to form the 14-membered ring. The present approach represents the most concise construction of any erythronolide reported, to date.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-888

발표분야: 유기화학

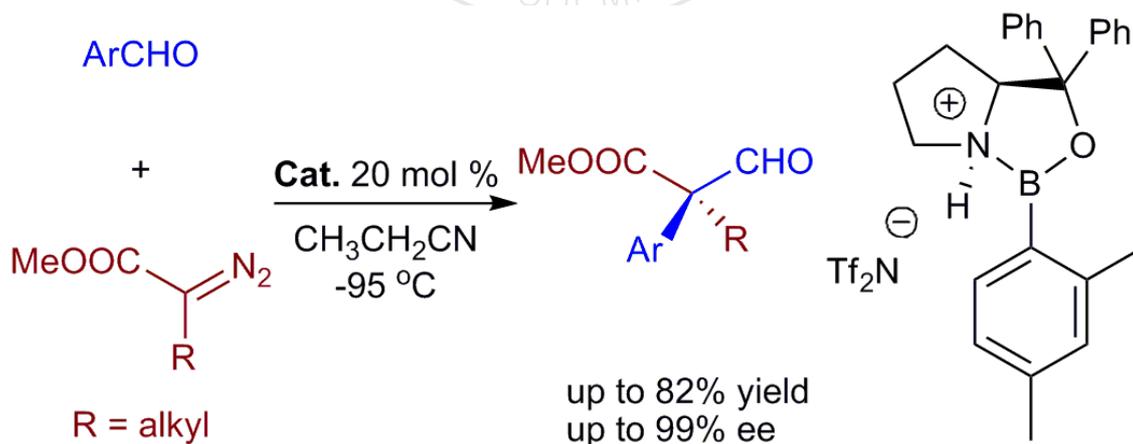
발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxazaborolidinium ion catalyzed stereoselective formal insertion of diazoacetates into aryl carbon-CHO bond: stereoselective construction of all-carbon quaternary carbon centers in acyclic systems

강병철¹ 심수용¹ 신성호¹ 류도현^{1,*}

성균관대학교 화학¹ 성균관대학교 화학과

This paper describes a catalytic enantioselective route to synthesize functional all-carbon quaternary aldehydes in acyclic systems, via boron Lewis acid-promoted formal C-C insertion of diazoesters into aryl carbon-CHO bond. In the presence of chiral (S)-oxazaborolidinium cation **1d** as a catalyst, the reaction proceeded in good yield (up to 82%) with good regioselectivity (up to 88:12) and excellent enantioselectivity (up to 99% ee). The synthetic potential of this method was illustrated by the preparation of β -amino and β -amino ester.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-889

발표분야: 유기화학

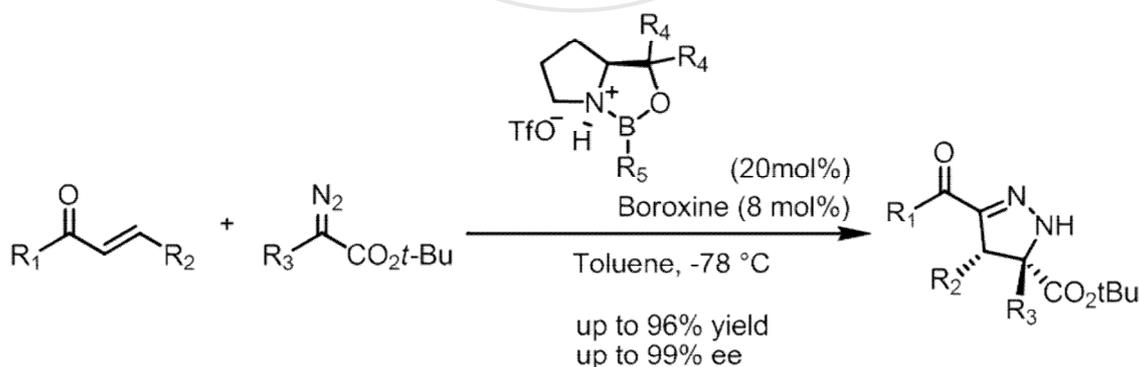
발표종류: 포스터, 발표일시: 수 16:00~19:00

CATALYTIC ENANTIOSELECTIVE ASYMMETRIC [3+2] CYCLOADDITION REACTION BETWEEN β -SUBSTITUTED ACYCLIC ENONES AND DIAZOACETATES

김가은 류도현* 신성호 강병철¹

성균관대학교 화학과¹ 성균관대학교 화학

Cycloaddition reactions of diazoalkanes with olefinic dipolarophiles have been widely utilized because the resulting pyrazolines can be converted into a variety of nitrogen-containing molecules. A catalytic synthetic route to highly functionalized chiral 2-pyrazolines was developed by an asymmetric [3+2] cycloaddition reaction of diazoacetates with β -substituted acyclic enones. In the presence of chiral (S)-oxazaborolidinium ion as a catalyst, the reaction proceeded in high yield with high to excellent enantioselectivity (up to 99% ee).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-890

발표분야: 유기화학

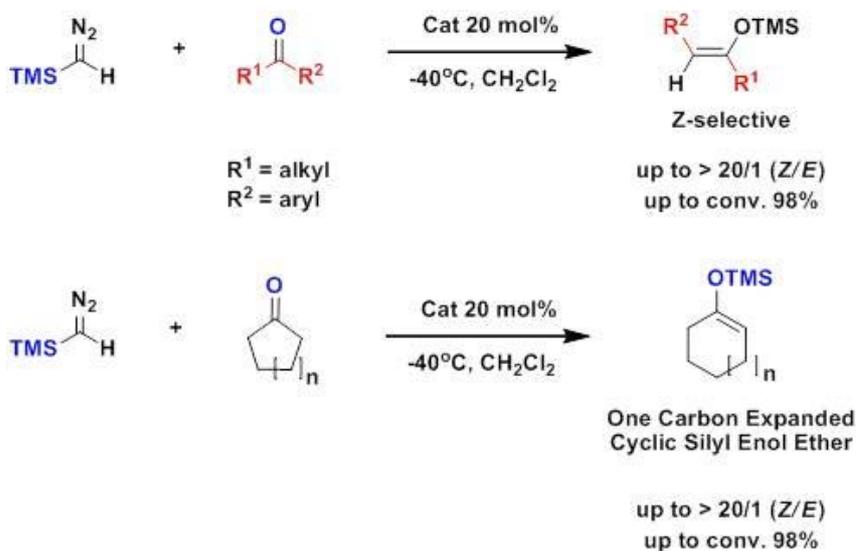
발표종류: 포스터, 발표일시: 수 16:00~19:00

A new stereoselective synthetic method of silyl enol ethers from alkyl aryl ketones and (Trimethylsilyl)diazomethane

심수용 강병철¹ 김가은 류도현*

성균관대학교 화학과 ¹성균관대학교 화학

Silyl enol ethers are one of the most useful substrates for a wide variety of organic reactions, including aldol, Michael, [4+2] cycloaddition reactions, alkylations, acylations, oxidative processes, and etc. The enolates can generally be prepared in situ from the corresponding carbonyl compounds and a base with control of regiochemistry determined kinetically or thermodynamically. However, Regioselectivity, chemoselectivity, and stereoselectivity (E or Z) are important topics in the synthesis of silyl enol ethers. Therefore, it is important to control regio- or stereoselectivity for a subsequent synthetic utility. In this research, highly (Z)-selective silyl enol ethers were prepared from alkyl aryl ketones and (trimethylsilyl)diazomethane by using oxazaborolidinium ion catalyst. Furthermore, one-carbon expanded cyclic silyl enol ethers were also successfully prepared from cyclic ketones.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-891**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cholate-based N-Oxide Amphiphiles for Membrane Protein Manipulation: Importance of Non-hydrocarbon Groups in the Hydrophobic Portion

sadafaiman 채필석^{1,*}

한양대학교 바이오나노공학과¹ 한양대학교 생명나노공학과

Integral membrane proteins, the fundamental part of the plasma membrane, mediate the transfer of materials and information between cells and their environments. The fact that more than 50% drugs target membrane proteins reflects the importance of these biomolecules' role in a disease or normal state of cells. Detergents are essential agents for membrane protein solubilization and stabilization. Therefore, many structurally-diverse amphiphiles have been developed to facilitate membrane protein study, but still information on detergent structure-property relationship is seriously limited. In the present study, we have prepared several cholate- or deoxycholate-based amphiphiles with N-Oxide head group. Our study reveals that these amphiphiles can be promising alternatives to conventional detergents for membrane protein study. In addition, our results give an insight into detergent structure-property relationship with respect to the role of non-hydrocarbon groups in the hydrophobic group.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-892**

발표분야: 유기화학

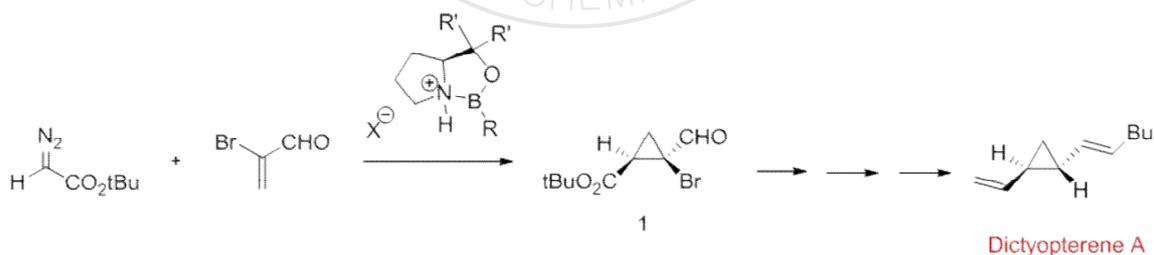
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Studies on Dictyopterene A, Sexual Pheromones for the Marine Brown Algae

김태형 백은희¹ 김재연 심수용 신성호 김가은 류도현*

성균관대학교 화학과 ¹성균관대학교 화학

Dictyopterenes are unsaturated C-11 hydrocarbons bearing a cyclopropane, and in particular a vinyl- and E-hexenyl-substituted ring in the case of dictyopterene A. These natural compounds were first isolated as major components from the odoriferous oil of the Hawaiian seaweeds, genus Dictyopteris. These compounds comprise a family of sexual pheromones for the marine brown algae, exhibiting remarkable activity including their sperm attracting physiological ability and the responsible for the intense ocean smell. We studied on the total synthesis of Dictyopterene A. The key intermediate 1 was prepared by asymmetric Oxazaborolidinium ion catalyzed Cyclopropanation.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-893**

발표분야: 유기화학

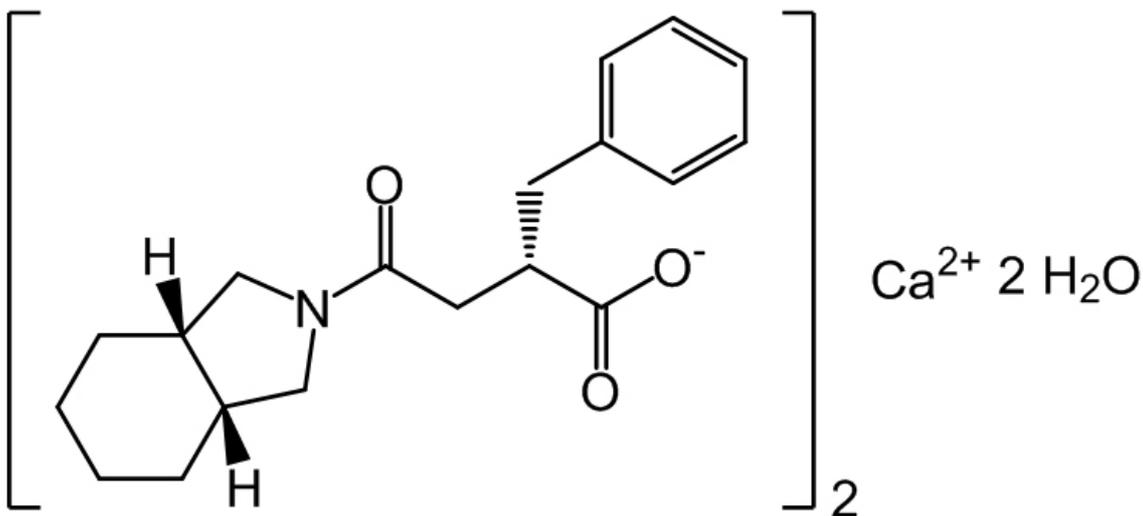
발표종류: 포스터, 발표일시: 수 16:00~19:00

Method for the preparation of mitiglinide calcium dihydrate

김관준 강용한*

한양대학교 응용화학과

Diabetes mellitus type 2 (formerly noninsulin-dependent diabetes mellitus (NIDDM) or adult-onset diabetes) is a metabolic disorder that is characterized by high blood glucose in the context of insulin resistance and relative insulin deficiency. Mitiglinide (INN, trade name Glufast) is a drug for the treatment of type 2 diabetes. Mitiglinide belongs to the meglitinide class of glucose-lowering drugs. In this study, we will introduce the method for the preparation of mitiglinide calcium dihydrate.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-894**

발표분야: 유기화학

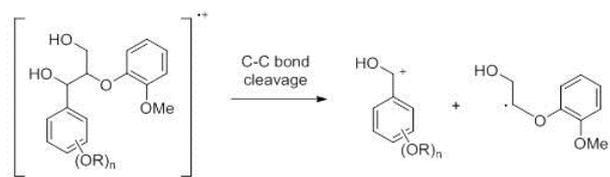
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of Alkoxy Groups on Arene Rings of Lignin beta-O-4 Model Compounds on the Efficiencies of SET Promoted Photochemical and Enzymatic C-C Bond Cleavage Reactions

임숙현 이진주 문경민 조대원*

영남대학교 화학과

To gain Information about how alkoxy substitution in arene rings of beta-O-4 structural units within lignin governs the efficiencies/rates of radical cation C1-C2 bond cleavage reactions, single electron transfer (SET) photochemical and lignin peroxidase catalyzed oxidation reactions of dimeric/tetrameric model compounds have been explored. The results show that the radical cations derived from less alkoxy substituted dimeric beta-O-4 models undergo more rapid C1-C2 bond cleavage than those of more alkoxy substituted analogs. These findings gained support from the results of DFT calculations, which demonstrate that C1-C2 bond dissociation energies of beta-O-4 radical cations decrease as the degree of alkoxy substitution decreases. In SET reactions of tetrameric compounds consisting of two beta-O-4 units, containing different degrees of alkoxy substitution, regioselective radical cation C-C bond cleavage was observed to occur in one case at the C1-C2 bond in the less alkoxy substituted beta-O-4 moiety. However, regioselective C1-C2 cleavage in the more alkoxy substituted beta-O-4 moiety was observed in another case, suggesting that other factors might participate in controlling this process. These observations show that lignins containing greater proportions of less rather than more alkoxy rings as part of beta-O-4 units would be more efficiently cleaved by SET mechanisms.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-895

발표분야: 유기화학

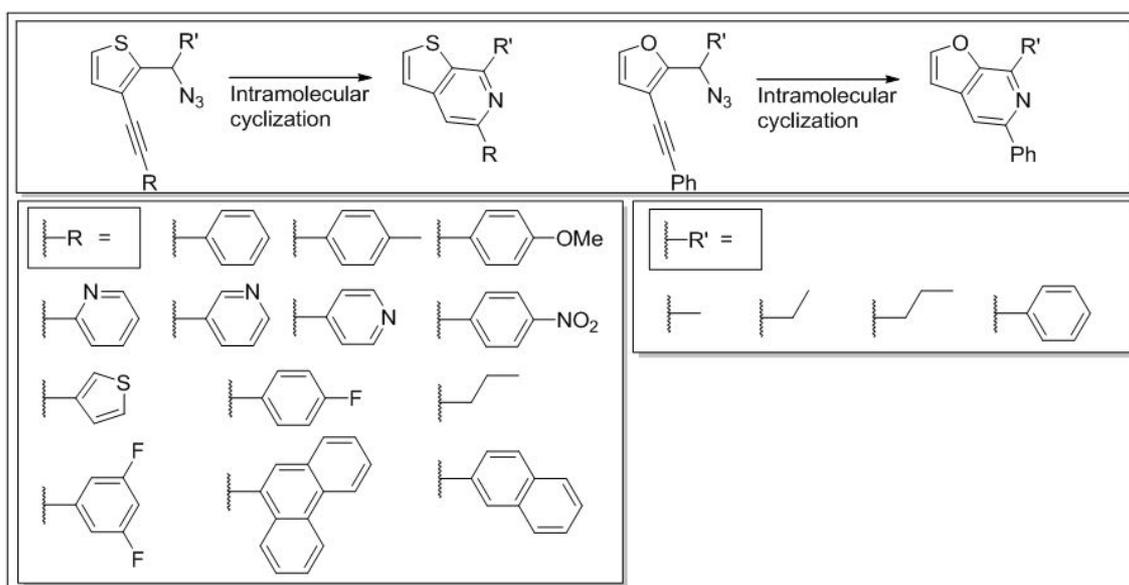
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Method for the Synthesis of Fused-pyridine Ring Compounds via Intramolecular Cyclization

정미진 이호규 이재탁 이원구* 하현준^{1,*}

서강대학교 화학과 ¹한국의국어대학교 화학과

Fused-pyridines ring compounds such as thienopyridine and furopyridine are used for pesticide, herbicide, dye, ligand, and diode. Additionally, some substituted Fused-pyridine ring compounds are pharmacologically and biologically active. Previously, several synthetic strategies for thienopyrine and furopyridine have been reported by Pomeranz-Fritsch, Larock, Yamamoto, Chen, and Queiroz. However, these methods require long reaction time, and harsh reaction condition to result low yield of product. In our previous work, we efficiently synthesized substituted azaindole by intramolecular cyclization reaction of azide and acetylene substituted pyrrole without catalyst. Applying the method, substituted thienopyridine and furopyridine were synthesized from thiophene and furan.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-896**

발표분야: 유기화학

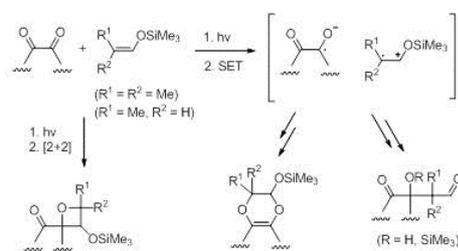
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photochemical Reactions of 1,2-Diketones with Silyl Enol Ethers

이진주 문경민 임숙현 조대원*

영남대학교 화학과

Results arising from the current study demonstrate that UV-irradiation induced photoaddition reactions of the 1,2-diketones, acenaphthenequinone, 9,10-phenanthrenequinone and benzil, with silyl enol ethers derived from propionaldehyde and isobutyraldehyde take place to form a variety of adducts. Product formation in these cases takes place mainly via two mechanistic pathways, one initiated by single electron transfer (SET) and the other by [2+2]-cycloaddition. In addition, observations show that the competition between these pathways depends on the nature of the substrates. An exploration of the photoreactions of acenaphthenequinone revealed that photoinduced SET is the predominant process occurring when the dimethyl-substituted silyl enol ether serves as a reactant, while cycloaddition and other excited state reactions become competitive with SET when the mono-methyl substituted silyl enol ether is used as a substrate. In the case of 9,10-phenanthrenequinone, photoreactions take place by [4+2]-cycloaddition routes regardless of the nature of silyl enol ether employed. Finally, irradiation of benzil in the presence of both silyl enol ethers leads to exclusive or predominant formation of products arising by [2+2]-cycloaddition and photoinduced, benzoyl radical forming alpha-cleavage.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-897**

발표분야: 유기화학

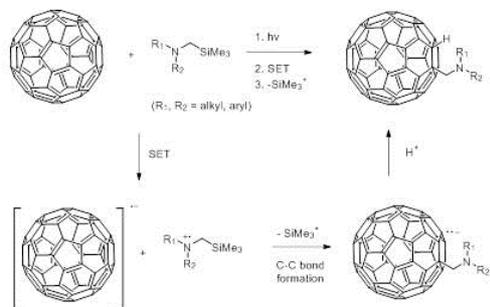
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of alpha-Aminofullerene Derivatives Using SET-Photochemical Reactions of Fullerene with alpha-Silyl-tertiary Amines

문경민 이진주 임숙현 조대원*

영남대학교 화학과

Single electron transfer (SET)-promoted photochemical reactions of C₆₀ fullerene with alpha-silyl tertiary amines to prepare alpha-aminofullerenes were carried out and their reaction mechanisms were explored. The results showed that 340 nm irradiation of 10% EtOH-toluene solutions containing amine donors and C₆₀ fullerene give rise to production of alpha-aminofullerenes with modest to high chemical yields. Electrochemical results and product distributions of photoreactions between alpha-silyl tertiary amine and C₆₀ fullerene have provided a plausible reaction mechanism. photoinduced SET from alpha-silyl tertiary amine to C₆₀ fullerene take place highly efficiently to form radical ion intermediates, alpha-silyl tertiary amine radical cations and C₆₀ radical anions, in which radical cations of alpha-silyl tertiary amines undergo rapid desilylation process to form alpha-amino carbon radicals. Consequently, C-C bond formation between alpha-amino carbon radicals and C₆₀ radical anion, followed solvent assisted protonation, produce 1,2-added alpha-amionfullerenes.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-898**

발표분야: 유기화학

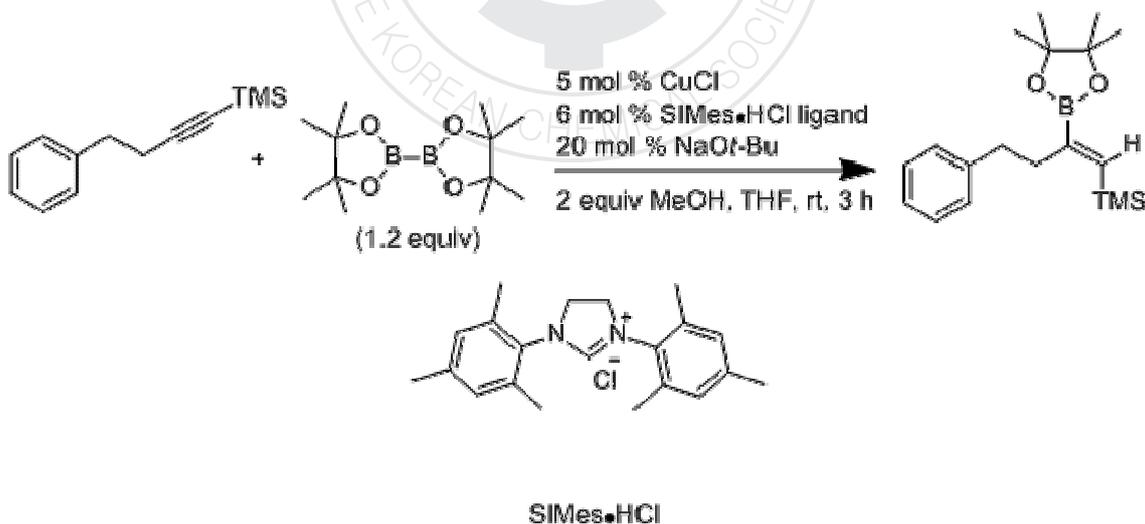
발표종류: 포스터, 발표일시: 수 16:00~19:00

SIMes-Cu Catalyzed Stereoselective Monoborylation of Silylalkynes

배준성 채영미 윤재숙*

성균관대학교 화학과

Copper-catalyzed boration of internal alkynes using diboron reagents in the presence of alcohol generates formally monohydroborated alkenylboron compounds with high chemo-, regio-, and stereoselectivity. In this study, we have investigated copper-catalyzed selective boron addition to internal silylalkynes by using various Cu-NHC catalysts. A range of alkyl-substituted substrates were examined and the results will be presented.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-899**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of nitrovinyl-substituted trimethoxystilbene derivatives as a potent tubulin polymerization inhibitors and antiproliferative agents

경민구 민동국 정만길*

연세대학교 화학과

Tans-trimethoxy resveratrol has superior pharmacokinetic characteristics when compared with resveratrol, including greater plasma exposure, longer elimination half-life, and lower clearance. Also, Bojja's group recently reported that stilbene analogues having a nitrovinyl side chain attached to the aromatic ring (β -nitrostyrenes) have been reported as proapoptotic anticancer agents, and the nitrovinyl moiety was identified as the pharmacophore for the activities : potent tubulin polymerization inhibition and antiproliferative property. In this study, we have synthesized novel nitrovinyl-substituted trimethoxystilbene derivatives as a potent tubulin polymerization inhibitors and antiproliferative agents.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ORGN.P-900

발표분야: 유기화학

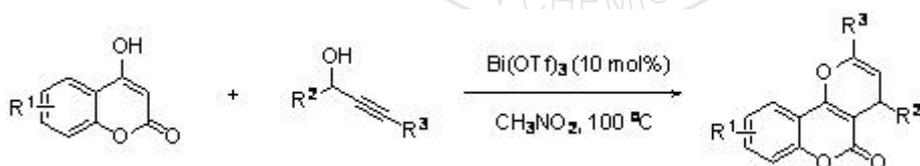
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of pyrano[3,2-c]coumarins via bismuth-catalyzed propargylation-cycloaddition tandem process between propargyl alcohols and 4-hydroxycoumarins

김재현 박정민 윤지희 이구연*

강원대학교 생명건강공학과

Pyranocoumarins are important class of heterocycles of wide occurrence in natural products as well as synthetic molecules, exhibiting a broad spectrum of biological activities such as antifungal, insecticidal, anticancer, anti-HIV, anti-inflammatory, and antibacterial activities. Herein, we have developed an efficient and highly regioselective tandem propargylation-cycloaddition of 4-hydroxycoumarins with propargyl alcohols catalyzed by $\text{Bi}(\text{OTf})_3$, which furnished various functionalized pyrano[3,2-c]coumarins in moderate to excellent yields.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-901**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A dendritic single-molecule fluorescent probe that is photostable and minimally blinking

양시경

전남대학교 화학교육과

Single-molecule fluorescence techniques have emerged as a powerful approach to understanding complex biological systems. However, a challenge researchers still face is the limited photostability of nearly all organic fluorophores. We have developed a new, monovalent probe that emits in the far-red region of the visible spectrum with properties desirable for single-molecule optical imaging. This probe is based on a ring-fused boron-dipyrromethene (BODIPY) core that is conjugated to a polyglycerol dendrimer (PGD), making the hydrophobic fluorophore water-soluble. This probe exhibits excellent brightness with an emission maximum of 705 nm. We have observed strikingly long and stable emission from individual PGD-BODIPY probes, even in the absence of anti-fading agents such as Trolox, a combined oxidizing/reducing agent often used in single-molecule studies for improving the photostability of common imaging probes. These interesting properties greatly simplify use of the fluorophore and overcome a significant obstacle in single-molecule fluorescence imaging.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-902**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Water-soluble ^{18}F -labeled prosthetic groups for facile bioconjugation with biomolecule

안혜진 지대윤^{1,*} 이병세²

서강대학교 유기화학 ¹서강대학교 화학과 ²(주)퓨처캡 표지화학연구소

Nucleophilic fluorinations of quaternary ammonium salt-containing sulfonate compounds were studied for fast and mild fluorination. The corresponding fluorinated compounds have water-soluble property, suited to bioconjugation in aqueous media because of quaternary ammonium salt functionality. A series of quaternary ammonium salt-containing sulfonate compounds were synthesized and fluorinated under mild condition, compared to a typical mesylate. As expected, the fluorinations of the new sulfonates in this study proceeded much faster (over several hundred times) than that of control mesylate compound due to ammonium salt moieties. The optimal sulfonate compound was radiofluorinated with F-18 in good yield. The bioconjugation of the resulting water-soluble ^{18}F -labeled compound to versatile biomolecules is now under investigation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-903**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct asymmetric aldol reaction using (L)-proline and isothiuronium salts

조은 김택현^{1,*}

전남대학교 신화학소재공학과 ¹전남대학교 응용화학공학부 광바이오사업단

The direct asymmetric aldol reaction constitutes one of the most powerful methodologies for the stereocontrolled formation of carbon-carbon bonds in the synthesis of chiral compounds. Isothiuronium salts have been explored quite recently as a new class of hydrogen-bonding subunit for anion recognition. Considering the probed ability of isothiuronium salts in anion recognitions, we contemplated the possibility of using isothiuronium salts as a novel activator in the aldol reactions. Co-catalytic system based on the combination of hydrogen-bond donation and chiral secondary amine catalysts for achieving highly enantioselective C-C bond formation. Herein, we report the results of the proline-catalyzed intermolecular direct aldol reaction between cyclohexanone and aldehydes using isothiuronium salts.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-904**

발표분야: 유기화학

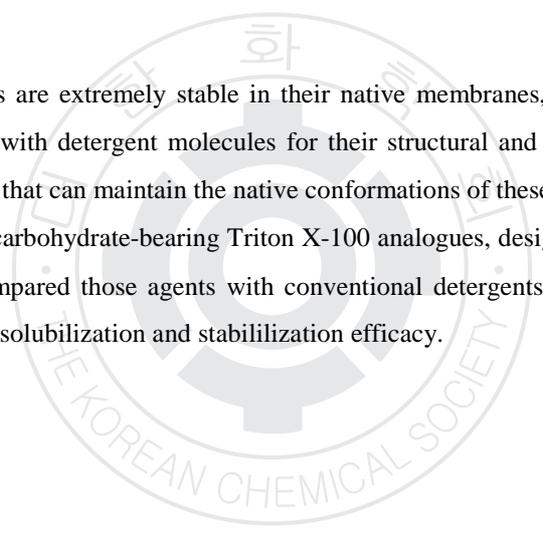
발표종류: 포스터, 발표일시: 수 16:00~19:00

Triton X-100 Analogues for Membrane Protein Study

배형은 채필석*

한양대학교 생명나노공학과

Integral membrane proteins are extremely stable in their native membranes, but tend to aggregate and denature when solubilized with detergent molecules for their structural and functional study. Thus, we need to invent novel agents that can maintain the native conformations of these bio-macromolecules. Here we designed and prepared carbohydrate-bearing Triton X-100 analogues, designated CGT (Chae's Glyco-Triton) detergents, and compared those agents with conventional detergents including Triton X-100 in terms of membrane protein solubilization and stabililization efficacy.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ORGN.P-905**

발표분야: 유기화학

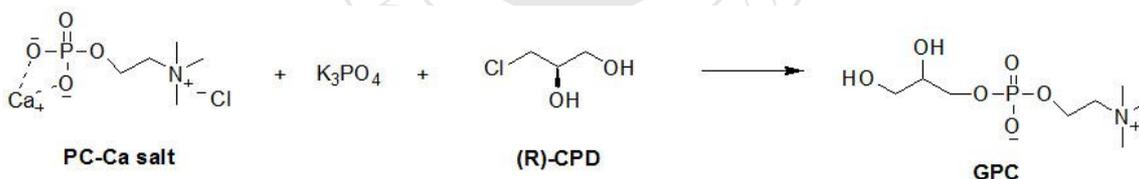
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot Synthesis of L- α -glycerophosphorylcholine(GPC)

안현석 이용우 이학준^{1,*}

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L- α -glycerophosphorylcholine(GPC), derived from soy lecithin is known for its use in the treatment of cerebrovascular disease, reduction of senile dementia (cognitive dysfunction) and also helps to improve learning ability and to promote non-REM sleep. The broad applications of GPC in medicine make its synthesis medicinally and industrially important. We report its efficient and economical one-pot synthesis from phosphorylcholine calcium salt and (R)-(-)-3-chloro-1, 2-propanediol followed by the purification using ion exchange resin to obtain pure L- α -glycerophosphorylcholine(GPC).



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

S-Benzyl isothiuronium iodide as an organocatalyst for the direct reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes using Hantzsch ester

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Reductive amination is one of the most powerful used methods of accessing different kinds of amines. In particular, when the carbonyl component is reacted directly with the amine and reducing agent, avoiding isolation of the imine intermediate. Hantzsch ester has 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 polyfunctional substrates. However, in some cases, this reducing agent was found to be ineffective without catalysis. Thioureas are powerful organocatalytic systems and can provide considerable reaction rate acceleration through hydrogen bond interactions. Isothiuroniums have been explored as prospective replacements of thioureas in the area of anion binding to enhance the acidity of the NH moieties and allow more hydrogen bonding. Isothiuronium salts have been explored quite recently as a new class of hydrogen-bonding subunit for the purpose of anion recognition. Herein, we will discuss the counter anions of S-benzyl isothiuronium effect the reaction rate and efficiency in the direct reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes using Hantzsch ester.

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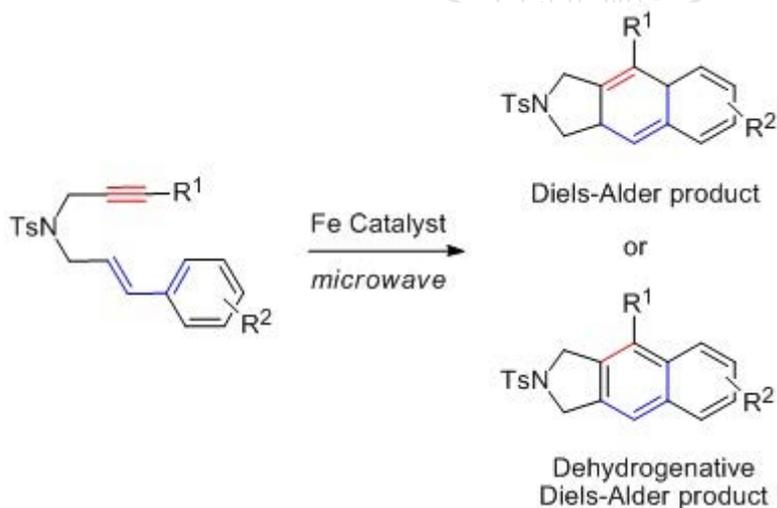
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fe-catalyzed dehydrogenative Diels-Alder reaction

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Iron salts can efficiently catalyze organic reaction as alternatives to traditional transition metal catalysts, showing advantages of being more sustainably produced and nontoxic. 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. Therefore, the quest to discover new variants of the Diels-Alder reaction remains important. The dehydrogenative cycloaddition of dieneynes, which possess a diene in the form of a styrene moiety and a dienophile in the form of an alkyne moiety, produces naphthalene derivatives when iron salt was used as a catalyst.



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E-beam Mediated Ligand Dissociation of Diyne-Dicobaltcarbonyl Complexes as Potential Photochemical Alkyne Precursor

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Arrayed alkynes on a solid surface have been used for electronic device coating, fluorescence nano-patterning, and surface reforming. In an effort to develop a photochemical alkyne precursor, we have synthesized diyne-cobalt complexes. We synthesize and studied diyne-cobalt complexes for this time. Diyne was synthesized from terminal alkyne by eglition coupling reaction. under e-beam irradiation diyne-cobalt complexes were fegmanteel into alkyne via CO ligand dissociation. These results suggested a potential application of the diyne-cobalt complex as alkyne precursor.

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발표코드: **MED.P-909**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of hybrid-nanocomposites for Diagnosis and treatment of tumor cells

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Hybrid nanocomposites have been widely used in medicinal chemistry, catalyst and industry. Using silica-gold, radioisotope can be used in the diagnosis and treatment of cancer is expected. Silica-gold nanocomposites were synthesized by template method, in order to increase water-soluble of nanocomposites using surfactant, its studies are in progress. Characterization of nanocomposites were measured by the XRD, SEM, TEM, Zetasizer, UV-Vis spectroscopy, ¹³C CP-MAS solid state NMR. The radioisotopes by the label on nanocomposites were used in PET (Positron Emission Tomography). ¹⁸F labeling multi-functional hybrid nanocomposites for PET imaging of breast cancer diagnostic reagents were used. In vitro, the accumulation on mouse colon cancer cell (CT-26) was observed by confocal laser scanning microscopy. In vivo, we confirmed that Silica-gold-¹⁸F used on the PET imaging. Later, the gold (¹⁹⁸Au) by neutron activation in a nuclear reactor for the treatment of cancer are expected to be available, in addition to other radioisotopes label as a drug for the treatment and diagnosis of cancer.

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발표코드: **MED.P-910**

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Synthesis of 5-HT₆ receptor PET Imaging probe precursors

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5-HT₆ receptors (5-HT₆R) are localized extensively in the brain. Antagonism of these receptors has been postulated to enhance cognitive performance. Evaluation of the 5-HT₆R expression and modulation in disease states, such as Alzheimer's, depression, or other forms of dementia could provide a valuable tool for probing the role of this target in these debilitating disease states. Positron emission tomography (PET) is a molecular imaging modality offering great promise for accelerating the process from preclinical discovery to clinical phases. Firstly developed 5-HT₆ imaging probe by GSK, [¹¹C]GSK215083 radiolabeled with [¹¹C] via methylation, is considered as a promising 5-HT₆ PET radioligand in vivo in humans. But [¹¹C]'s half life(T_{1/2} = 20.38min) is shorter than [¹⁸F](T_{1/2} = 109.8min), which limits its use to sites with a cyclotron and restricts PET studies to radiotracers of relatively fast kinetics. For this reason, the Flourine-18-labeled imaging probe is extensively needed, but the [¹⁸F] labeled 5-HT₆ probe has not been yet developed until recently. Therefore, we designed an [¹⁸F] labeled 5-HT₆ probe based on the GSK215083's structure, and synthesized two PET imaging precursors. One is nitro-precursor which enables to radio-lable by [¹⁸F] nucleophilic substitution. The other is tin-precursor which can be converted to radiofluorinated compound. In this presentation, the detailed synthetic adversities and overcomes will be discussed in this work.

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Discovery of Q203, a potent clinical candidate for the treatment of tuberculosis

강선희 서민정 서무영 서정제 이수미 강주희 고윤애 최인희 이진화¹ 김재승*

한국파스티르연구소 의약화학그룹¹ 한국파스티르연구소 late discovery program(LDP)

The most urgent clinical need is to discover potent agents capable of reducing the time of M-XDR tuberculosis therapy with a success rate comparable to susceptible tuberculosis. The last decade has seen the discovery of promising new agent classes for the management of tuberculosis, several of which are currently under clinical development. However, given the high attrition rate during clinical development and emergence of resistance, the discovery of additional clinical candidates is clearly needed. We reported on a promising class of ImidazoPyridine Amide (IPA) compounds that block Mycobacterium tuberculosis growth by targeting the respiratory cytochrome bc-1 complex. The optimized IPA compound Q203 inhibits the growth of M-XDR M. tuberculosis clinical isolates and was efficacious in vivo at a dose below 1 mg/kg, making this compound one of the most potent discovered to date. In addition, Q203 displays pharmacokinetic and safety profiles compatible with once daily dosing. Together, our data indicates that Q203 is a promising novel clinical candidate for the treatment of tuberculosis. (Nature Medicine, published online on August 4th, 2013, doi:10.1038/nm.3262)

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발표코드: **MEDI.P-912**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and SAR of urotensin-II receptor (UT) antagonists

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학

The urotensin-II (U-II), a cystein-linked cyclic undecapeptide, is widely expressed through cardiovascular, central nervous and renal system and is known as the one of the most potent vasoconstrictor. U-II ligand binds to an urotensin-II receptor (UT) as specific G-protein coupled receptor, which plays an important role in the regulation of cardiorenal function. In addition, UT is considered to be promising target for treating heart failure. As part of our ongoing drug discovery project on the the development of novel and potent UT antagonists, we previously found that several pyridine substituted derivatives exhibit highly potent UT binding activities. In order to more improve UT binding activity and proper pharmacokinetic properties, we further examined replacement of benzoxazinone with various aryl amide with holding pyridinyl substituted amine moiety. The synthesis biological evaluation and structure-activity relationship (SAR) results will be presented in detail.

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발표코드: **MED.P-913**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Cell test for synthesis of radiopharmaceuticals of tumor diagnosis

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Recently, the design of surface-modified nanoparticles have been interested greatly in nanobiotechnology (NBT) due to the major applications, such as contrast media. Among the various nanoparticles, iron oxide was used to have applications in tagging for biosensing, probe of drug delivery and contrast media for magnetic resonance imaging (MRI). This research was focus on developing of nano-bio targeting composites using Fe_3O_4 nanoparticles and Ga-68 radioisotope, which could be useful for therapy in hyperthermia and diagnosis in the fields of PET and MRI applications. The surface of Fe_3O_4 nanoparticles that are used MRI imaging and hyperthermia can be reformed by citric acid to increase hydrophilic property. Nano-bio targeting composites can be obtained by combining Fe_3O_4 nanoparticles and NOTA as bifunctional chelating agent with Ga-68 radioisotope.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Trifluoperazine(TFP) derivatives as new scaffold for glioblastoma

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Glioblastoma is the most common and aggressive primary brain tumor. Treatment of glioblastoma usually involves a multidisciplinary approach such as surgery, radiotherapy and chemotherapy. Temodar, one of the chemotherapeutic agent, extends survival period only by few months. Therefore, more effective chemotherapy is needed with better efficacy than Temodar for first-line. Calcium signaling is associated with many physiological processes in cancer cell proliferation and motility, and also involved in growth of glioblastoma. Based on this hypothesis, new derivatives as calmodulin inhibitors were prepared and examined. To obtain new and selective calmodulin inhibitors, trifluoperazine derivatives were designed and synthesized. A series of compounds was evaluated for in vitro assay using calcium imaging method. Compounds that showed activities above 70 % were evaluated further in vitro assay, MTT, NSC cell line and GBM 28 cell line. Further in vitro assay such as invasion, colony formation and in vivo assay using cancer disease animal model will be performed for several derivatives that showed comparable in vitro activities with reference compound.

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T-type Calcium Channel Blockers: Pyrrolidine Derivatives-Design, Synthesis and *In vivo* Assay

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Introduction : T-type calcium channels play a crucial role in pathologies including hypertension, heart failure, sleep disorders, epilepsy, drug addiction and neuropathic pain. Cav3.2 is the predominant T-type channel subtype in the dorsal root ganglion (DRG) with lower expression of both Cav3.1 and Cav3.3 detected. The major function of T-type Ca^{2+} channels in DRG sensory neurons is to support acute nociceptive signals. Cav3.2, therefore, is strongly implicated as contributing to the development of neuropathic pain. Objectives : The goal of this study is to identify compounds that block the Cav3.2 channels and to evaluate their *in vitro* and *in vivo* efficacies. Methods : Several pyrrolidine derivatives were designed using a 3D ligand based pharmacophore model. The synthesized compounds were evaluated *in vitro* in HEK293 cells which stably express both Cav3.1 and Cav3.2 using FDSS6000 assay and *in vivo* rat assay. Results : It was demonstrated that the *in vivo* efficacy of KKPG0001 is comparable to that of gabapentin with regard to two behavioral experiments (mechanical and thermal allodynia) in both the SNL model and STZ-induced diabetic neuropathy model.

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Acetylcholinesterase Inhibition Activity of Some Quinolinyl Substituted Triazolothiadiazole Derivatives

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A series of aralkanoic acids was converted into aralkanoic acid hydrazides through their esters formation. The aralkanoic acids hydrazides upon treatment with carbon disulfide and methanolic potassium hydroxide yielded potassium dithiocarbazinate salts which on refluxing with aqueous hydrazine hydrate yielded 5-aralkyl-4-amino-3-mercapto-1,2,4-triazoles. The target compounds, 3-aryl-6-(substitutedquinolinyl)[1,2,4]triazolo[3,4-b][1,3,4] thiadiazoles were synthesized by condensing various quinolinyl substituted carboxylic acids with 5-aralkyl-4-amino-3-mercapto-1,2,4-triazoles in phosphorus oxychloride. The structures of the newly synthesized compounds were characterized by IR, ¹H NMR, ¹³C NMR and elemental analysis. All the synthesized compounds were screened for their acetylcholinesterase inhibition activities. Some of the compounds exhibited excellent acetylcholinesterase inhibition activity as compared to the reference inhibitor.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-inflammatory and Anti-hyperglycemic Activities of Some New Triazole Derivatives

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A new series of 3,4-disubstituted 1,2,4-triazol-5(4H)-one, bearing various methoxyphenyl-, fluorophenyl- and tolyl groups, was synthesized by the dehydrocyclization of hydrazinecarboxamides by refluxing in 2N sodium hydroxide solution. Hydrazinecarboxamides was synthesized by the condensation of corresponding aralkanoic acid hydrazides with fluoro-, tolyl- and methoxyphenylisocyanates. The newly synthesized compounds were characterized by IR, ¹H NMR and ¹³C NMR analysis. All synthesized compounds were screened for their anti-inflammatory and anti-diabetic (α -glucosidase and α -amylase inhibition) activity in the perspective of identifying new drugs which might be useful in preventing the damages related to diabetes and inflammation. Some of the compounds showed excellent anti-inflammatory and anti-hyperglycemic activity.

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Regioselective one-pot synthesis of 1,4-disubstituted 1,2,3-triazoles from in situ generated potassium arylethynyltrifluoroborates

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1,4-Disubstituted 1,2,3-triazole derivatives, which are obtained from terminal alkynes and azides via 1,3-dipolar cycloaddition, are important small-molecule building blocks for complex compounds, and hence find significant application in organic synthesis, pharmaceutical sciences, and development of functional materials. Terminal alkynes are expensive, have low molecular weights and boiling point, have a short shelf life(storage-instable), and are difficult to handle; these problems hinder the widespread use of terminal alkynes as 1,3-dipolar cycloaddition partners of azides. Potassium arylethynyltrifluoroborates, the intermediates generated by the Sonogashira reaction of potassium ethynyltrifluoroborate with various aryl halides, were directly coupled with azides in the presence of a stoichiometric amount of CuI under aqueous conditions, and the desired 1,4-disubstituted 1,2,3-triazoles were isolated in good yields. Both electron-donating and electron-withdrawing substituents on the potassium arylethynyltrifluoroborates gave moderate-to-excellent isolated yields.

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4-Substituted Azetidine derivatives as triple reuptake inhibitor

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(KIST) 화학키노믹스연구센터 ³한국과학기술연구원(KIST) 생체과학연구부

Triple reuptake inhibitors (TRIs) are emerging a new therapeutic target for major depressive disorder by the inhibition of reuptake of three monoamine neurotransmitters (serotonin, norepinephrine and dopamine) in a synapse. As a part of our continuing efforts to develop of new TRIs, we designed 4-substituted azetidine derivatives by a structure analysis and a molecule modification of the fifteen kinds of commercially available antidepressant in the market. Syntheses of target compounds considering a chemical diversity and their inhibitory reuptake activities against three monoamine neurotransmitters will be presented. Herein we will also report their structure-activity relationship. A few compounds showed better TRIs biological activity than that of previously reported compounds.

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발표코드: **MEDI.P-920**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and synthesis of novel 3-aminoazetidine derivatives as triple reuptake inhibitor

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Major depressive disorder is a common and serious illness with the potential to become the leading cause of disability worldwide. An important recent development in antidepressant therapy has been achieved with the discovery of triple reuptake inhibitors (TRI), broad spectrum antidepressants that are capable of inhibiting the reuptake of neurotransmitters (5-HT, NE or DA) by one molecule. However, any TRI is not yet available in the market. As a part of our continuing efforts to develop novel TRI, we designed 3-aminoazetidine derivatives by the structure analysis and molecular modification of compounds which possess antidepressant activity and TRI pharmacophore modeling. Herein we will report synthesis of target compounds and their biological activities against 5-HT, NE or DA reuptake inhibition as well as their structure-activity relationship.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Mitochondrial dysfunction modulator for Alzheimer's disease

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Alzheimer's disease (AD) is the most common form of dementia but doesn't have any therapeutic agent till now. According to the pathophysiology research, amyloid β -protein ($A\beta$) aggregation, called senile plaque, is reported as the most powerful cause of AD. In normal neuronal cells, mitochondrial permeability transition pore (mPTP) is supposed to be closed. But binding $A\beta$ to Cyclophilin D (Cyp D) can promote calcium-induced mPTP opening. That results in mitochondrial dysfunction and eventually leads to apoptosis. Interaction between Cycloporin A (CsA) and Cyp D which is an isoenzyme of cyclophilin family blocks mPTP. Cyclophilin A (Cyp A) is also a subtype of cyclophilin families and has a high affinity with CsA. Based on these findings, the development of mPTP blockers were designed from Cyp A inhibitor. In this research, overall 51 compounds were synthesized as mPTP blockers and evaluated for JC-1 assay. Further study will proceed to find new hit compound for AD and these new approach will be guidelines to obtain mPTP blockers with novel made of acting for Alzheimer's disease.

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발표코드: **MEDI.P-922**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Arrest of Peroxiredoxin Repair Achieved by Putative Allosteric Inhibition of Sulfiredoxin

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Peroxiredoxins (Prxs), one type of the antioxidant peroxidases in the cells, are thioredoxin-dependent peroxidases which play a crucial role in decreasing reactive oxygen species (ROS) levels in the cells. 2-Cys Prxs undergo oxidation of their thiols by reacting with hydrogen peroxide (H₂O₂) yielding cysteine sulfenic acid (Cys-SPOH). Under the moderate ROS levels, the sulfenic acid undergoes reduction by thioredoxin (Trx) through a disulfide intermediate. Whereas, when ROS levels increased above certain levels, the cysteine sulfenic acid Prx (Cys-SPOH) can be oxidized into sulfinic acid (Cys-SPO₂H) showing loss of its antioxidant function. Since sulfiredoxin (Srx), a 2-Cys Prx sulfinic acid-reducing protein enables 2-Cys Prxs to maintain antioxidant capacity, Srx plays an important role in regulating ROS levels in the cells. The fact that cancer cells are more dependent on their antioxidant system and the function of Srx suggests a novel approach for the development of anticancer drugs by increasing oxidative stress in cancer cells. In order to sieve Srx inhibitor molecules, we conducted high-throughput screening (HTS) and obtained a lead compound (J14). Molecular docking onto Srx was performed and novel derivatives were designed. Among the newly synthesized molecules based on the ligand binding mode, LMT-328 showed the most potent inhibitory activity (IC₅₀=6.7μM) as well as the best growth inhibitory activities against several cancer cell lines. Molecular modeling studies suggested the hypothetical arrest of Prx sulfinic acid reduction through Srx inhibition. It is thought that LMT-328 tightly binds into the hydrophobic pocket of the Srx surface rather than the ligand binding site. In addition, further studies with the crystal structure of Srx?Prx I complex substantiated that the allosteric inhibition of Srx could result in the arrest of Prx repair mechanism. These in silico and in vitro data suggest a novel approach for anticancer chemotherapy. More detailed result will be presented in the presentation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Target identification of an imidazopyridine amide (Q203) as a novel anti-Tuberculosis agent: homology modeling and docking of the Cytochrome bc1 complex

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Tuberculosis caused by *Mycobacterium tuberculosis* (TB) is considered as a disease that is under control but it is still being a serious world health problem. Despite of the availability of effective chemotherapy, multiple-drug resistant TB (MDR-TB) and extensively-drug resistant TB (XDR-TB) strains are rapidly arising. Consequently, there is an urgent need for an effective drug against MDR-TB and XDR-TB strains. Imidazo pyridine amide (IPA) series was identified via high-contents screening (HCS) as a highly effective TB agent which is also active against MDR-TB and XDR-TB. The cytochrome b subunit of the cytochrome bc1 complex (QcrB) was identified as a drug target in TB (Rv2196) for IPA compounds by generating spontaneous mutants. Subsequently, the substitution of Thr313 into Alanine confirmed resistance to activity of IPA compounds, especially Q203. In addition, the rapid ATP depletion by Q203 in TB grown under both aerobic and anaerobic conditions confirmed that the primary mode of action of Q203 is the inhibition of cytochrome bc1 activity. Herein, we built the homology model of TB QcrB based on the sequence similarity with other species' cytochrome bc1 complex of x-ray structures: *Rhodobacter sphaeroides*, *Paracoccus denitrificans*, yeast and bovine. The overall 3D structure of TB QcrB model was similar to those of known structures. From the structural validation results, the model with the best quality was selected for docking. These insightful information will be beneficial to the further development of IPA series as novel anti-tuberculosis drugs.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-speed, Microwave-assisted Combinatorial Chemistry of Novel 1,3,4-Oxadiazole Drug-like Library

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Recently, combinatorial chemistry has become a powerful strategy in medicinal chemistry. In an effort to make various drug-like library, we studied thiohydantoin-containing 1,3,4-oxadiazole derivatives based on the combinatorial chemistry. 1,3,4-Oxadiazole moiety has been reported to produce substances of interest in numerous biological areas, such as anti-inflammatory, antimicrobial, anticonvulsant, and antihypertensive. In this reason, we were highly interested in the 1,3,4-oxadiazole moiety and we tried to establish the thiohydantoin-containing 1,3,4-oxadiazole libraries. At first, we screened various kind of reagent such as *p*-TsCl, TMSCl, EDC·HCl and POCl₃ to formate desired 1,3,4-oxadiazole moiety from semicarbazide. As a result of this screening, POCl₃ was the most effective reagent and it showed us less byproduct. However, formation of 1,3,4-oxadiazole moiety with POCl₃ required long reaction times and relatively high temperature. So, we employed microwave-assisted synthesis in order to formate desired 1,3,4-oxadiazole moiety. In this way, we synthesized the 1,3,4-oxadiazole with minimized byproduct and reduced the reaction times effectively.

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장소: 창원CECO

발표코드: **MEDI.P-925**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Construction of Drug-like 1,3,4-Oxadiazole Analogues Library via Solid-Phase Organic Synthesis

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동국대학교 화학과

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 have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as antiinflammatory, antimicrobial, anticonvulsant, and antihypertensive. In addition, these heterocycles serve as intermediates in the preparation of various biologically important compounds. In this reason, we developed synthetic method of 1,3,4-oxadiazole analogues on the solid-phase. The key step on this solid-phase synthesis involves the preparation of polymer-bound 2-amino-1,3,4-oxadiazole resin by cyclization reaction of thiosemicarbazide resin. The thiosemicarbazide resin is produced by addition of various benzhydrazide to the isothiocyanate-terminated resin and serve as a key intermediate for the linker resin. This core skeleton 2-amino-1,3,4-oxadiazole resin undergoes functionalization reaction with various electrophiles such as alkyl halide and acid chloride to generate N-alkylamino and N-acylamino-1,3,4-oxadiazole resin respectively. Finally, 2-amino and 2-amido-1,3,4-oxadiazole derivatives are then generated in good yields and high purities by cleavage of the respective resin under trifluoroacetic acid(TFA) in dichloromethane(DCM).

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발표코드: **MED.P-926**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of a Novel Drug-like 2,5-Piperazinedione Derivatives Using Various Amino Acids by Microwave-assisted Organic Synthesis

이석형 이지형 곽세훈 공영대*

동국대학교 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for six-membered ring heterocyclic compound, which are core components of a large number of substances that possess a wide range of interesting biological activities. The potential of the piperazinedione scaffold to serve as a privileged structure for the generation of drug-like libraries in drug discovery programs has been plentifully demonstrated in medicinal chemistry. Piperazinedione is a class of compounds which are of significant interest in biology and drug discovery. Their peculiar heterocyclic system found in several natural products constitutes a rich source of new biologically active compounds. The wide range of their biological properties points to various therapeutic possibility. Some of the most important biological activities of piperazinedione are related to the inhibition of plasminogen activator inhibitor-1 (PAI-1) and alteration of cardiovascular and blood-clotting functions. And then compounds containing amino acids are attractive class of scaffolds in drug research, due to its chiral nature, rigid structure. Also it was well known that the use of microwave ovens dramatically accelerated the rate of many organic reactions. Since then, microwave heating has been applied not only to reduce reaction times but also to improve yields and selectivity. Therefore we have concentrated our efforts on describing a solution-phase strategy for the preparation of a small molecule library based on the piperazinedione by using microwave reaction. As a result, we reported a useful method for the synthesis of 1-(1,3,4-oxadiazol-2-yl)piperazine-2,5-dione derivatives using various amino acids and several residue.

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장소: 창원CECO

발표코드: **MEDI.P-927**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of N-Substituted-4H-benzo[d][1,3]thiazin-2-amine Derivatives on BAL Resin

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동국대학교 화학과

Solid-phase Synthesis has become an extremely powerful technique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. Therefore, we have been exploring the potential of resin-bound benzo[d][1,3]thiazine derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Especially, we were interested in construction the various N-substituted-4H-benzo[d][1,3]thiazin-2-amine library because of their broad biological activities such as antitumor, cardiovascular, neurodegenerative pathologies, antiproliferative activity. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of N-substituted-4H-benzo[d][1,3]thiazin-2-amine library through resin-bound benzo[d][1,3]thiazine on BAL resin.

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장소: 창원CECO

발표코드: **MEDI.P-928**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-inflammatory Activity of *N*-(2,2-Disubstituted-2*H*-cromene-6-yl)-*N'*,*N''*-disubstituted-guanidine Derivatives

이지형 김하영 공영대*

동국대학교 화학과

Inflammation is a kind of immune response such as pathogens, damaged cells, or irritants and a protective attempt by the organism to remove the injurious stimuli. Chronic inflammation can also lead to a host of diseases, such as hay fever, periodontitis, atherosclerosis, rheumatoid arthritis, and even cancer. Asthma is a common chronic inflammatory disease of the airways characterized by variable and recurring symptoms, reversible airflow obstruction, and bronchospasm. The enzyme GSNO reductase (*S*-nitroglutathion reductase; GSNOR) is an important in the metabolic regulation of *S*-nitroglutathion that is a endogenous bronchodilator and maintenance of nitric oxide(NO). According to reports in animal models using ovalbumin as antigen, volume of GSNOR increased at respiratory tract. Consequentially, volume of GSNO decreased. N30 Pharmaceuticals have conducted clinical testing of N6022 as a potential inhibitor of GSNOR. In that regard, we concentrated our effort to construction of a novel small organic drug-like lead compound without side-effect of existing anti-inflammatory drugs. Herein we report our recent progress on this project, which includes the construction of benzopyran coreskeleton library as commonly scaffolds on which pharmacophores are arranged to provide potent and selective drugs. As a result, we synthesized *N*-(2,2-Disubstituted-2*H*-cromene-6-yl)-*N'*,*N''*-disubstituted-guanidine Derivatives

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI.P-929**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid-phase Organic Synthesis of Drug-like 1,3,4-Thiadiazole Analogues via Desulfurative Cyclization of Thiosemicarbazide Intermediate

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동국대학교 화학과

Solid-phase synthesis has been situated in powerful technique for the generation of drug-like small organic molecule libraries in medicinal chemistry. And Heterocyclic compounds play a role as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. Especially, core components containing five-membered ring hetero cyclic compounds have a wide range of interesting biological activities. In a preceding study, 1,3,4-oxadiazole analogues shown potent biological activity in Wnt signaling which has been regulate cell proliferation, differentiation and morphogenesis. In this respect, we have a interest in synthesis both 1,3,4-oxadiazole and 1,3,4-thiadiazole as a bioisostere. However, we couldn't obtain 1,3,4-thiadiazole analogues in our previous study. In this reason, we tried to develop another synthetic method. Herein, we report our new synthetic strategy to synthesize 1,3,4-thiadiazole analogues on the solid-phase.

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발표코드: **MED.P-930**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of Novel 3-Arylethynyl-substituted Thieno[3,4-*b*]pyrazine Derivatives as a Human Transglutaminase 2 Inhibitor

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Transglutaminase 2 (TGase 2) is a calcium dependent multifunctional enzyme, of which functions generally involve either the protection or prevention of body injury, or tissue assembly and repair. It catalyzes various post-translational modifications including amine incorporation, deamination, protein crosslinking formed by acyl transfer reaction between the amino group of protein and the carboxyl group of a glutamine. TGase 2 is related to various diseases including Celiac disease, Huntington's disease, inflammation, neurodegenerative diseases, diabetes and cancers. Specially, TGase 2 is associated with drug resistance of cancer cell. Through activation of nuclear factor- κ B (NF- κ B), TGase 2 expression is closely associated with NF- κ B activity in drug-resistant breast cancer cells. And, in turn, NF- κ B activation gives cancer cells resistance against the apoptotic chemotherapeutic agents. In agreement to the reports described above, TGase 2 inhibitor has shown to reduce NF- κ B activity of cancer cells in a dose dependent manner. We screened 1000 small heterocyclic compounds and identified the five number of 3-arylethyl thieno[3,4-*b*]pyrazine derivatives as Transglutaminase 2(TGase 2) inhibitors. In the optimization process, we developed a novel core skeleton of thieno[3,4-*b*]pyrazine via the GK-13 compound. These derivatives were shown to inhibit TGase 2 activity in cancer cells. Some of the hit compounds such as the arylethynyl group-coupled thieno[3,4-*b*]pyrazine derivatives were shown to hold promise for use as potential therapeutic small-molecules in renal cancer by inhibiting TGase 2 activity.

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발표코드: MED.P-931

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Disruption of Interactions between Hydrophobic Residues on Nonpolar Faces is a Key Determinant in Decreasing Hemolysis and Increasing Antimicrobial Activities of α -Helical Amphipathic Peptides

이유리 현순실 유재훈*

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Owing to the fact that they have amphipathic character, most cationic antimicrobial peptides facilitate the disruption of membranes in pathogens. However, because of this property, these types of peptides also cause disruption of host cell membranes, giving rise to severe side effects. With the goal of designing side effect-free antimicrobial peptides, an amphipathic α -helical peptide composed of Leu and Lys (LK) was selected and mutated with a variety of amino acids to reduce its hemolytic activity. In this series, the mutant LK-L8N was observed to have more than an 8,000-fold reduced hemolytic activity. Surprisingly, LK-L8N also displays an 8-fold improved antimicrobial activity against *E.coli*, affording a 64,000-fold increased therapeutic index. This strategy was applied to the truncated version of a natural cationic antimicrobial peptide, LL-37, which also possesses segregated amphipathic α -helices. Incorporation of hydrophilic residues on the hydrophobic face of LL-37 leads to an approximate 8-fold reduction in its hemolytic activity and a retained antimicrobial activity against *E.coli*, which corresponds to an 8-fold increase in its therapeutic index. Disruption of the segregated hydrophobicity by incorporation of neutral hydrophilic residues induces a significant reduction of the α -helicity and hydrophobicity of amphipathic peptides. Both of these changes are reflected in reduced hemolytic activities, while not affecting or increasing the specificity determinant against *E.coli*. The strategy employed in this investigation could be generally useful in the design of side effect-free antimicrobial peptides.

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장소: 창원CECO

발표코드: **MED.P-932**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemical suppression of AIMP2-DX2, oncogenic splicing variant

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Aminoacyl-tRNA synthetase-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. We found that a series of maleic acid derivatives inhibited the expression of AIMP2-DX2 through selective degradation of AIMP2-DX2 mRNA transcript. Herein, we report that 1) how new scaffolds were designed and validated; 2) optimization process through 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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발표코드: **MED.P-933**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of natural product inhibitors against Hsp90 folding machinery

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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 EGFR 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. 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 six essential hallmarks of cancer, including EGFR, Her2, Met, Akt, Raf, HIF-1 and MMP2. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways. Kava (*Piper methylsticum*) is a native plant traditionally used as a medicine and social drink in the South Pacific islands, including Fiji, Vanuatu and Western Samoa. Flavokawain B, one of chalcone component isolated from kava extract, has been reported to exhibit strong anti-proliferative effects against several cancer cell line. In this study, we discovered that a natural product, flavokawain B disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer (H1975). The result suggested that flavokawain B could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

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발표코드: **MED.P-934**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Purification and Structure Determination of anti-oxidative and anti-cholinesterase compounds from *Sargassum ringgoldianum*

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In our continuing search for anti-oxidative and anti-holinesterase compounds from marine alga, *Sargassum ringgoldianum* was examined and here we report the progress on the purification and biological activities of the purified compounds. From the 100 % methanol extract of *S. ringgoldianum*, solvent partition fractions were prepared by using n-hexane, chloroform, butanol and water, and among them chloroform fraction showed strong anti-oxidative and BuChE inhibitory activities. The chloroform fraction of *S. ringgoldianum* showed about 56 % DPPH radical scavenging activity and 86 % BuChE inhibitory activity at 0.1mg/mL. Using various chromatographic methods and by the bioassay-guided fractionation, the chloroform fraction was separated into five fractions, and each fraction showed anti-oxidative activity as 56.0, 72.0, 77.9, 43.7, 31.5% at 0.1mg/mL, respectively. Among them, the most anti-oxidative fraction 3 was further purified by HPLC and the structure determination and biological activities of the purified compound will be reported. * BuChE : butyrylcholinesterase

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장소: 창원CECO

발표코드: **MED.P-935**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of mGluR1 Negative Allosteric Modulators for treatment of CNS disorders

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Glutamate is one of the neurotransmitters that exhibit excitatory effect in central nervous system and peripheral nervous system. Glutamate receptors are related to mediate glutamate for post-synaptic excitation in neural cell. Thus, they are involved in pathologies of many brain diseases. There are two types of glutamate receptors depending on their mechanism of activation; ionotropic glutamate receptors (iGluRs), metabotropic glutamate receptors (mGluRs). There are eight mGluRs classified into three groups based on pharmacology and signal transduction mechanism. Among them, Group I mGluRs have been implicated in the pathogenesis of several diseases. In particular, it has been reported that knockdown of spinal mGluR1 alleviates neuropathic pain in SNL rat model. Therefore, negative allosteric modulators (NAM's) of mGluR1 will be potential therapeutic candidates for the treatment of neuropathic pain. In this presentation, we will present novel quinolines/quinazolines as selective mGluR1 NAM's. The preliminary result of in vitro assay against mGluR1 through high throughput screening system and their structure-activity relationship will be discussed.

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장소: 창원CECO

발표코드: **MED.P-936**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of the 2,4-disubstituted phenols as Pim kinase inhibitors

박종성 HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

The Pim protein kinases are frequently overexpressed in leukemia, lymphoma and solid tumors such as prostate cancer. Pim kinases are serine/threonine kinases that are involved in the control of cell growth, survival, apoptosis and differentiation. So, pim kinases are a very promising therapeutic target for the treatment of cancer. The present report describes the discovery of pim kinases inhibitors with high potency. Novel series of 2,4-disubstituted phenols derivatives were designed and synthesized. Compounds showed potent inhibitory activity against Pim kinases. The most potent compound exhibited IC50s of 0.5 nM for Pim-1, 1.4 nM for Pim-2 and 0.5 nM for Pim-3.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-937**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of 2-acetamidothiophene-3-carboxamide derivatives against *Leishmania donovani*

오상미 권보성 공선주 이진화¹ 송릿다*

한국파스티르연구소 의약화학 연구실 ¹한국파스티르연구소 late discovery program(LDP)

Leishmaniasis is one of the most neglected tropical diseases caused by *Leishmania*, a protozoan parasites transmitted by the bite of female phlebotomine sandflies.¹ More than 1.2 million people worldwide are estimated to be infected by *Leishmania* and more than 50,000 deaths are reported every year. Despite efficacy for leishmaniasis with some of the current drugs on the market, there are urgent unmet medical need due to the low efficacy, high toxicity, difficult administration, and emergence of drug resistant parasites. Here, we report the synthesis and anti-leishmanial activities of 2-acetamidothiophene-3-carboxamide derivatives which were tested against both *L. donovani* promastigotes and intracellular amastigotes.² A high-throughput (HTS) and high-content screening (HCS) campaign of a commercial library identified this scaffold as a novel class of anti-leishmanial agents. A series of chemical modification was done in three parts and the compounds were evaluated their anti-leishmanial activities *in vitro* against not only extracellular promastigotes but also intracellular amastigotes. Compounds 6a showed promising anti-amastigote activity (EC₅₀, 6.41 μM) against *L. donovani* without any cytotoxicity (CC₅₀, > 50 μM) toward human macrophages. [Reference]1. Akopyants, N. S.; Kimblin, N.; Secundino, N.; Patrick, R.; Peters, N.; Lawyer, P.; Dobson, D. E.; Beverley, S. M.; Sacks, D. L. Science 2009, 324, 265.2. Siqueira-Neto, J. L.; Moon, S.; Jang, J.; Yang, G.; Lee, C.; Moon, H. K.; Chatelain, E.; Genovesio, A.; Cechetto, J.; Freitas-Junior, L. H. PLoS Negl. Trop. Dis. 2012, 6, e1671.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-938**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of substituted pyrazol-4-yl pyridazinone derivatives as novel c-Met kinase inhibitor

강승태 김은영¹ 강가애² 정희정³ 김형래³ 하재두^{3,*} 조성윤^{3,*}

성균관대학교 ¹성균관대학교 화학과 ²한국화학연구원 난치성질환치료제연구그룹 ³한국화학연구원 난치성질환치료제연구센터

Receptor tyrosine kinase (RTK) family is an attractive target for cancer therapy. c-Met kinase is a member of this family with its ligand, hepatocyte growth factor (HGF) or scatter factor (SF) which is crucial for normal mammalian development. c-Met is known to be over-expressed and mutated in a variety of human cancer types. c-Met is accountable proliferation, scattering, invasion, and metastasis of tumor cells. In an effort to search c-met kinase inhibitors, substituted pyrazol-4-yl pyridazinone derivatives were synthesized and evaluated toward c-Met kinase inhibitory activity. Some of the compounds displayed excellent activity in vitro enzymatic and cell-based assay.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-939**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anaplastic Lymphoma Kinase (ALK) inhibitors for Cancer Treatment

latifmuhammad 이광호^{1,*} 김형래² 채종학³ 윤창수⁴

과학기술연합대학원대학교(UST) 의약화학 ¹한국화학연구원 신물질본부/난치성 ²한국화학연구원
난치성질환치료제연구센터 ³한국화학연구원 신물질연구본부/신약플랫폼기술팀 ⁴한국화학
연구원 신약연구본부 의약화학연구센터

Anaplastic lymphoma kinase (ALK) is a receptor tyrosine kinase (RTK) belonging to the insulin receptor superfamily and was first identified as a part of NPM-ALK fusion protein derived from a chromosomal translocation detected in anaplastic large cell lymphoma (ALCL) patients. EML4-ALK, the fusion of ALK gene with echinoderm microtubule-associated protein-like4 (EML4), has been identified in Japanese non-small cell lung cancer patients during Crizotinib (Xalkori?, Pfizer) clinical study. Recently many other ALK-fusion proteins have been reported such as FN1-ALK responsible to ovarian cancer, TPM3-ALK to inflammatory myofibroblastic tumors (IMT), KIF5B-ALK to NSCLC and so on. Despite of dramatic response to Crizotinib, Crizotinib resistant ALK gene mutation occurs within a year including ALK L1196M, F1174L, R1275Q and G1269S and so on. To address this limitation, new ALK inhibitors have been studied and under development. Herein, we wish to report recent KRICT ALK study.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-940**

발표분야: 의약화학

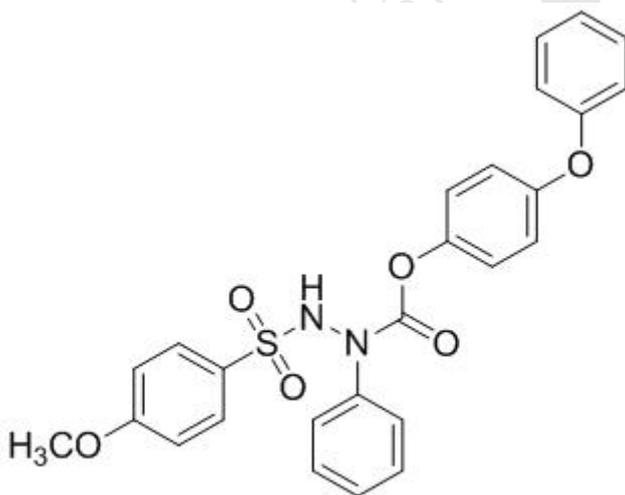
발표종류: 포스터, 발표일시: 수 16:00~19:00

***N*-Sulfonyl-*N'*-phenoxy-carbonylhydrazine Derivatives as a Novel Class of mPGES-1 Inhibitor**

강승목 주동준 이재열*

경희대학교 화학과

N-Sulfonyl-*N'*-phenoxy-carbonylhydrazine Derivatives were synthesized and evaluated for the inhibitory activities on LPS-induced PGE₂ production in RAW 264.7 macrophage cells. Hydrazine as main scaffold was easily obtained using one of three synthetic methods. Among the compounds investigated, 4-Phenoxyphenyl 2-((4-methoxyphenyl)sulfonyl)-1-phenylhydrazinecarboxylate (MPO-0052) showed a strong inhibitory activity (IC₅₀ = 17.06 nM) of PGE₂ production.



MPO-0052 (IC₅₀ = 17.06 nM)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-941**

발표분야: 의약화학

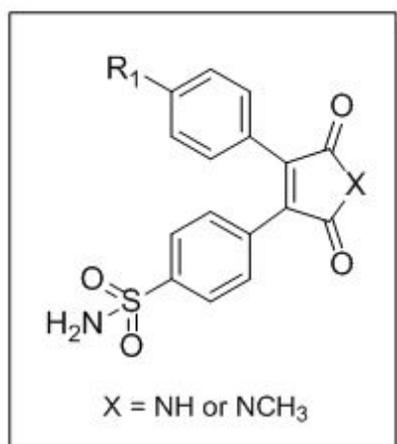
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Pharmacological Evaluation and Molecular Docking Study of Pyrrole-2,5-dione Derivatives as Selective COX-2 Inhibitor

이진성 주동준 이재열*

경희대학교 화학과

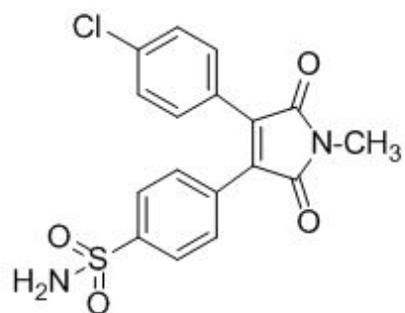
A series of pyrrole-2,5-dione derivatives was synthesized and evaluated for COX-1/COX-2 inhibition and PGE2 production inhibition. Compounds MPO-0024, MPO-0025, MPO-0029 were proved to be potent COX-2 inhibitors with IC₅₀ range of 5.95-85.05 nM. In vitro COX-1/COX-2 inhibition studies identified compound MPO-0029 as highly potent (IC₅₀=5.95 nM) and an extremely selective [COX-2 (SI) > 1,000] compared to celecoxib [COX-2 (SI) = 110]. A molecular modeling study was carried out through docking MPO-0029 into the COX-2 binding site to predict if this compound has analogous binding mode to the COX-2 inhibitors. Molecular modeling (docking) study showed that MPO-0029 inserted deep inside the pocket of the COX-2 active site. It formed six hydrogen bonds with Leu338, Ser339, Gln178, Phe504, Arg499 and Ser516. As a result, docking study of MPO-0029 into the active site of COX-2 revealed a similar binding mode to celecoxib, a selective COX-2 inhibitor.



Compound library

Screening

for PGE₂
production
inhibition &
COX-2



MPO-0029

IC₅₀ = 5.95nM against COX-2



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI.P-942**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Molecular Docking Study Azaindole Derivatives as a JAK1 Inhibitor

신희립 김미경 정유훈*

건국대학교 생명공학과

The discovery of somatic Jak1 mutations in patients with various cancers has led to significant interest in discovering selective Jak1 inhibitors for use in treating these disorders. A series of azaindole derivatives has been designed and synthesized as inhibitor of Janus kinase 1. The molecular docking study was also performed to elucidate the molecular mechanism of the JAK1 inhibitory potency of azaindole derivatives. The results indicated that azaindole derivatives interact with the key amino acid residues at the ATP binding cavity of JAK1 protein. The 1-amino and 7-amino groups of the azaindole bind to the hinge part of the kinase through two hydrogen bonds with adjacent backbone amides (Glu957, Leu959). The compound is further evaluated for its biological activity to lead to the discovery of potent JAK1 kinase inhibitor.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI.P-943**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of safe and effective polyphenol conjugate-based chemosensitizers for reversing multidrug resistance

김미경 정유훈*

건국대학교 생명공학과

Multidrug resistance (MDR) is a severe impediment to successful chemotherapy of cancer, which refers to cancer cells exhibiting simultaneous resistance to several structurally unrelated drugs of no common mechanism of action. MDR cancer cells are known to be sensitized to anticancer drugs when treated with a P-gp inhibitor, called a chemosensitizer. The first-generation chemosensitizers showed side effects at doses required for clinical effect. Thus, development of new chemosensitizers with higher selectivity and potency has been in demand. The search for chemosensitizers with advantages of stability with low toxicity has led much of the research interests to polyphenol. In this study, novel polyphenol conjugates were designed, synthesized, and evaluated for their cytotoxicity and multidrug resistance-reversing activity in in-vitro assay systems. The chemosensitizing activities of the polyphenol conjugates against representative human sarcoma cells (MES-SA) and doxorubicin-resistant human sarcoma cells (MES-SA/Dx5), which overexpress the MDR/P-gp drug efflux pump responsible for drug resistance, were evaluated by MTT assay. Treatment of drug-resistant MES-SA/Dx5 cells with polyphenol conjugates completely restored the cytotoxic effect of doxorubicin against resistant cancer cells at 5 μM . In particular, two quercetin conjugates, Q-7-O-POM ($\text{IC}_{50}=5.3 \mu\text{M}$) and Q-7-O-Glu ($\text{IC}_{50}=1.7 \mu\text{M}$), showed MDR-reversal activity similar to that of verapamil ($\text{IC}_{50}=0.7 \mu\text{M}$), a wellknown MDR modulating compound. Q-7-O-POM and Q-7-O-Glu showed increase Rh123 accumulation in MDR cells, which suggests that these compounds may act by inhibiting the P-gp transport activity. Design, synthesis, and MDR-reversing activities (in vitro and in vivo) of the polyphenol conjugates would be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-944**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The analysis of water network for kinase selectivity

장우대 강남숙*

충남대학교 신약전문대학원

We carried out the effect of water molecules correlated with hydrophobic environment by analyzing hydrogen-bonded water network using molecular dynamics simulations to explain kinase selectivity within two example systems, a variant of Gleevec and a series of substituted JNK ligands. We carried out the analysis of five-membered ring (R5) structure for water molecules, which is a dominant structure in aqueous solutions containing hydrophobic solutes due to hydrophobic effects. The patterns of water network using R5 structure are well mapped to the selective activity profile for the kinase inhibitors.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-945**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study on the heterocyclic compounds for the application to protein kinase inhibitor generating

문지영 송치만¹ 정낙철 정찬성^{1,*}

고려대학교 화학과 ¹한국과학기술연구원(KIST) 화학키노믹스연구센터

Diversification of small molecule is one of the key step in drug discovery. As a target of anticancer drug, protein kinases are involved in cellular signaling, homeostasis, cell growth and development. Therefore, it is possible that the anticancer effect can be obtained by inhibiting these actions by well-modulated small molecule. Among various kinds of molecular scaffolds, pyrimidine derivatives have been used as the kinase inhibitor of PI3K, Btk, etc. In the previous our studies in the new drug development, pyrimidine derivatives have shown high biological activities and beneficial physical properties, bioavailability. Based on these data, we have synthesized several heterocyclic compounds using pyrimidine analogue as starting material, which was transformed by anionic alkylation, oxidation and cyclization. During these progresses, reaction condition and new synthetic methods were investigated. These synthesized compounds will be tested for kinase inhibition capability.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-946**

발표분야: 의약화학

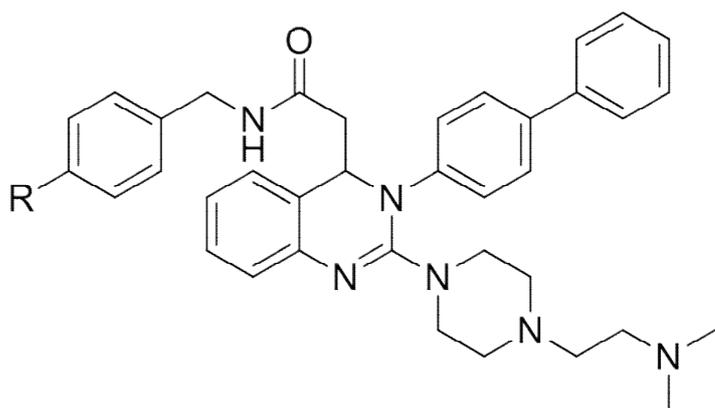
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cell Cycle Arrest and Anticancer Effect on Human Ovarian Cancer Cells by T-Type Calcium Channel Blockers

조세현 주동준 이재열*

경희대학교 화학과

The growth inhibition of human cancer cells via T-type Ca^{2+} channel blockade has been well known. Herein, a series of new 3,4-dihydroquinazoline derivatives were synthesized via a brief SAR study on KYS05090 template and evaluated for both T-type Ca^{2+} channel (Cav3.1) blockade and cytotoxicity on three human ovarian cancer cells (SK-OV-3, A2780 and A2780-T). Most of compounds except 6i generally exhibited more potent cytotoxicity on SK-OV-3 than mibefradil as a positive control regardless of the degree of Ttype channel blockade. In particular, eight compounds (KYS05090, 6a and 6c-6h) showing strong channel blockade ($>45\%$ @ $1 \mu\text{M}$) exhibited almost equal and more potent cytotoxicity (IC_{50} values of 1.06-1.65 μM) on A2780 when compared to mibefradil (IC_{50} value of 24.23 μM). On A2780-T paclitaxel-resistant human ovarian carcinoma, two compounds (KYS05090 and 6d) were 20-fold more active than mibefradil. With respect to cell cycle arrest effect on A2780 and A2780-T cells, KYS05090 induced large proportion of sub-G1 phase (71.4 and 95.4 % @ 8 μM , respectively) in the cell cycle progression of A2780 and A2780-T, meaning the induction of cancer cell death instead of cell cycle arrest via blocking T-type Ca^{2+} channel. In the case of new analogues 6g and 6h, two compounds induced cell cycle arrest at G1 phase of A2780 and A2780-T cells in concentration-dependent manner, indicating the cancer cell growth inhibition by blocking T-type Ca^{2+} channel. Therefore, our findings suggest that our T-type Ca^{2+} channel blockers have potential chemotherapeutic value for the treatment of human ovarian cancer via various modes of action.



6g (R = F)

6h (R = OCH₃)



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-947**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and synthesis of 2-(2-Aminopyrimidin-4-yl)phenol derivatives as Pim kinase inhibitors

이지훈 HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

The Pim kinases are a small sub-family of serine/threonine protein kinases within the CAMK family, comprising Pim-1, 2, and 3. Pim kinases are cell function regulators that mediate most of the signal transduction pathways involved in cell growth, metabolism, differentiation and apoptosis. Overexpression of these kinases leads to many hematopoietic cancers and some solid tumors. So, Pim kinases are a very promising therapeutic target for the treatment of cancer. Novel series of 2-(2-aminopyrimidin-4-yl)phenol derivatives were synthesized and screened against Pim kinases.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-948**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In vitro Antiinflammatory Activity of the Components from Amomum tsao-ko in Murine Macrophage Raw264.7 Cells

최춘환 홍성수¹ 오좌섭^{2,*}

경기과학기술진흥원 천연물신약연구소¹ 경기과학기술진흥원 천연물연구팀² 단국대학교 약학대학

This research was undertaken to find the in vitro antiinflammatory action of the components from Amomum tsao-ko (Zingiberaceae) herbs. In vitro bioassay-guide revealed that the methanol (MeOH) extract of the whole plant of Amomum tsao-ko showed NO inhibitory activity by assessing their effects on the Murine Macrophage Raw264.7 Cells. Phytochemical study of the MeOH extract of this plant led to the isolation of ten compounds; 1,2-benzeneidol (1), 1,4-benzeneidol (2), 4-hydroxy-3-methoxy-benzoic acid (3), (-)-hannokinol (4), (+)-hannokinol (5), coumaric acid (6), 4-hydroxy-benzoic acid (7), (+)-epicatechin (8), (-)-catechin (9), myrciaphenone A (10). The results showed that the isolated components, benzeneidol (1), 1,4-benzeneidol (2), (+)-epicatechin (8) and (-)-catechin (9) inhibited the production of nitric oxide significantly in lipopolysaccharide (LPS)-treated RAW 264.7 cells. Cell viability was determined by MTT assay after treatment with various dilutions of the compounds.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MEDI.P-949**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of cancer targeted oleanolic acid-conjugated PET/MR dual contrast agent

채민경 조장근¹ 이철현* 유은경*

한국기초과학지원연구원 자기공명연구부 ¹중앙대학교 화학과

Research into multifunctional nanoparticles is focused on creating an agent for use in an all-in-one multimodal imaging system that includes diagnostic imaging, drug delivery, and therapeutic monitoring. We designed a new dual-modality tumor-targeting agent with a new tumor-targeting molecule, oleanolic acid (3 β -hydroxy-olea-12-en-28-oic acid, OA), which is derived from a natural compound and coupled with a macrocyclic chelating agent such as 1,4,7-triazacyclononane-1,4,7-triacetic acid (NOTA), iron oxide nanoparticles (IONP), and radiolabeling components such as ⁶⁸Ga for dual-modality positron emission tomography (PET)/magnetic resonance imaging (MRI). We obtained PET and MRI tumor images as well as fusion PET/MRI images of the tumors using ⁶⁸Ga-NOTA-OA-IONP from HT-29 cancer models. It showed that the dual-modality cancer-targeting radiolabeled nanoparticle is a potent imaging agent for PET, MRI, and it also has the advantage of not only detecting tumor functionality, but also simultaneously aiding in tumor resolution.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MED.P-950**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure-based design of TTR kinetic stabilizers that can prevent TTR fibril formation

김보영 최성욱^{1,*}

충남대학교 신약전문대학원 신약개발학과 ¹충남대학교 신약개발학과

Transthyretin(TTR) is a homotetrameric protein composed of 127-amino-acid, β -sheet-rich subunits. The established physiological functions of TTR are to bind to and transport the thyroid hormone thyroxine(T4) and holo-retinol binding protein in the blood and cerebrospinal fluid(CSF). TTR is one of more than 30 nonhomologous human amyloidogenic proteins, whose misfolding and/or misassembly appears to elicit the proteotoxicity and cell degeneration, which cause the amyloidoses. TTR fibril formation requires the rate-limiting tetramer dissociation and misassembly of partially denatured monomeric subunits. Small molecules that bind to T4 binding site stabilize the ground state of tetrameric TTR and raise the kinetic barrier for dissociation, imposing kinetic stabilization on TTR and preventing aggregation. There are two symmetrically equivalent T4 binding sites for ligands in each tetrameric TTR. To design small molecules can bind to T4 binding site, the designed quinoline derivatives were synthesized and evaluated possibilities for TTR kinetic stabilizer, using stagnant acid-mediated turbidity assay, cell cytotoxicity assay and fibril disruption assay.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MED.P-951

발표분야: 의약화학

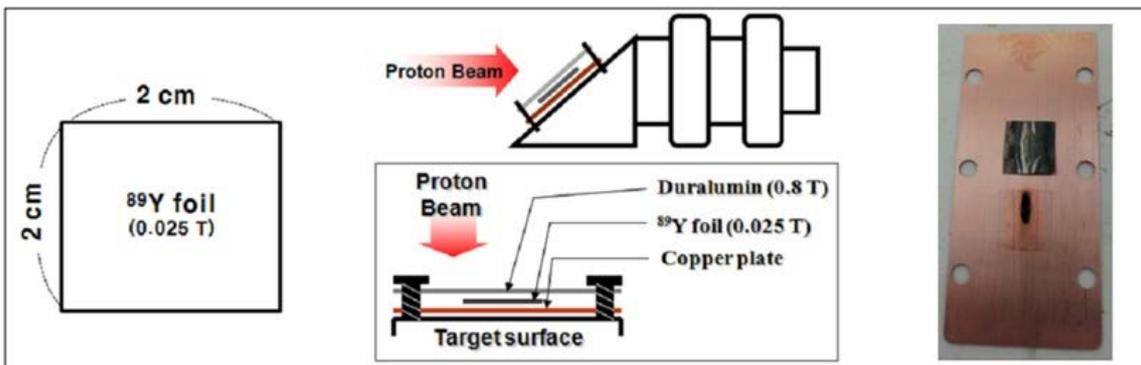
발표종류: 포스터, 발표일시: 수 16:00~19:00

Production and its Evaluation of Medical Radioisotope Zr-89 by KIRAMS Experience

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Objective: One of positron emission radiometals Zr-89 (half-life 3.27 days) has recently been reported to be particularly effective in immuno-PET. The development of radiopharmaceuticals based on this Zr-89 depends on a good chelator and proper antibody for specific binding in tumor cell. However, the production of Zr-89 has never been studied in Korea. The aim of our study was to widen the use of Zr-89 in molecular imaging based on Korean PET technology. Material & Method: The Zr-89 production used here was prepared by 50 MeV cyclotron according to simple method modified from the target of yttrium foil (0.025 mm). For Zr-89 nuclear reaction, we carried out Y-89(p,n)Zr-89 under about 10-30 μ A for a hour and used the proton beam of about 18 MeV, which was reduced by the degrader composed of Al and Ta foil. In particular, we could design the disposable Sep-PaK column (hydroxamate resin) for Zr-89 purification and the melting method of yttrium target using mixing acids. Result: The radiometal Zr-89 was easily purified by short column and its radiochemical purity was over 99%. The averagely production yield of Zr-89 was obtained as 4 mCi/h at 30 μ A in chemical form of Zr oxalate. In addition, we have obtained an interesting result to quickly dissolve the radioactivated yttrium target with a solution made by the regular ratio of hydrochloric acid and nitric acid. By the use of multichannel analyzer installed HPGe detector, we were able to identify the energy of Zr-89 gamma ray at 511 and 909 KeV as reported previously. The purified Zr-89 was also showed good labeling yield of over 80% with DFO and DTPA under pH 7. On the other hand, the PET images of Zr-89 were found to have low quality than that of F-18 at the same phantom. Conclusion: This development of Zr-89 production may be extended to the synthesis of new radiotracer for molecular imaging and tumor therapy.



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Synthesis and Biological Evaluation of 18 kDa Mitochondrial Translocator protein (TSPO) ligands for the Treatment of Alzheimer's Disease

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분부

The role of mitochondrial β -Amyloid peptide ($A\beta$) has been highlighted in Alzheimer's disease (AD) pathogenesis. $A\beta$ is produced from transmembrane amyloid precursor protein (APP) by sequential actions of β - and γ -secretase. $A\beta$ is implicated in the pathogenesis of Alzheimer's disease by interaction with cyclophilin D (CypD). CypD, adenin nucleotide translocator (ANT), voltage-dependent anion channel (VDAC), and 18kDa Translocator protein (TSPO) compose the mitochondrial permeability transition pore (mPTP). $A\beta$ enhances both mPTP opening and influx of cytosolic solutes into the mitochondrial matrix. Consequently, $A\beta$ can cause mitochondrial swelling and apoptotic cell death. The TSPO ligand inhibiting mPTP can be an effective therapeutic strategy in AD. Based on the pharmacophore-based virtual screening, we identified KKPN0001 and KKPN0002 which are novel TSPO ligand scaffolds. These two compounds were synthesized and their biological evaluations were performed. We measure biological effects of each compound in five in vitro cell-based assays; JC-1 assay, ATP assay, MTT assay, Calcein AM assay, and ROS assay. And then, several selected compounds were injected into $A\beta$ -induced acute AD mouse model for a behavioral test. The in vivo assay results of the Y-maze spontaneous alternation test showed that KKPN0001 improved memory and cognitive functions. For the optimization study of KKPN compounds, KKPN derivatives (KKPT compounds) were synthesized and biologically evaluated in our in vitro assay system. Their cell-based in vitro data showed the improvement in symptoms of AD. Now, more than 100 KKPT compounds were synthesized and their optimization process is still in progress.

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Synthesis of Functionalized Amino Acids and Effect on Blocking of NMO-IgG binding to Aquaporin-4

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단

Protein is an essential material that is needed for development and maintenance of cellular tissue and is used to form hormones, enzymes, antibody, and neurotransmitter. It is composed of amino acids which are biologically important organic compounds and play significant role in variety of functions in metabolism. In present research, various functional groups are applied to the 20 amino acids to build a Functionalized Amino Acid (FAA) library for screening of biologically active compounds. Neuromyelitis optica (NMO) is an inflammatory disease in the CNS caused by anti-aquaporin-4 (AQP4) autoantibodies to AQP-4 on astrocytes. We used the FAA library to seek a lead compound for blockers of Neuromyelitis Optica (NMO) immunoglobulin G binding to Aquaporin-4.

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Development of screening system for blockers of NMO-IgG binding to aquaporin-4

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Neuromyelitis Optica (NMO) is a demyelinating autoimmune disease of optic nerve and spinal cord triggered by binding of NMO-specific Immunoglobulin-G autoantibodies (NMO-IgG) to astrocyte water channel aquaporin-4 (AQP4). We prepared human M23-AQP4-expressing U87MG cells and set up a screening system for small molecule blockers against the binding of NMO-IgG to AQP4 measuring lactate dehydrogenase release for complement dependent cytotoxicity. Furthermore, we performed high-throughput small molecule inhibitor screening system by quantitative measurement of two immunofluorescence ratio imaging on binding of NMO-IgG to AQP4 using high content screening (HCS). Our development of screening system on small molecule inhibitors of NMO-IgG to AQP4 would lead to further pathogenesis and therapeutic researches.

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Molecular Dynamics study for Perturbations of Amyloid Fibrils by small molecules

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The beta-amyloid (A β) is the major peptide constituent of neuritic plaques in Alzheimer's disease, and its aggregation is believed to play a central role in the pathogenesis of the disease. Current research has indicated that small compound could interfere with β -amyloid fibril growth and have the ability to disassemble preformed folded structures. This compound, which possesses both hydrophilic and hydrophobic moieties and binds to peptides/proteins, is a potential candidate against amyloidogenesis. The molecular mechanisms have not been elucidated in detail yet. Here the effects of compound on preformed fibrils are investigated by replica-exchanged molecular dynamics method. Molecular dynamics simulations are used to identify those features which play a key role in the destabilization of the aggregates. The computational analysis suggests that dissociation of peptides from the amyloid superstructures could take place along the fibril axis and be primarily determined by the cooperative rupture of the backbone hydrogen bonds and of the Asp-Lys salt bridges.

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Synthesis and biological evaluation of tetrahydrothieno[2,3-c]pyridine derivatives as mGluR1/5 negative allosteric modulators

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Glutamate (L-glutamic acid), the major excitatory transmitter in the mammalian central nervous system (CNS), exerts its effects through both ionotropic and metabotropic glutamate receptors, thereby generating the fast excitatory synaptic responses at the majority of CNS synapses and involved in pathologies of many brain diseases. While ionotropic glutamate receptors are ligand-gated ion channels responsible for mediation of glutamate fast transmission, the metabotropic glutamate receptors (mGluR) belong to family C of the Gprotein- coupled receptors (GPCRs) and modulate the strength of synaptic transmission and they are divided into three groups with eight subtypes on the basis of their sequence homology, pharmacology, and signal transduction mechanism. Group 1 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 show that selective mGluR5 antagonists may play a role in the treatment of neuropathic pain and other brain diseases. In this study, we report the synthesis and biological evaluation of novel tetrahydrothieno[2,3-c]pyridine derivatives as mGluR5 antagonists for treatment of neuropathic pain.

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Radio immunoassay of [123I]iodohypericin for HER-2 receptor as inhibitor

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The aim of this study is synthesis and evaluation the radio labelled hypericin as radiopharmaceutical for cancer cell diagnosis and therapy. The labeling of ¹²³I was performed in [123I]NaI solution (159 MBq/100 uL). 0.5 M H₃PO₄, 32% peracetic acid with hypericin solution in ethanol (1 mg/mL) then stirring for 10 minutes. The compound was purified by RP-HPLC. Cell uptake experiments Both of the breast cancer cells MCF-7 and SK-BR-3 cell lines were seeded at in 24 well plates at 1 mL per well and incubated at 37 °C in a 5% CO₂ for 24 h for an adherence and growth. To each well in 2-[123I]iodohypericin (185 KBq) was added. Cells were washed twice in cold phosphate buffered saline (PBS) at designated time point (10 min, 30 min, 60 min and 120 min). The cell pellets were counted by gamma counter. Data was presented as a percentage of the injected radioactivity dose (%ID). The synthesis of Iodohypericin was confirmed by ¹H-NMR spectroscopy. Purification of [123I]iodohypericin was carried out by a RP-HPLC using ammonium acetate and ethanol. As a result, the peak was found about 35 minutes. The cellular uptakes of 2-[123I]iodohypericin increased in a time dependent manner for both breast cancer cell lines (SK-BR-3 and MCF7). We have synthesized and evaluated 2-[123I]iodoemodin on human breast cancer cells (SK-BR-3 and MCF-7) which express of HER-2 receptor. The results of this study can be used as a breast cancer imaging reagent for PET

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Radio immunoassay of [123I]iodoemodin for HER-2 receptor as inhibitor

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The aim of this study is synthesis and evaluation the radio labelled emodin as radiopharmaceutical for cancer cell diagnosis and therapy. The labeling of 123I was performed in [123I]NaI solution (1110 GBq/100 μ L). 0.5 M H₃PO₄, 32% peracetic acid with emodin solution in methanol (3 mg/mL) then stirring for 10 minutes. The compound was purified by RP-HPLC. Cell uptake experiments Both of the breast cancer cells MCF-7 and SK-BR-3 cell lines were seeded at in 24 well plates at 1 mL per well and incubated at 37 °C in a 5% CO₂ for 24 h for an adherence and growth. To each well in 2-[123I]iodoemodin (185 KBq) was added. Cells were washed twice in cold phosphate buffered saline (PBS) at designated time point (10 min, 30 min, 60 min and 120 min). The cell pellets were counted by gamma counter. Data was presented as a percentage of the injected radioactivity dose (%ID). The synthesis of Iodoemodin was conformed by ¹H-NMR spectroscopy. Iodone was found to be introduced at the 2-positron of the emodin from the disappearance of the proton signal of the 1H NMR spectrum at 6.6 ppm. Purification of [123I]iodoemodin was carried out by a RP-HPLC using ammonium acetate and methanol. As a result, the peak was found about 25 minutes. The cellular uptakes of 2-[123I]iodoemodin increased in a time dependent manner for both breast cancer cell lines (SK-BR-3 and MCF7). We have synthesized and evaluated 2-[123I]iodoemodin on human breast cancer cells (SK-BR-3 and MCF-7) which express of HER-2 receptor. The results of this study can be used as a breast cancer imaging reagent for PET

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NON-REACTIVATING PROPERTIES OF OXIME REACTIVATORS

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Current treatment of organophosphorus (OP) poisoning, originating as irreversible inhibition of acetylcholinesterase (AChE) and resulting as the overstimulation and of cholinergic receptors by acetylcholine (ACh), consists of the administration of atropine and oxime reactivators. The reactivators' mechanism of action seems to be simple: restore the activity of OP-inhibited AChE. However, rather complex mechanism has been ascribed to oxime reactivators. They act at several levels of the cholinergic transmission including synthesis, release, inactivation and re-uptake of the transmitter, especially the interaction with muscarinic and nicotinic receptors may be of therapeutic benefit in the treatment of OP poisoning. Our study focuses on this non-reactivation properties of oximes, especially on the interaction with postsynaptic muscarinic and nicotinic receptors. Furthermore, the effect on AChE and re-uptake transport system (HACU) has been investigated as well. Both in vitro receptor binding studies, isolated organ's contraction studies, patch-clamp etc and in vivo techniques were used. The results confirmed that oxime reactivators are also inhibitors of AChE (IC₅₀ in micromolar range) and may influence the release of ACh via the interaction with re-uptake transport system (HACU) a key-regulatory system, which delivers choline for the synthesis de novo. In-vitro and in-vivo experiments comprehensively proved inhibitory effects of studied oximes on nicotinic receptors. Although, the IC₅₀ values were in the hundreds of micromoles, even a weak inhibition may speak in favor of the treatment with reactivators. Especially when atropine does not affect nicotinic receptors at all and nicotinic symptoms are usually responsible for the death of a victim. Muscarinic antagonism has also been described by both in-vitro and in-vivo experiments as well. Although, the mechanism of binding has not been satisfactorily explained a weak inhibition was observed (atropine had at least 3-fold higher efficacy). However, even a weak inhibition may play an important role in the treatment of OP poisoning, in particular, in the case of

“aging”. We can conclude that oxime reactivators’ mechanism of action represents much more complex system than only reactivation. This work was supported by the grant of Ministry of Health (Czech Republic) No. NT12062 and A long — term organization development plan 1011



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Development of M₁ selective muscarinic acetylcholine receptor agonists with cyclic oxime moiety

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Muscarinic acetylcholine receptors (mAChRs) mediate the metabotropic action of the neurotransmitter acetylcholine (ACh) in the peripheral and central nervous system, and consist of five muscarinic receptor subtypes, M₁—M₅. The M₁ receptor subtype of them is abundant in cerebral cortex and hippocampus of central nervous system (CNS), and has been considered as potential therapeutic target for the treatment of cognitive dysfunction and impairment observed in Alzheimer's disease (AD) and schizophrenia patients. Our efforts have been focused on developing novel M₁ selective mAChR agonists with low side effects for the treatment of AD. We designed and synthesized new analogs that have (1) *N*-methyltetrahydropyridine moiety, (2) cyclic oxime moiety and (3) various substituents at 5 position of isoxazoline ring. We assayed the analogs in HEK293 cells transiently transfected with each human mAChR, and found an M₁ selective compound and further examined the effect of the compound on ERK1/2 phosphorylation.

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Hydrocarbon-Bridged α -Helix Mimetics Small Molecules

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The α -helix-mediated protein-protein interactions (PPIs) are considered one of the most important focus in chemical biology and medicinal chemistry. Because many cellular events occur via protein-protein interaction (PPI) where protein secondary structure, such as α -helix or β -turn, plays an important role as a recognition motif. Previously, we constructed a one-bead-one-compound (OBOC) combinatorial library of triazind-piperazine-triazine-based α -helix mimetics and found a hit compound showing low micromolar affinity to MCL-1. In this research, we modified the structure of the hit compound by macrocyclization with a series of different length of linkers (C8 - C12) to reduce rotational movement of α -helix scaffold. As the result of in vitro binding assay using fluorescence polarization (FP) method, one of those macrocyclic compounds showed higher binding affinity to MCL-1 than the original hit compound. In summary, macrocyclization of the α -helix mimetics in the view of structure-activity relationship study (SARS) might be able to give structural rigidity and enhance the inhibition for PPIs.

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Design, Synthesis, and Biological Evaluation of Phenyl-Piperazine-Triazine-Based α -Helix Mimetics

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포항공과대학교 화학과

α -Helices, which account for 30% of protein secondary structure, are involved in many protein-protein interactions (PPIs) as recognition motifs. It is, therefore, of great interest to target α -helix-mediated-PPIs by developing small molecule α -helical mimetics as a modulator of such interactions. Current α -helix mimetic small molecules have several important drawbacks such as poor water solubility and synthetic difficulty. Here we describe the design and efficient solid-phase-synthesis of phenyl-piperazine-triazine scaffold as a novel class of α -helix mimetic small molecules. Our library compounds had higher synthetic accessibility, and showed improved water solubility. Additionally, the subsequent screening of a focused library molecules identified a potent inhibitor of Mcl-1/BH3 and Bcl-XL/BH3 interaction, demonstrating their ability to act as inhibitors of α -helix-mediated PPIs. Consequently, our scaffold, along with simple synthetic route, will provide an excellent source of PPI modulators.

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고용량 커패시터 전극을 위한 나노구조 ruthenium 셀 제조

박민한 김효혜¹ 정현민*

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금속산화물 전극물질로 사용하는 슈퍼 커패시터 개발에서 고용량의 정전용량을 갖기 위한 다양한 구조와 금속산화물-카본 복합물질이 연구되어왔다. 본 연구에서는 나노구조의 ruthenium oxide 셀을 형성하여 정전용량을 극대화하는 효과를 얻고자 하였다. 나노구조의 ruthenium oxide 셀은 polystyrene 을 템플리트로 사용하여 ruthenium(III) chloride 을 프리커서로 하여 제조한다. 제조된 나노구조의 ruthenium oxide 셀 구조는 SEM 과 TEM 을 이용하여 확인하고, XPS 를 이용하여 Ru 의 결합특성을 확인하였다. 기존의 ruthenium oxide 파우더와 비교해 나노구조의 ruthenium oxide 셀의 향상된 정전용량은 galvanostatic charge-discharge 를 이용하여 확인하였다.

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***In Situ* Investigation on Pore Opening during Wet-Chemical Etching of the Barrier Layer of Nanoporous Anodic Aluminum Oxide: Nonuniform Impurity Distribution in Anodic Oxide**

박상준 이우*

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Nanoporous anodic aluminum oxide (AAO) with hexagonally arranged hole arrays have drawn enormous attention on account of its tunability in pore dimension (*i.e.*, diameter and length), pore interval, and internal pore diameter as well as readily accessible fabrication process by simply anodizing Al under proper conditions (*i.e.*, anodization electrolyte and voltage). In light of this, AAO has widely been adopted in various applications such as fabrication of functional nanomaterials and optoelectronics [1-4]. Through-hole AAO membranes are more prospective in terms of practical applications. They can be readily obtained by opening of the barrier oxide layer at the pore bottom of AAO by either wet-chemical or dry etching. The former renders more simple and economical way of preparation of through-hole AAO membranes compared to the latter. Inspired from this, we performed systematic investigation on controlled wet-chemical etching of the barrier layer of AAO by employing a newly-designed setup for explicit *in situ* detection of pore opening point during chemical etching of the barrier oxide layer as well as scanning electron microscopy (SEM), secondary ion mass spectrometry (SIMS). We disclosed that opening of the barrier oxide layer by wet-chemical etching can be significantly affected by anodization time (tanodi). From the result of SIMS analyses, barrier oxide of porous AAOs prepared from long-term anodization found to be less contaminated by anionic impurity in comparison to one obtained from the short-term anodization, leading to retarded pore opening during the wet-chemical etching. This observation comes from the progressive decrease of the electrolyte concentration upon anodization. Based on the quantitative comparison on the outer pore wall etching rates for the upper and lower part of AAO, the etching rate of the former is lower than the one of the latter on account of the lower level of impurity content in that region. This observation suggests that a spatial concentration gradient of anionic impurity

in the outer pore wall oxide might be established along both the vertical and radial directions of cylindrical pores. The results of the present work are expected to offer viable information not only for practical utilization of nanoporous AAO in nanotechnology but also for deeper understanding of the self-organization behaviors of oxide nanopores during anodization.

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장소: 창원CECO

발표코드: MAT.P-965

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Control of Oxygen Vacancies in TiO₂ by Plasma Enhanced Atomic Layer Deposition (PEALD) as its implication on resistive switching behavior

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TiO_x is one of the strong candidates for resistive switching (RS) devices. It has generally been believed that the resistive switching (RS) in TiO_x-based RS devices is ascribed to the formation of oxygen deficient Magn?li phase by field-driven drift and ordering of oxygen vacancies (V_O) [1,2]. Accordingly, it is important to study the influence of oxygen vacancy concentration on the RS behaviors of TiO_x-based RS devices. Stoichiometry of TiO_x has clear relation to the oxygen vacancy concentration [3]. In this regard, Pt/TiO_x/Pt capacitors with different values of x were prepared in this study to explore the effect of oxygen vacancy on RS behavior. TiO_x films were grown by plasma enhanced atomic layer deposition (PEALD) using titanium (IV) tetraisopropoxide (TTIP; Ti[OCH(CH₃)₂]₄) and mixture gas of pure O₂ and N₂ (99.999% for both) as Ti precursor and reactant, respectively. Stoichiometry of TiO_x (*i.e.*, x value) is deliberately controlled by adjusting flow ratio (*R_F*) of O₂ gas to N₂ + O₂ mixture gas from 0.25 to 1.00.

Microstructure and properties of the resulting films were characterized by Rutherford backscattering spectrometry (RBS), transmission electron microscopy (TEM), X-ray diffraction (XRD), confocal Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and spectroscopic ellipsometry (SE). According to RBS result, x in TiO_x was found to be varied from 1.62 to 1.70 for RF range from 0.25 to 1.00. PEALD TiO_x films were observed to be amorphous at *R_F* = 0.25, whereas nanocrystalline anatase at *R_F* = 1.00. Another evidence for dependence of the film crystallinity on RF was obtained from Raman spectroscopic analysis. It turned out from the deconvolution of the O1s XPS peaks that non-lattice oxygen content increase from 15.3 to 20.7% with decreasing the *R_F* from 1.00 to 0.25, which indicates increase of oxygen vacancies in PEALD TiO_x film with *R_F*. It was revealed from SE analyses that the absorption originated from defect states below bandgap, monotonously increases with decrease of x, *i.e.*, increase of oxygen

vacancy concentration. Based on these results, systematic studies on the influence of oxygen vacancy on resistive switching (RS) behaviors of TiO_x -based RS devices were carried out [4].

References

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일시: 2013년 10월 16~18일(수~금) 3일간

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발표코드: MAT.P-966

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Size-controlled synthesis of platinum nanoparticles using Proton Beam Irradiation

이윤지 송재희*

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이 실험에서는 실온에서 용액 상태인 백금이온에 양성자 빔을 조사하여 백금 나노입자로 합성 할 수 있었다. 이때 계면활성제는 cetyltrimethyl ammonium bromide(CTAB)과 sodium dodecyl sulfate(SDS)를 사용하였다. 그리고 계면활성제와 백금의 이온 혼합용액에 IPA 을 첨가함에 따라 나노입자 크기가 커지는 것을 확인 할 수 있었다. 그리고 다양한 빔 전류와 조사시간을 통해 백금 나노입자의 크기와 모양을 조절하였다. 합성된 Pt 나노입자는 UV-Vis absorption spectroscopy 와 Transmission Electron Microscopy(TEM), energy dispersive X-ray spectroscopy(EDS) 분석을통해 확인되었다.

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장소: 창원CECO

발표코드: MAT.P-967

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Wafer-scale GaN nanorod structure fabricated using self-assembled PS nanosphere and dry etching process

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Wafer-scale GaN nanorod arrays were fabricated on 2-inch sized GaN wafers by combination of self-assembled PS nanosphere, reactive ion etching (RIE) and ion coupling plasma (ICP) etching processes. A Cr and SiO₂ films as mask for etching of GaN were coated on 2-inch sized GaN wafer by thermal evaporation and plasma enhanced chemical vapor deposition (PECVD) process, respectively, forming Cr/SiO₂/GaN structure. 960nm sized PS monolayer then was coated on the Cr/SiO₂/GaN structure via scooping transfer technique. PS/Cr/SiO₂ layers on GaN wafer were thinned and etched by RIE process, forming SiO₂ nanorod/GaN. Subsequently, SiO₂ nanorod/GaN structure was etched via ICP etching process. Finally, SiO₂ residues on GaN nanorod were eliminated using wet etching process with HF solution. The structural, morphological and optical properties of GaN nanorod arrays were investigated by scanning electron microscopy (SEM), photoluminescence (PL) and cathode luminescence (CL) measurements.

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장소: 창원CECO

발표코드: **MAT.P-968**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of blue emitting Cu₃P/ZnS quantum dots

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Cu₃P/ZnS quantum dots (QDs) were synthesized by a solvothermal method using toluene, 1-octadecene, 1-dodecanthiol as solvent without stirring to realize blue emitting QDs. We optimized the Cu₃P/ZnS QDs by changing core growth time and ratio of Cu and Zn precursors. As increasing the core growth time, the photoluminescence (PL) quantum yields (QYs) of QDs were increased. Dominant wavelength of blue emitting QDs is around 475 nm. Optical properties of QDs were observed by UV-vis spectroscopy, photoluminescence (PL) spectroscopy.

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발표코드: MAT.P-969

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and characterization of white phosphor-converted light-emitting diode using AgIn₅S₈/ZnS quantum dots coated glass bead composite

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In this study, we designed white phosphor converted light emitting diode (white pc-LED) using dodecanthiol-capped AgIn₅S₈-ZnS (AIS/ZS) alloyed quantum dots (QDs) coated glass beads (GB) composites (QD-GB composites) in order to confirm the scattering effect by changing the glass bead size (5um and 100um). The AIS/ZS QDs were synthesized by using colloidal hot injection method. The quantum yield of QDs is over 50%. To successfully disperse the AIS/ZS alloyed QDs on GBs, the surface of glass beads was treated by trichloro(octadecyl)silane (OTS) for changing hydrophilic surface to hydrophobic surface. The QD-GB composites were prepared by mixing and vacuum drying process. The white pc-LED was realized by putting the mixture of Si-binder and QD-GB composite into LED cup. The synthesized QD was characterized by UV-Vis spectroscopy and photoluminescence (PL). The morphological and optical properties of QD-GB composite were measured by scanning electron microscopy (SEM) and PL spectroscopy. The white pc-LED was measured by electroluminescence (EL).

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장소: 창원CECO

발표코드: MAT.P-970

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of green and yellow emitting AgIn₅S₈/ZnS quantum dots for white light-emitting diodes

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In this study, we synthesize green and yellow emitting AgIn₅S₈/ZnS (AIS/ZS) core/shell quantum dots (QDs) for white light-emitting diodes (W-LEDs) using hot injection method. The AIS/ZS QDs are good candidates for W-LEDs due to their broad emission band from donor-acceptor emission. To realize green and yellow emission, the AIS/ZS QDs were optimized by changing core temperature, core reaction time, and shell injection conditions such as concentrations of shell precursors, number of shell injection, and temperature. The W-LEDs containing AIS/ZS QDs were prepared by mixing with Si-binder and AIS/ZS QDs and putting the mixed binder into LED cup. The AIS/ZS QDs were characterized by using photoluminescence (PL), electroluminescence (EL), UV-Vis spectroscopy, X-ray diffraction (XRD) and transmission electron microscopy (TEM).

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장소: 창원CECO

발표코드: MAT.P-971

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An effective route for room temperature synthesis of Pd nanomaterials in aqueous solution

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순천대학교 화학과

We present a facile one-pot synthetic route for the production of palladium nanoparticles via a simple proton beam irradiation process at room temperature. The synthesis of size-controlled palladium nanostructures was realized just by changing the mean current of the proton beam and by controlling the molar concentration ratios of surfactants to Pd precursors in an aqueous phase-based solution without the addition of any harsh reductants. As the beam current was increased under the same Pd ion concentration conditions, the average diameter of the prepared Pd nanoparticles tended to be decreased. We also found that the size of the synthesized Pd nanocrystals was decreased as the molar ratio of surfactants to palladium ion was increased.

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장소: 창원CECO

발표코드: MAT.P-972

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemodosimetric detection of explosives using polymer-based chromogenic nanoparticles

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Developing a sensitive and selective detection method to explosives is one of the most important research subject in scientific society. The method is mainly used for detecting environmental pollution, terrorism prevention, and military purposes; for instances, forensic research, land-mine detection, and environmental effects of explosive residues. As terrorism activities have been increased recently around the world, there are more possibilities to have more IEDs (Improvised Explosive Devices). With all this in mind, canine teams, GC-MS, Raman, X-ray, and IMS have been used for detecting these chemicals. They have their own distinct cons, as well as pros such as lack of portability and low sensitivity with certain interfering compounds. Therefore, recent researches for detecting explosives have been focused to have better sensitivity and selectivity with lower costs. Optical detection techniques are popular recently in order to study biological events through quantifying and imaging biological molecules in supramolecular chemistry. It is beneficial to have better sensitivity of color and fluorescence changes with various simple devices. In fact, different protocols of chemosensors have been widely applied to the design of probes for anions, cations, and, to a lesser extent, to explosives. In this research, we'll discuss how to detect nitroaromatic explosives (TNT, DNT, and PA) by applying new polymer-based chromogenic nanoparticles.

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장소: 창원CECO

발표코드: **MAT.P-973**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ordered Mesoporous Porphyrinic Carbons with Very High Electrocatalytic Activity for the Oxygen Reduction Reaction

천재영 사영진 주상훈*

울산과학기술대학교(UNIST) 나노생명화학공학부

Ordered mesoporous porphyrinic carbons (M-OMPC; M = Fe, Co, or, FeCo) were synthesized via a nanocasting method, using mesoporous silica as a template and metalloporphyrins as a precursor, respectively. Among the family of M-OMPC catalysts, the Fe and Co co-doped OMPC (FeCo-OMPC) showed an extremely high electrocatalytic activity towards oxygen reduction reaction (ORR) in acidic media. In addition, FeCo-OMPC showed higher kinetic current at 0.9 V than Pt/C catalysts, as well as superior long-term durability and methanol-tolerance. Density functional theory calculations coupled with extended X-ray absorption fine structure analysis revealed a weakening of the interaction between oxygen atom and FeCo-OMPC compared to Pt/C. This effect and high surface area of FeCo-OMPC appear responsible for its significantly high ORR activity.

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발표코드: MAT.P-974

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ordered Mesoporous Co_3O_4 Spinels as Stable, Bifunctional, Noble-Metal Free Oxygen Electrocatalysts

사영진 천재영 주상훈*

울산과학기술대학교(UNIST) 나노생명화학공학부

Ordered mesoporous Co_3O_4 spinels (meso- Co_3O_4) with two different pore structures were prepared by nanocasting KIT-6 mesoporous silica with cubic $Ia3d$ mesostructure, and were used as bifunctional catalysts for both oxygen evolution and reduction reactions (OER and ORR, respectively). The meso- Co_3O_4 nanostructures showed high activity for OER in an alkaline medium, which makes them comparable to the most active Ir/C catalyst and better than Co_3O_4 nanoparticles (NPs) and the Pt/C catalyst. Furthermore, meso- Co_3O_4 exhibited enhanced stability, compared to Co_3O_4 NPs, possibly due to the structural stability of the gyroid network structure. The meso- Co_3O_4 nanostructures also showed promising activity for ORR in an alkaline medium, and exhibited a methanol-tolerance superior to the Pt/C catalyst. The total overpotential of meso- Co_3O_4 for OER and ORR was on a par with noble metal-based catalysts.

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발표코드: MAT.P-975

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon Nanotubes/Heteroatom-Doped Carbon Core-Sheath Nanostructures as Highly Active, Metal-Free Oxygen Reduction Electrocatalysts for Alkaline Fuel Cells

사영진 주상훈*

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An ionic liquid (IL)-driven, facile, scalable route to new carbon nanostructures comprising pure carbon nanotube cores and heteroatom-doped carbon sheath layers (CNT/HDC) has been developed. The design of the CNT/HDC nanocomposite allows for combining electrical conductivity derived from the CNTs with the catalytic activity of the heteroatom-containing HDC sheath layers. The CNT/HDC nanostructures showed excellent electrocatalytic activity for the oxygen reduction reaction (ORR) in an alkali medium, evidenced by their high half-wave potential. The ORR activity of CNT/HDC nanostructures is one of the best performances among the heteroatom-doped nanocarbon catalysts in terms of half-wave potential and kinetic current density. The kinetic parameters of the CNT/HDC nanostructures, including 4-electron selectivity and exchange current density, compared favorably with those of a Pt/C catalyst. The CNT/HDC nanostructures also exhibited highly superior long-term durability and poison-tolerance relative to Pt/C. In addition, the CNT/HDC nanostructures showed high current and power densities when employed as a cathode catalyst in alkaline fuel cell, which sheds light on their practical applicability.

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발표코드: MAT.P-976

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ordered Mesoporous Carbon Arrays Embedding Molybdenum Disulfides Nanosheets as Highly Active Electrocatalyst for Hydrogen Evolution Reaction

서보라 천재영 사영진 주상훈*

울산과학기술대학교(UNIST) 나노생명화학공학과

Ordered mesoporous carbon arrays embedding molybdenum disulfides nanosheets ($\text{MoS}_2\text{@OMC}$) have been prepared by sequential formation of carbon and MoS_2 nanostructures inside the nanopores of mesoporous silica templates followed by etching of the latter. This design of $\text{MoS}_2\text{@OMC}$ structures combines the electrical conductivity of carbon frameworks as well as the formation of MoS_2 nanosheets with a high density of edge sites. The $\text{MoS}_2\text{@OMC}$ exhibited very high electrocatalytic activity for hydrogen evolution reaction (HER). Significantly, the HER activity by mesoporous $\text{MoS}_2\text{@OMC}$ showed an oscillating phenomenon with a change of layer number in MoS_2 nanosheets.

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장소: 창원CECO

발표코드: MAT.P-977

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Low-Temperature Atomic Layer Deposition of Nickel Sulfide Thin Films

한규석 성명모*

한양대학교 화학과

We developed nickel sulfide thin films by atomic layer deposition with [nickel(1-dimethylamino-2-methyl-2-butanolate)₂] [Ni(dmamb)₂] and hydrogen sulfide (H₂S) at low temperatures of 90-200 °C. The film growth rate was 0.35nm/cycle at deposition temperature of 140~180°C. A linear growth rate characteristic of ALD was observed, with no chemical contamination. Film properties are studied using XPS, XRD and Hall measurements. SEM images show that the films are polycrystalline with grain size increasing with film thickness. The prepared nickel sulfide thin films were used as counter electrode of dye-sensitized solar cell. The catalytic properties of nickel sulfide films was comparable to platinum counter electrode.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-978**

발표분야: 재료화학

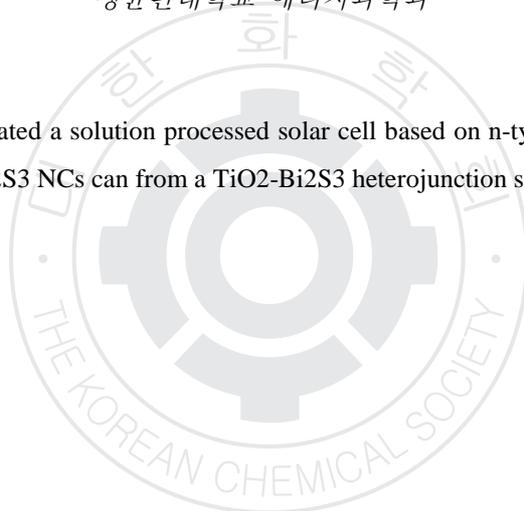
발표종류: 포스터, 발표일시: 수 16:00~19:00

Near IR-Sensitive Inorganic-organic heterojunction Solar cells Employing Bi₂S₃ quantum dot

서갑석 안태규*

성균관대학교 에너지과학과

We have recently demonstrated a solution processed solar cell based on n-type Bi₂S₃ nanocrystals(NCs) and we have shown that Bi₂S₃ NCs can form a TiO₂-Bi₂S₃ heterojunction structure.



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발표코드: **MAT.P-979**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Blue Light Emitting Material

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경상대학교 화학과 ¹경상대학교 자연과학대학 화학과 ²경상대학교 나노신소재공학부

The use of π -conjugated organic compounds as electroluminescent materials in organic light-emitting diodes (OLEDs) was introduced by Tang and Van Slyke over two decades ago. Since then, organic electroluminescent (EL) materials have been widely researched for their applications in high-efficiency, low-drive-voltage, large-display-area, full-color flat-panel displays. In order to develop high performance materials with desirable properties and devices with optimized architecture to develop marketable OLEDs, great effort has been made. Whereas, compared with red- and green-light-emitting devices, the EL properties of blue-light-emitting ones need to be enhanced, especially in terms of color purity and efficiency. In this work, we have designed and synthesized new blue-light-emitting material.

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장소: 창원CECO

발표코드: MAT.P-980

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Melting Assisted Solvent free Synthesis of Ordered Mesoporous Carbon

JINXING 김지만*

성균관대학교 화학과

Ordered mesoporous carbon (OMC) materials are recently aroused great research interest because of their widespread applications in many areas such as sorbents for separation processes and gas storage, as supports for many important catalytic processes, and as electrode materials for batteries, fuel cells, and supercapacitors. The synthesis of mesoporous carbon using hard ordered mesoporous silica (OMS) as the template. Their approach includes the following four steps: a) preparation of silica with controlled pore structure, b) impregnation of the silica template with monomer or polymer precursors using the incipient wetness impregnation method, c) cross-linking and carbonization of the organic precursors, and d) dissolution of the silica template. Generally, the OMC was impregnation of the silica template with carbon precursor solution. After drying the solvent 100 °C and 160 °C for 6 and 6 h, and then the 2nd impregnation and drying procedure was repeated once (Scheme 1). Here, we have developed a simple and facile synthesis of OMC by using melting assisted solvent free method by using carbon precursor of Phenanthrene (Phen), 1,10-Phenanthroline (1,10-Phen) and p-toluenesulfonic acid (p-TSA) with low melting point around 101 °C, 117 °C and 103 °C, respectively. And compare with the OMC by used different method.

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발표분야: 재료화학

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Direct double stranded DNA detection based on graphene oxide

이지연 민달희*

서울대학교 화학과

Sequence-specific DNA detection plays a crucial role in the diagnosis and monitoring the genetic related diseases and fatal virus infections. Although the sequence recognition methods by Watson-Crick base pairing are extensively chosen for DNA sensing in most laboratories, they are generally required denaturation and/or rehybridization steps because the target DNA strand usually forms a duplex with complementary strand. Recently, several approaches which does not require denaturation and/or rehybridization has been proposed. These direct detection methods have utilized dsDNA binding probes such as zinc finger DNA binding proteins, polyamide and triplex-forming oligonucleotides (TFOs). However, most of these probe molecules has several fundamental drawbacks in their own stability during the detection of target and limitation in recognition length or sequence. Therefore, it is important to establish a direct, simple and efficient platform for dsDNA detection. Here, we report a double stranded DNA (dsDNA) detection method based on the invasion capability of peptide nucleic acid (PNA) and preferential binding of single-stranded PNA (ssPNA) over DNA/PNA duplex to graphene oxide (GO). GO can be used as an efficient nano-quencher because it adsorbs single stranded PNA followed by long range energy transfer from dye. By measuring the quenching and recovery of fluorescence of dye conjugated to PNA probe, dsDNA could be analyzed quantitatively. Moreover, the high binding affinity of PNA for GO allows to overcome the drawbacks of conventional DNA probe and make the field of limited GO based sensor broader. We believe that this new direct GO-based dsDNA sensor will be a widely applicable tool in the field of DNA diagnostics.

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Active Ester-Functionalized Conducting Cell Scaffolds

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Electrically conducting polymers exhibiting biological activity have gained much attention as materials capable of intimately interacting cells and tissues both in biological and electrical ways. In this regard, a study is performed on the electropolymerization of 3'-carboxyl-2,2':5',2''-terthiophene (TThCOOH), which contains carboxylic acid (-COOH) functionality that can be easily modified with biological moieties at the surface of the polymer scaffolds. The resultant functionalized polymer, PTThCOOH, exhibit a good conductivity, 1.22 ± 0.15 S/cm. The chemical structure of this scaffold is characterized by X-ray photoelectron spectroscopy (XPS), which verified the presence of carboxylic acid (-COOH) functionality at the surface. The PTThCOOH surface is grafted with a cell-adhesive Arg-Gly-Asp (RGD) motif, and the attachment and growth of normal human dermal fibroblast (NHDF) cells are studied to assess the ability of RGD-grafted PTThCOOH surfaces to interact with cells using fluorescence microscopy and an MTS viability assay, consequently demonstrating the conductive PTThCOOH as a promising bioactive scaffold for tissue engineering application.

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High Surface Area Conducting Polypyrrole Scaffolds

이주운

한국교통대학교 교양학부 - 화학

In the present study, the successful fabrication of 3-dimensionally porous-structured PPy cell scaffolds is demonstrated, and the viability of such films for cell adhesion and proliferation is evaluated using an MTS cell proliferation assay. The porous-structured PPy was prepared by electrochemical PPy polymerization through the interstitial voids of a thermo-sensitive agarose gel ($T_{Gel} \sim 20 \text{ }^{\circ}\text{C}$) template. Selective removal of the template from the agarose-PPy matrix immersed in boiling water yielded porous-structured PPy cell scaffolds. The morphology and chemical surface composition of the PPy scaffolds were evaluated by SEM and XPS, respectively. A model human umbilical vein endothelial cells (HUVECs) were seeded and cultured over the PPy scaffolds to quantify the cell viability. The PPy with high surface area and interconnected porous network exhibited enhanced cell adhesion and proliferation compared to conventional non-porous PPy films. This research was supported by a grant from the Academic Research Program of Korea National University of Transportation in 2013.

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용액공정으로 150°C 저온 소성한 ZnO 산화물 반도체 소자의 산화막 두께와 소성법에 따른 전기적 성질에 관한 연구

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ZnO TFTs 는 낮은 온도에서 성막하여도 좋은 전기적 성질을 나타내고, 공기 중에서도 높은 안정성을 나타내는 장점 때문에 최근 박막 트랜지스터로의 응용에 큰 관심을 끌고 있다. 본 연구에서는 전구체를 이용한 합성을 통해 얻은 물질로 용액 공정을 통해 ZnO TFTs 소자를 구성하여 전기적 성질과 안정성을 연구하였다. 합성된 $\text{Zn}(\text{OH})_2 / \text{NH}_4 \text{OH}$ 용액은 5wt %까지 용액화 할 수 있고, 높은 농도의 용액으로 성막된 ZnO 박막 두께는 선형적으로 증가한다. 용액공정 ZnO TFTs 는 gate electrode 로 P-도핑 된 Si 기판에 100nm 의 SiO_2 절연체 층을 이용한 소자와 gate patterned device 를 구성하기 위해 $\text{ZrO}(\text{NO}_3)_2$ 을 전구체로 이용한 절연체층을 적용하였다. 2wt% $\text{Zn}(\text{OH})_2 / \text{NH}_4 \text{OH}$ 용액으로 150°C 열처리 공정을 통해서 SiO_2 절연체를 이용한 bottom gate 소자인 경우 ZnO 층 두께는 ~30nm 이며, 이동도는 ~0.6 $\text{cm}^2/\text{V} \cdot \text{s}$ 을 나타낸다. 반도체 막 두께 조절을 통해 ~50nm 의 ZnO 층 두께인 소자는 1.17 $\text{cm}^2/\text{V} \cdot \text{s}$ 의 이동도를 나타냈다. 또한, 새로운 소성법을 이용해 4wt% $\text{Zn}(\text{OH})_2 / \text{NH}_4 \text{OH}$ 용액을 사용한 소자의 경우는 2.91 $\text{cm}^2/\text{V} \cdot \text{s}$ 의 이동도를 얻을 수 있었다. passivation layer 없이도 ZnO 의 TFTs 는 수개월 동안 안정적인 이동도를 유지했다.

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Size dependent interaction of calcium carbonate materials with plasma and blood cells

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We have investigated interaction between calcium carbonate materials and blood components according to the particle size of calcium carbonate. Three calcium carbonate materials with different primary particle size and distribution were purchased: submicron-sized, nano-sized with either broad or narrow distribution. In order to evaluate the biological interaction, calcium carbonates were mixed with plasma or whole blood obtained from rat. According to X-ray diffraction patterns, it was confirmed that all the samples preserve their highly crystalline Calcite even after exposure to plasma. However, zeta-potential values of all the samples significantly decreased suggesting possible surface interaction of calcium carbonates with plasma proteins. Time-dependent protein fluorescence quenching ratio was determined that nano-sized calcium carbonate have higher interaction than submicron-sized ones. The red blood cells treated with three calcium carbonate materials were visualized with both optical and electron microscopy images to confirm the morphological change, and results suggested that nano-sized particles interact more actively with blood cells. Acknowledgement This research was supported by a grant (13182MFDS608) from Ministry of Food and Drug Safety in 2013.

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Interaction between biological matrix and different sized calcium carbonate materials

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Nano-sized materials, due to their large surface area, often exhibit unexpected effect when they interact with various molecules. Especially, their interactions with biological molecules are important in developing biological application of nanomaterials. We evaluated the particle size dependent interaction of calcium carbonate with biological matrix such as plasma protein, digestive protein and electrolyte. Three calcium carbonate materials with different particle size and distribution were purchased. Those calcium carbonate samples were added to simulated physiological solutions mimicking gastric, intestinal and plasma environment. From scanning electron microscopy, it was revealed that the overall morphology of calcium carbonates was preserved regardless of particle size and physiological conditions. However, the zeta-potential of calcium carbonate changed significantly according to the particle size and treated condition, showing that the particle size effected the interaction between calcium carbonate and biological matrices. In order to study the interaction between calcium carbonate materials and proteins precisely, we also carried out time dependent protein fluorescence quenching assay as well as protein adsorption analysis. Acknowledgement This research was supported by a grant (13182MFDS608) from Ministry of Food and Drug Safety in 2013.

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The Fluorescent 2-[2-(2-Fluorophenyl)acetyl]-N-(m-tolyl)hydrazinecarboxamide as Ni Ion Sensor

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The fluorescent 2-[2-(2-fluorophenyl)acetyl]-N-(m-tolyl)hydrazinecarboxamide was synthesized by the condensation of 2-(2-fluorophenyl)acetohydrazide with 1-isocyanato-3-methylbenzene, which showed effective fluorescence emission signal at 339 nm, upon chelation with 1-equivalent nickel (II) chloride, while there was no fluorescence signal for competitive ion (Cr³⁺, Cd²⁺, Pb²⁺, Zn²⁺, Hg²⁺, Co²⁺, Ni²⁺, Ca²⁺, Mg²⁺, Ag²⁺, Mn²⁺, Sr²⁺, Cs²⁺, Na⁺, K⁺, Li⁺) in this range recorded at neutral pH. The fluorescence emission was quenched in basic solution while acidic pH does not show any effect on the emission intensity. The synthesized aromatic semicarbazide derivative can be used for selective detection of Ni ion in micromolar concentration level.

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In vitro behavior and in vivo absorption of different sized calcium carbonate materials

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Calcium carbonate is widely used as food additives or dietary calcium supplement. Its physical properties including particle size and shape are known to affect its chemical interaction with biological substances during digestive processes. In this study, we analysed physico-chemical properties and biological behaviours of three different calcium carbonate materials: bulk, food grade nano and reagent grade nano calcium carbonate. The powder X-ray diffraction patterns showed that all the samples had highly crystallized Calcite structures (JCPDS 47-1743). Dynamic light scattering analysis confirmed that all the samples made agglomerate in water suspension showing 2 ~ 6 μm size. In order to evaluate biological behaviors of three different calcium carbonates during digestive process, simulated body fluids, gastric and intestinal solution and collected digestive fluids from rats were treated to calcium carbonates. According to the X-ray diffraction patterns, the calcite structure of all the calcium carbonates were well preserved while some unknown impurity phase evolved in food grade and reagent grade nano samples. Inductively coupled plasma-atomic emission spectroscopy revealed that small particles more dissolve than large particles. The calcium carbonates were orally administered to rats and their pharmacokinetic parameters were evaluated. The results showed that smaller particles shorten the half life, while the total absorption amount was not significantly affected according to sample type. Acknowledgement This research was supported by a grant (13182MFDS608) from Ministry of Food and Drug Safety in 2013.

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Copper Electrode Materials Using Copper Amine/Diamine Complex for Printed Electronics

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Previous researches have successfully produced conductive thin films from inks based on organo-metallic compounds. Nonetheless, some inks, like those made from copper salt and amines, tend to move during thermal annealing and thus, affecting the conductive pattern on the substrate. In this study, conductive inks were synthesized by forming complexes of copper with amines and/or blended amines. A diamine was added to the complex to build-up an organo-metallic framework. The prepared inks were coated on glass substrate and were annealed on a hot plate at 170 °C under the gaseous mixture of formic acid and methanol for 5 minutes. It was observed that there were less movements and better fixation on the substrate during annealing. Inks with blended amines produced films with lower resistivities. The lowest electrical resistivity recorded was 4.99 Ω·cm. To increase the metal content of the films and reduce the porosity, copper nanoparticles and copper nanopowders were added to the new formulation of the ink.

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Thermally modified metal-insulator transition of vanadium dioxide crystals prepared by hydrothermal method

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부경대학교 화학과

The clear insulator (Monoclinic-VO₂) to metal (Rutile-VO₂) transition (IMT) was observed in electrical conductivity and differential scanning calorimeter(DSC) measurements at around 340 K, IMT temperature (T_H), in the hydrothermally prepared VO₂ crystals. The occurrence of metal to insulator transition (MIT) temperature (T_C) was observed below 333 K during the first resistance measurement cycle in most of case. The sudden jump of the electrical resistance at MIT was amplified several times than that of the first cycle during the repeated successive thermal cycles (heating and cooling across the IMT and MIT temperature). The T_C and T_H moved to higher temperature by the repeated successive thermal cycles. The transition temperatures moving will be related to the relaxation process of mechanical stress between the VO₂ crystals. However, the starting point of MIT, T_{CS} = ~336 K, and the starting point of IMT, T_{HS} = ~338 K, keep almost constant. These temperatures may be related to the intrinsic properties of the VO₂: the phase transitions initiated at these temperatures. The neat surface of the VO₂ crystals was severely damaged after more than 70 times of the repeated thermal cycles. The damaged surface, originated from the crystal volume change during the first order transition of the VO₂, will reduce the probability of the electrical conduction between the VO₂ single crystals and will result the amplified jump at the repeated MIT.

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Electrical properties and Raman analysis of gold nanoparticles attached carbon nanotubes with the diameter of various size

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A convenient route is developed to fabricate the gold nanoparticles(AuNPs) attached carbon nanotubes (Au-CNTs) with the diameter of various sizes through the carbonization of sucrose with anodic aluminum oxide (AAO) template. A thermal decomposition of HAuCl_4 within AAO template produced the high crystalline AuNPs of ~20 nm size. The diameter of Au-CNTs with 40 ~ 250 nm size could be controlled by nanochannel diameter of AAO template. The morphology of Au-CNTs with 40 nm in diameter was the flexible bamboo-like tubes, whereas the shapes of CNTs above 80 nm in diameters were the neat and straight tubes. These differences of morphology with respect to the diameter of CNTs are related to crystallinity of carbon phase. The enlargement of graphite particle size and the high crystallinity of the graphitized carbon phase depending on the increase of the diameter of CNTs were confirmed by the broadening of G and D band appeared in Raman shift. The electrical conductivity of Au-CNTs according to the diameter of CNTs showed the fairly high value up to $\sim 10^4$ S/cm due to their graphitized carbon crystals. And, the Au-CNTs exhibit the small band gaps on the order of 20 meV.

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Fabrication of Graphene Nano-ring Arrays using Au@Pt Nanodisk as a Pattern Mask

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The arrangement and fabrication of distinctive graphene shape such as nanomesh and nanoribbon has gained a great deal of attention for applications such as electronic devices. Here, we fabricate 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 control the shape of graphene frames by changing the Au@Pt nanoplates. This fabrication method for graphene nano-rings will suggest the future graphene electronics.

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Fabrication and Characterization of 3-Dimensional Cu@SnO₂@Ppy Nanorods for Lithium-Ion Batteries

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We fabricated 3-dimensional (3D) Cu nanorods (NRs) coated with SnO₂ and polypyrrole (Ppy) on Cu foil by assisted anodized alumina oxides (AAO) template. The anode active materials of SnO₂ on Cu NRs array were synthesized by using cyclic voltammetry (CV), followed by coating of Ppy via cathodic electrodeposition method. Then, we confirmed that the electrode without Ppy showed a decrease of specific capacity continuously. On the other hand, the electrode coated with Ppy steadily maintains its capacity over 50 cycles. It is speculated that Cu@SnO₂@Ppy NRs electrode has more stability in terms of specific capacity than that without Ppy electrode since Ppy outer layer suppresses the volume expansion of SnO₂. As-prepared samples were characterized with various techniques such as SEM, TEM, XPS and XRD.

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Three-dimensional silicon as anode coated on Cu NRs for lithium-ion battery

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성균관대학교 에너지과학과 ¹성균관대학교 화학과

We synthesized three-dimensional silicon as anode electrode coated on Cu nanorods arrays which were prepared by electropulse deposition as current collector. Silicon is also electrodeposited in glove box because silicon readily oxidized on exposure to air. Silicon is one of the most promising anode materials because it has the highest known theoretical capacity. However silicon is hindered by poor cyclability because of its large volume change associated with the insertion and extraction of lithium. Volume change during lithiation and delithiation cause pulverization of silicon, which lead to a loss of electrical contact and eventual fading of capacity. Three-dimensional nanostructure which silicon is coated on cu nanorods is possible to overcome volume change. Coated silicon on cu nanorods led to reversible capacity and more stable cycle life.

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Facile Synthesis of Pd@Pt Core-shell Nanotubes Array with Controllable Pores and Their Enhanced Catalytic Performance for Methanol-oxidation

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In this work, we demonstrate for the first time that vertically aligned Pd@Pt core-shell nanotubes array is able to be successfully synthesized using anodic aluminum oxide (AAO) template-assisted electro-deposition, and resulting nanostructures exhibit higher catalytic activity in methanol oxidation than either individual constituent (Pt or Pd). The facile synthesis of Pd@Pt tubular nanostructure was inspired by the previously developed thin-walled Pd nanotubes formation mechanism, which takes advantage of surface hydroxyl chemistry of AAO template and comparable reduction potential of Pd complex anions and hydrogen cations. The thickness of Pt layer in Pd@Pt core-shell nanotubes could well controlled by electro-depositon method. The inner and outer wall of perpendicular opened Pd@Pt nanotubes enhanced the ratio of surface area to mass relative to solid nanorods structure, resulting in higher current density in methanol oxidation. More importantly, synergistic electronic effect between Pt and Pd gives rise to the enhanced catalytic activity in methanol oxidation, as evidenced from comparisons in onset potentials and CO oxidation behaviors. Thus, vertically aligned Pd@Pt nanotubes may potentially act as upgraded catalyst in methanol oxidation compared to Pt nanorods structure counterpart.

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Synthesis and Electrochemical Studies of Ligand-Protected Quantum-Sized Gold Nanoclusters

표경립 광규주 고은솔 이동일*

연세대학교 화학과

For the past few years, owing to high chemical and thermodynamic stability, gold nanoclusters(AuNCs), protected with ligands, have been one of the most extensively studied nanomaterials. In the present research, we synthesized and studied the properties of two different types of AuNCs, which were separately protected with hexanethiol and 3-mercapto-1-propylsulfonate ligands(MPS). The synthesis was carried out in a mixed solvents by reducing gold(III) salt with sodium borohydride in the presence of the specific ligands. By comparing these two types of AuNCs we found out that AuNCs showed different properties depending on the sizes as well as the ligands protecting them. The AuNCs protected with hexanethiol ligands were soluble in organic solvents while the ones stabilized with MPS ligands(MPS-AuNCs) were soluble only in aqueous solvents. Both AuNCs showed unique stair-wise UV-vis spectra and size-dependent electrochemical properties. Water soluble MPS-AuNCs were phase-transferred to organic phase for electrochemistry studies. The presence of sulfonate terminal groups on the end of the ligands enabled facile phase transfer by ion-pairing with hydrophobic cations. Observing the electrochemistry of AuNCs it was found to be stable and redox active allowing the possibility for being used in diverse applications such as biosensors and catalysts.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-997

발표분야: 재료화학

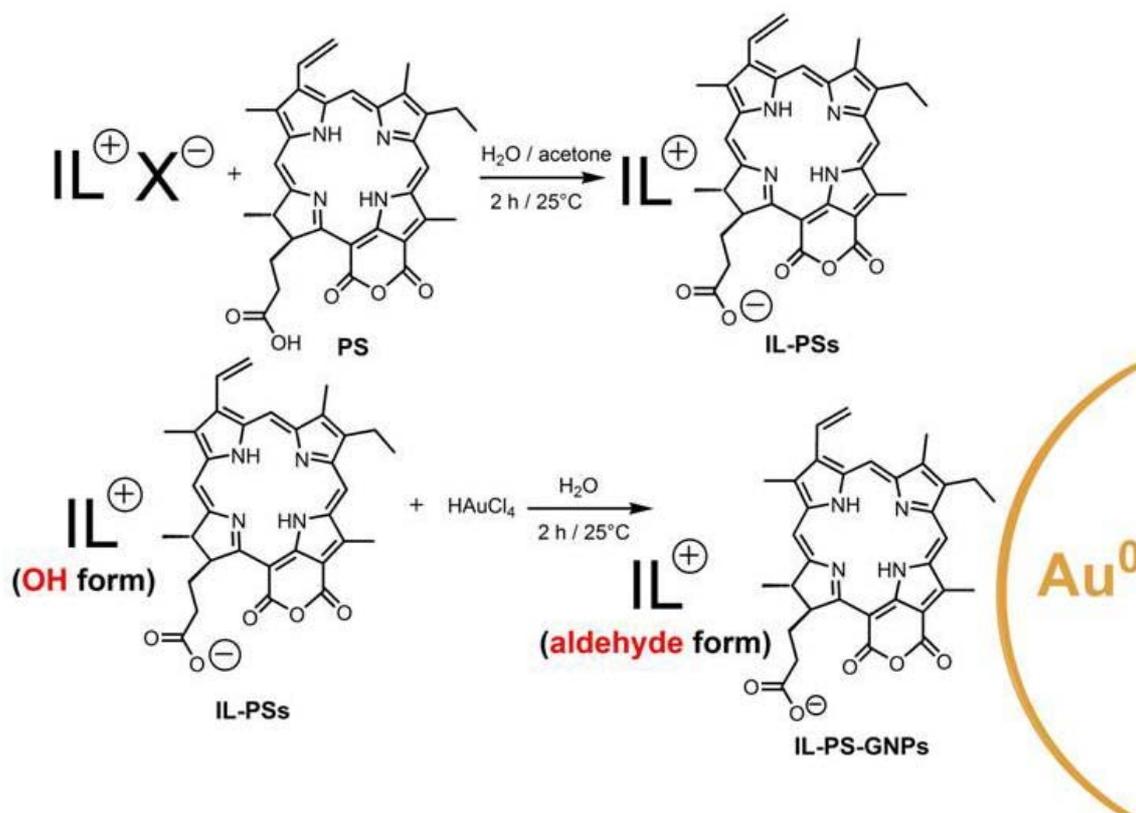
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ionic Liquid Type Purpurin-18 Derivatives and Gold Nanoparticles for Photodynamic Therapy

윤일* 이태현¹ 심영기^{1,*}

인제대학교 PDT 연구소 ¹인제대학교 나노공학부

Generally, most of the PSs are hydrophobic, which may afford disadvantage to make the PSs insoluble under physiological conditions and hinders to reach the accumulation in the tumor sites. Therefore, in order to increase uptake of PSs into tumor cells, it is very important to keep suitable hydrophobic/hydrophilic balance of PSs, for which use of gold nanoparticles (GNPs) has a great interest as efficient carriers of PS. Ionic liquids (ILs) are useful materials for generating GNPs complex with high stability. IL type PS (ILPS) may help PSs capable of increased solubility in aqueous system as well as support attachment of PSs on GNPs surface through stable electrostatic interactions between ILs and PSs. In this work, four different kinds of ILs 1?4, such as morpholinium, cholinium, imidazolium, and ammonium type, were prepared and used to form GNPs from a reaction between ILPSs 1?4 (containing Purpurin-18) and Au(III) without any additional reducing agents and surfactants. The hydroxyl groups and positive charge units of ILs 1?4 have important roles as a reducing agent as well as a stabilizer through the electrically charged functional groups in forming the GNPs complexes 1?4. PDT efficacy of the ILPSs 1?4 and the corresponding GNPs complexes 1?4 was investigated by MTT assay against A549 and HeLa cell lines. The GNPs complexes showed higher cell viability compared to the corresponding free ILPSs, respectively, due to higher cell penetration based on excellent delivery effect of the GNPs. Among the complexes, the relative PDT activity difference was depend on the property of the ILPSs (e.g. different reduction strength of Au(III)).



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장소: 창원CECO

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발표분야: 재료화학

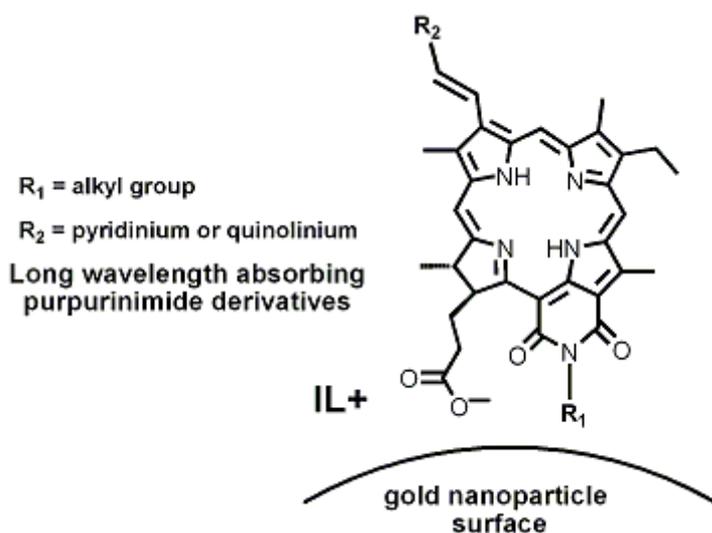
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photodynamic Activities of Novel Gold Nanoparticles as Long Wavelength Absorbing Photosensitizers

윤일* 이태현¹ 심영기^{1,*}

인제대학교 PDT 연구소 ¹인제대학교 나노공학부

Synthesis of novel long wavelength absorbing photosensitizers (PSs) using purpurin-18-N-butylimide and pyridinium or quinolinium moiety at 32 position of the purpurinimide molecule and its ionic liquid (IL) type gold nanoparticles (GNPs) is described. The structures of the purpurinimide derivatives and its IL type GNPs are confirmed by ¹H-NMR spectroscopy, mass spectrometry, UV-vis spectroscopy, TGA and TEM measurements. In addition, photodynamic activity of the purpurinimide compounds and its GNPs are evaluated against A549 and HeLa cell lines. Cell viability results are calculated by MTT assay, and cell penetration and accumulation of the GNPs are confirmed by confocal laser scanning microscopy measurement.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-999

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Asymmetric Material for Organic Light-Emitting Diodes(OLEDs)

전찬우 황재영¹ 김란² 한승훈² 김윤희^{2,*}

경상대학교 자연과학대학 화학과 ¹경상대학교 그린에너지융합연구소 ²경상대학교 화학과

We have synthesized asymmetrical organic light-emitting diodes (OLEDs) material based on anthracene. The advantages of anthracene are easy substitution at the 9 and 10 positions, high thermal stability and high electronic stability. Anthracene derivatives have been widely used as emitting materials in OLEDs, because these derivatives have excellent photoluminescence (PL). In principle, the asymmetric structure can control the electronic properties due to different dipoles and can also inhibit intermolecular interaction due to reduced stacking, compared with a symmetric structure. In this study, we designed and developed new asymmetrical material with anthracene. We expect in foreseeable future this material using blue OLED material.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1000

발표분야: 재료화학

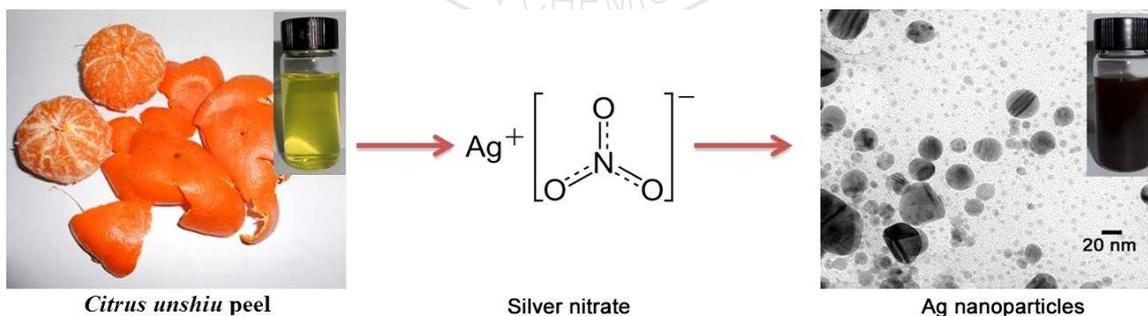
발표종류: 포스터, 발표일시: 수 16:00~19:00

Green Synthesis of Silver Nanoparticles Using Satsuma Mandarin (Citrus Unshiu) Peel Extract

BASAVEGOWDANAGARAJ 이용록*

영남대학교 화학공학부

Silver nanoparticles (AgNps) were synthesized by using Satsuma mandarin peel extract as a simple, non-toxic, eco-friendly without adding external surfactant and capping agent. When the aqueous silver (Ag⁺) ions were exposed to Satsuma mandarin peel extract, silver nanoparticles were reduced in the size range from 5-20 nm. The silver nanoparticles were characterized by UV-Vis spectroscopy, fourier transform infra-red spectroscopy (FT-IR), x-ray diffraction (XRD) and transmission electron microscopy (TEM) with energy dispersive x-ray analysis (EDAX). This study shows the feasibility of using fruit waste material for the synthesis of AgNps which is potentially more scalable and economic due to its lower cost.



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장소: 창원CECO

발표코드: MAT.P-1001

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

상온 고체전해질의 합성 및 전기화학 CO₂ 가스센서로의 응용

이형근

한국전자통신연구원 부품소재연구부문/나노융합센서연구실

지구 온난화의 영향으로 CO₂ 가스의 감지 및 저감에 많은 연구가 진행되고 있다. CO₂ 가스를 측정하는 센서는 광학식, 전기화학식, 반도체식 가스센서 등이 연구되고 있다. 광학식 CO₂ 가스 센서는 정밀하고 신뢰도 높은 장점이 있으나, 복잡하고 부피가 크다는 단점과 높은 생산가격으로 인해 넓은 영역의 대기에서 CO₂ 가스 감지를 위한 응용에는 적합하지 않다. 반도체식 가스센서는 아직 개발 초기 단계이며, 그 동작 메커니즘이 정확히 밝혀지지 않은 상태이다. 이에 상대적으로 동작 신뢰도가 확보되고, 초박형 저전력화 가능한 고체전해질 전기화학식 CO₂ 센서를 개발하고자 한다. 고체전해질 전기화학식 CO₂ 센서는 알칼리 카보네이트 계열의 감지물질이 고온에서 산소와 이산화탄소로 분해되는 반응을 이용하며, 이때 생성되는 리튬이온의 양을 고체전해질 상의 기준전극과 감지전극 간의 기전력을 측정하여 대기의 CO₂ 농도를 결정하게 된다. 본 연구에서는 고온(400~500도)에서 동작하는 고체전해질 전기화학식 CO₂ 센서의 동작온도를 저감하기 위한 상온 고체전해질 개발과 그 결과물인 CO₂ 센서의 동작 특성에 대해 발표하고자 한다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1002

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new Mussel-Inspired Polydopamine Phototransistor with Ultra-High Photosensitivity

남혜진 차준호¹ 정덕영^{2,*}

성균관대학교 기초과학연구소 ¹성균관대학교 화학 ²성균관대학교 화학과

We first demonstrated a polydopamine (PDA)-based organic phototransistor (OPT) showing excellent photo-controlled switching properties at low voltages as well as good adhesion with SiO₂/Si substrates. PDA thin film with a dense and conformal surface was prepared by self-polymerization using O₂ gas as an oxygen source instead of a conventional air stream. The PDA exhibited ultra-high photoresponsivity and efficient light detection ability. The single-step deposition process and precise control of the PDA thin film by micropatterning led to fabricate high-performance OPTs. The PDA-based OPTs exhibited p-type semiconducting characteristics and ultra-high photoresponse properties with I_{light}/I_{dark} ratio of 6.9×10⁴ and photoresponsivity of 1050 AW⁻¹ depending on incident light intensity. The excellent device performance producing an extremely high photocurrent at a low voltage provides potential applications in low-cost, high-density organic optoelectronics.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1003

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemical reaction of metal hydroxides in aqueous solutions

이상남 정덕영* 차지현 차준호¹ 이한경 박승욱 김유중 배상미

성균관대학교 화학과 ¹성균관대학교 화학

We reported the syntheses of precursor materials for Cu-In-Ga-S-Se absorber layer and characterization of chemical properties. Advantages of hydroxide-based precursor synthesis by using a co-precipitation method were stability of ambient atmosphere and easy of synthesis. We prepared the metal hydroxides with various molar ratios and added an aqueous alkali hydroxide solution at room temperature. The obtained metal precursors confirm hydroxide form by TGA, to be dehydration and dehydroxylation. The metal the hydroxide precursors were mixed with the aqueous SeO_3 to prepare the salt precursor [CIG]- $[\text{SeO}_3^{2-}]$ through acid-base reaction. On the basis of TGA and Raman spectroscopy results, we demonstrated the formation of [CIG]- $[\text{SeO}_3^{2-}]$. The as-prepared precursors and heat-treated samples were characterized by SEM, XRD and XRF and ICP-AES.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1004**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

pH-Induced Aggregation of Gold Nanoparticles-Photosensitizer complex for Photothermal/Photodynamic dual Therapy

정영재 윤일¹ 김승범² 이우경*

인제대학교 나노공학부 ¹인제대학교 PDT 연구소 ²인제대학교 나노시스템

Smart gold nanoparticles that is designed to aggregate in weak acidic intracellular environments by its hydrolysis-susceptible citraconic amide surface. When pH was changed, the gold nanoparticle surfaces are engineered to have both positive and negative charges. In this experiment, cis-aconitic amide was used instead of citraconic amide to link gold nanoparticle and photosensitizer for photothermal/photodynamic dual therapy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1005

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Conductive Silver Paste using SiO₂@Ag Core-Shell Nanocomposite

길현석 차민혁 김상호 이석우*

공주대학교 화학과

In this study, we have prepared the silver nanocomposite using silica beads and silver precursor, and investigated the application of nanocomposite to conductive silver paste. The silver nanoparticles (AgNP) were prepared by the chemical reduction method using trisodium citrate (Na₃Cit) as a surfactant and hydrazine as a reducing agent. The SiO₂@Ag core-shell nanocomposite was synthesized by controlled growth method after formation of seed on the silica surface. The composites were characterized by SEM, EDS, powder XRD, ICP-AES, and UV/Vis analyses. The dispersability of AgNP was investigated in various solvents. Finally, conductivity of silver pastes prepared using AgNP and composite was investigated as a function of sintering temperature.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1006**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

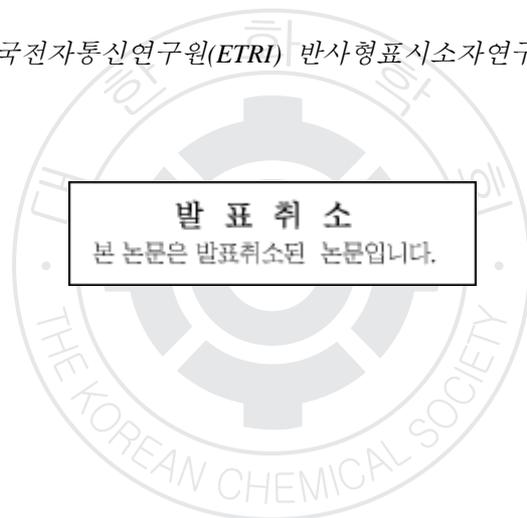
**[발표취소] Optical and electrical properties of high transparent
electrochromic optical shutter**

아칠성* 류호준

한국전자통신연구원(ETRI) 반사형표시소자연구실

발 표 취 소

본 논문은 발표취소된 논문입니다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1007**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Behaviors of Silicon/Pitch and Graphene Oxide Composite as Anode materials for High Capacity Lithium Ion Secondary Battery

임태진 박수진*

인하대학교 화학과

In this work, to avoid volume expansion of silicon during intercalation/de-intercalation of lithium we coated pitch on silicon particle. Carbon/silicon composites were synthesized by mixing silicon powders with petroleum pitch and subsequent heat treatment. And we used GO as Conductive material to improve electriccal conductive. The physical characteristics of the synthesized composites were analyzed by SEM and XRD. In addition, their electrochemical properties were examined by the electrochemical analysis techniques such as charge/discharge performance, cyclic voltammetry.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1008

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Microporous Carbon Supports on Electrochemical Behaviors of Pt-Ru/Carbons as Catalysts for Direct Methanol Fuel Cells

임태진 박수진*

인하대학교 화학과

In this work, microporous carbons were prepared by a conventional zeolite templating method using furfuryl alcohol for catalysts supports in direct methanol fuel cells (DMFCs). The Zeolite templating carbons (ZTCs) were conducted KOH activation with different activation temperatures. We deposited 30 wt% of Pt-Ru metals on activated ZTCs (A-ZTCs) by chemical reduction method. The crystalline and structural features of Pt-Ru/ZTCs were investigated by X-ray diffraction (XRD). The textural properties of activated ZTCs (A-ZTCs) were investigated by N₂/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and BJH method. The surface morphology was characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The electrochemical properties of Pt-Ru/ZTCs catalysts were also analyzed by cyclic voltammetry measurements.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1009

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Masking Nanoparticle Surfaces for Sensitive and Selective Colorimetric Detection of Proteins

김병호 이재승*

고려대학교 신소재공학부

We have developed a convenient and efficient colorimetric detection system for protein targets using aptamer-gold nanoparticle conjugates. We take advantage of the correlation between the catalytic properties and the exposed surface area of the nanoparticles, which is inversely proportional to the amount of the aptamer-bound protein targets. As the concentration of the protein target increases, the nanoparticle surface area becomes more masked, thus increasing the reduction time of 4-nitrophenol for the color change. We also reduce the detection time by either redesigning the aptamer sequences or regulating their density. This detection system is highly selective, discriminating the target protein even at a concentration 1000 times higher than the limit of detection (LOD). Importantly, to the best of our knowledge, the LOD with the unaided eye in this work is the lowest for a colorimetric detection system using lysozyme as a model protein (16 nM). Lysozyme in chicken egg whites is directly analyzed using our detection system, whose results are in excellent agreement with the ELISA analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1010

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cobalt redox couple in back illuminated dye-sensitized solar cells with Ti foil substrate

김점중 성기현¹ 김보람¹ 윤용진^{1,*}

한국전자통신연구원 IT부품산업기술연구부 ¹경상대학교 화학과

Dye-sensitized solar cells (DSSCs) have been considered as a next generation solar cell because they are cost-effective and eco-friendly with relatively high efficiency. To commercialize the DSSCs, a module with 10% efficiency may need to be priced at US\$ 20 - 30m⁻². Due to the high cost of transparent oxide (TCO) layer, low cost of DSSCs which replaced one or two TCO-coated glasses with metal foil(s) are considered as a highly promising cell type in DSSCs. In particular, Ti foils as a substrate of photoanode have shown a plenty of advantages, such as low sheet resistance, good flexibility, excellent corrosion resistance and high-temperature stability. However, the solar light should be irradiated from Pt coated counter electrode, i.e., back illumination. That means that solar light have to pass through the I₃⁻ / I⁻ redox couple before reaching to photoanode. Inherently, some wavelengths of solar energy will be scattered and absorbed by the electrolyte, which decrease the cell efficiency significantly. In back illuminated dye-sensitized solar cells (DSSCs) with Ti foil, it is demonstrated that the cobalt redox couples can replace the conventional I₃⁻ / I⁻, which had limited photovoltaic performance and large scale production. By simultaneous effects of the higher transmittance of cobalt redox electrolyte and thermally formed oxides layer on Ti foil, a 7.12% of highly efficient power conversion efficiency (PCE) has been accomplished, which overcomes that (5.7%) of DSSCs based on the I₃⁻ / I⁻ electrolyte.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1011**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

WO₃-based Core-shell Photoanodes for Photoelectrochemical Water Splitting

이현주 aqi 이민형*

경희대학교 응용화학과

The solar-driven production of hydrogen from the water splitting can provide renewable and green source of energy. Here, we report WO₃/CuWO₄ and WO₃/BiWO₆ core-shell nanowires as photoanode components for a water-splitting photoelectrochemical (PEC) cell. The core-shell nanowires were synthesized by chemical and heat treatment on WO₃ nanowires grown by chemical vapor deposition (CVD). The core-shell nanowires showed enhanced PEC performance compared to WO₃ nanowires due to increased light absorption in the visible light. Also, the core-shell nanowires exhibit excellent chemical stability in a wide pH range and long-term stability against photocorrosion. Furthermore, plasmon-assisted photocurrent generation using the core-shell nanowires decorated with plasmonic nanoparticle will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1012

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Tin Chalcogenide Nanocrystals Using Laser Photolysis and their composition tuning

임형순 박정희^{1,*} 장동명¹ 정찬수¹ 임영록¹ 박기동²

고려대학교 미세소자공학협동/마이크로소자공학 ¹고려대학교 소재화학과 ²고려대학교 미세
소자협동과정

Narrow band gap IV-VI semiconductors, typically have narrow band gaps, leading to efficient absorption of incident solar radiation, constitute an important class of materials for photovoltaic applications. We developed a novel synthesis method for polytypic tin chalcogenide NCs with facile phase and composition control. They were synthesized by gas phase reaction using a 1064 nm Nd:YAG pulsed laser in a closed glass reactor. Sn(CH₃)₄, H₂S, and Se(CH₃)₂ were chosen as precursors of Sn, S, and Se, respectively.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1013

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Laser-Induced Graphitization of Nanodiamond for Oxygen Reduction Reaction

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에너지 공학과 대학원 ³고려대학교 미세소자협동과정

Graphitic layered nanodiamonds were conveniently prepared by the pulsed laser irradiation of colloidal solution. The fraction of graphite/diamond phases was simply controlled by the irradiation time. They exhibit remarkably electrocatalytic activity for oxygen reduction reaction (ORR). They were doped with pyrrolic-type nitrogen that ensures four-electron pathway of ORR.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1014

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Quaternary Composition GaP-ZnS Nanowire

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Semiconductors with direct band gaps corresponding to the energy of visible light have many important applications such as light emitting diodes and photocatalysts. The GaP-ZnS nanowires have been synthesized via catalyst-assisted chemical vapor transport method under vapor-liquid-solid mechanism. The morphology, chemical composition, and crystal structure of the as-synthesized nanowires were investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, and X-ray diffraction pattern. Herein, we observed that GaP-ZnS quaternary alloy nanowires exhibit improved photoluminescence, and the band gaps smaller than that of either GaP or ZnS.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1015

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In-situ HRTEM observation of phase transition in GeTe-Bi₂Te₃ nanowire driven by thermal annealing

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Solid-state structural transformation coupled with an electronic property change is an important mechanism for nonvolatile information storage technologies, such as phase-change memories. Herein we aim to exploit the phase-change materials of germanium bismuth telluride (GeTe-Bi₂Te₃) pseudobinary nanowires. High-quality GeTe-Bi₂Te₃ nanowires have been synthesized via thermal evaporation method under vapor-liquid-solid mechanism. The morphology, chemical composition, and crystal structure of the as-synthesized GeTe-Bi₂Te₃ nanowires were investigated by scanning electron microscopy(SEM), energy dispersive X-ray spectroscopy(EDX), high-resolution transmission electron microscopy (HR-TEM), and X-ray diffraction pattern(XRD). In-situ TEM technique was used to study the metastable crystal structures to the stable thermodynamic phase transition in GeTe-Bi₂Te₃ via thermal heating.

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장소: 창원CECO

발표코드: **MAT.P-1016**

발표분야: 재료화학

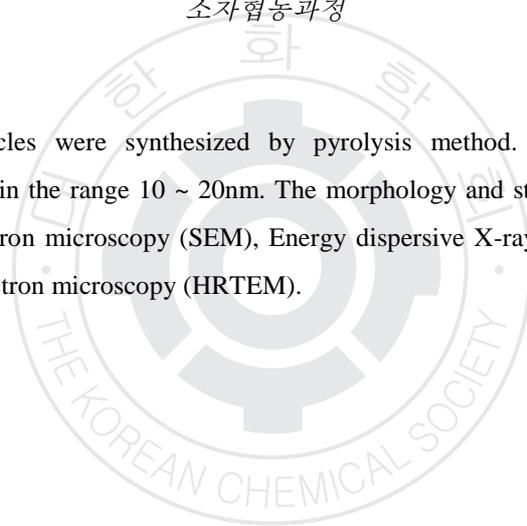
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of high yield Iron Nanoparticles and Their Application

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소자협동과정

high-yield Iron nanoparticles were synthesized by pyrolysis method. The diameter of the iron nanoparticles is controlled in the range 10 ~ 20nm. The morphology and structure of the products were analyzed by scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HRTEM).



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1017

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ionic liquid-doped and p-NIPAAm-based temperature responsive copolymer: Extraordinary entrapping and releasing behaviors of BSA at 36-42 °C

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단국대학교 WCU ¹ 단국대학교 나노바이오의과학

Positive charge doping on the temperature responsive polymer p-NIPAAm was achieved by radical copolymerization of N-isopropyl acryl amide (NIPAAm) and 1-butyl-3-vinylimidazolium bromide ([BVIIm]Br) to give a new temperature responsive copolymer (p-NIBIm). The resulted cationic copolymer chain was found to be composed of about 97 mol% of NIPAAm and 3 mol% of [BVIIm]Br moieties by ¹H-NMR analysis. The p-NIBIm copolymer showed the highly increased Zeta potential value and the LCST (lower critical solution temperatures) value, respectively, +9.8 mV at pH=7 and 38.3 °C, compared to those (+0.3 mV at pH=7 and 32.1 °C) of p-NIPAAm without the cationic moiety. It was confirmed in SEM microgram that the cationic copolymer molecules exist in micellar form with the size of less than 300 nm in diameter created via spontaneous self-assembly during drying at 45 °C. The dependence of the p-NIBIm micelle sizes on the temperatures ranging from 25 to 45 °C also was determined using Zeta Sizer under aqueous condition, showing a certain size contraction from 253 to 90.5 nm in diameter (about 95.4 % contraction in volume). The thermo-sensitive behaviors to entrap BSA protein at the body temperature (36-37 °C) and to release the protein near the LCST (38-42 °C) also were tested by sizing of the complexes of p-NIBIm/BSA using Zeta Sizer and by a colorimetric assay method using Bio-Rad DC Protein Assay II kit, resulting in a maximum entrapment of 70 g BSA for 1 mg polymer at the body temperature (36-37 °C) and in a maximum release of 51 g BSA for 1 mg polymer (about 73 % releasing of the entrapped amount) at the temperature range of 38-42 °C. These results revealed that the cationic and temperature responsive co-polymeric systems have a very high applicability as a novel delivery system for negatively charged molecules as a natural (or synthetic) drug and DNA.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1018**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic H₂ Production of MoS₂ catalyst loaded *p*-InP Photocathodes

이정은 진하정 이민형*

경희대학교 응용화학과

Molybdenum disulfide (MoS₂) has been widely studied as a low-cost and efficient catalyst for hydrogen evolution reaction. Here, we synthesized MoS₂ nanoparticles with different morphologies using hydrothermal synthetic method. The synthesized MoS₂ particles showed high crystallinity, and provided excellent catalytic activity in hydrogen evolution reaction. To evaluate co-catalytic performance of MoS₂ in photoelectrochemical (PEC) water splitting, electrochemical performance of *p*-InP cathodes decorated with MoS₂ were investigated. PEC performance of *p*-InP photocathodes depending surface area of catalytical active edge termination of MoS₂ particles will be discussed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1019**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Full-color-emitting $\text{Eu}^{2+/3+}$ - and Tb^{3+} -codoped LaAlO_3 phosphors

이민호 정우식*

영남대학교 화학공학부

Full-color-emitting lanthanum aluminate (LaAlO_3) phosphors were prepared by calcining a mixture of alumina and Eu(III)/Tb(III) -codoped lanthanum carbonate hydroxide (LaCO_3OH) powders in Ar atmosphere. The LaCO_3OH powders were obtained from boiling an aqueous solution containing La(III) salt, Tb(III) salt, EuF_3 and urea. The LaAlO_3 powders were characterized by powder X-ray diffraction, SEM, IR and luminescence spectroscopy. The EuF_3 compound, which thermally decomposed to EuF_2 , made the formation temperature of LaAlO_3 powders lowered. The full-color-emission lines can be tuned by varying concentrations of EuF_3 and Tb(III) salt, reaction temperature, and duration time.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1020

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Inorganic Light Reflecting Material using Mica treated with TiO₂ Nanoparticles

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공주대학교 화학과

In this work, we have prepared the nanocomposite by the reaction of synthetic mica and titanium oxide, and investigated the application of nanocomposite to UV protecting creams. Titanium tetraisopropoxide was used as a precursor for titanium oxide and the preparation of nanocomposite was carried out in an acidic aqueous solution. Nanometer-sized titanium oxide particles were attached on the surface of layered mica. Phase transition in calcined composite was observed after annealing at 1000 °C. The composite were characterized by SEM, EDS, powder XRD, and DRS UV/Vis analyses. Finally, we measured monochromatic protection factor (MPF) of ultraviolet protection creams manufactured by using mica composite treated with titanium oxide in the range of 280~400 nm. The nanocomposites developed in this work might be applicable as inorganic light reflecting materials for UV protecting creams.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1021

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Polymer/Inorganic Light Protecting Material using Poly(ferulic acid) and ZnO Nanoparticles

송혜연 길현석 이석우*

공주대학교 화학과

본 연구에서는 중합체/무기 혼합 자외선 차단제를 제조하기 위하여, 피부 보호 효과를 갖는 나노미터 크기의 구형 중합체와 무기 재료 자외선 차단제인 ZnO 를 혼합하여 복합 재료를 제조한 후, 자외선 차단 효과를 살펴보고자 하였다. Ferulic acid 와 methacrylic acid 의 공중합체 합성 시, 첨가되는 가교제인 EGDMA 의 양에 따라 입자 크기를 조절하였으며, ZnO 와 배합하여 크기와 조성에 따른 자외선 차단 효율을 고찰하였다. SEM 이미지 분석, 입도 분석을 통하여 중합체의 모양과 크기를 확인하였으며, FT-IR, TGA, DSC, 원소 분석을 통해 제조된 물질의 물리화학적 특성을 규명하였다. DRS-UV/Vis 분석을 통해 제조된 복합 재료의 광반사 및 흡수 능력을 확인하였으며, 최종적으로 표준 프로토콜에 의해 제조된 자외선 차단용 배합물의 MPF 를 측정하여 자외선 차단 능력을 확인하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1022

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid and facile synthesis of $(\text{Zn}_x\text{Ag}_y\text{In}_z)\text{S}_2$ nanocrystal library via sono-combichem method and its characterization

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연세대학교 화학과 ¹한국화학연구원 나노기술융합연구단 ²한국화학연구원 형광물질연구팀

The ultrasound-based ZAIS nanocrystal synthesis can be utilized as a novel, simple and rapid method for creating a library of $(\text{Zn}_x\text{Ag}_y\text{In}_z)\text{S}_2$ NCs. The emission colors of the resulting NCs are tunable from blue to red, depending on their chemical composition. According to our characterization, the ZAIS NCs seem much brighter than QDs up to about 10 times and more photostable due to lack of photoblinking. Perhaps those are the most important features of these NCs because they allow more reliable fluorescence studies including single particle tracking. Their compact sizes about 4 nm, regardless of the emission colors, can also be an added value as fluorescence probes. Moreover, ZAIS NCs are non-toxic to cells as evidenced using two cell types, HCC-1954 and MCF-7, thereby showing a feasibility of their use for bio-imaging. In addition, the library of $(\text{Zn}_x\text{Ag}_y\text{In}_z)\text{S}_2$ NCs could assist photocatalyst, quantum dot-like solar cells applications and other relevant areas.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1023

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Carbon-Encapsulated Iron Nanoparticles and A Facile Separation Process between the Iron and Hollow Carbon Shell

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한국화학연구원 나노기술융합연구단 ¹연세대학교 화학과 ²한국화학연구원 형광물질연구팀

Spherical iron oxide and carbon-encapsulated iron nanoparticles have been prepared by ultrasonic irradiation followed by annealing at various temperatures. As the annealing temperature of the as-prepared α -Fe₂O₃ nanoparticles was increased, the sample transformed into γ -Fe₂O₃, Fe₃O₄, and Fe nanoparticles by reduction process without any additional reducing agent such as H₂ gas and created a carbon shell in the iron nanoparticles. By controlling the experimental conditions, (such as sonic irradiation time and ratio of binary solvent), Fe nanoparticles with various sizes can be formed with a diameter in the range of 100 - 800 nm and these nanoparticles are tightly encapsulated by 20 nm carbon shells. Because of their high saturation magnetization of 212 emu/g, the carbon-encapsulated Fe nanoparticles can be used for magnetic resonance imaging (MRI) with an dramatically enhancement efficiency comparable to commercially available T₂ contrast agents. A separation between the carbon shell and the Fe particle was observed when the annealing temperature was sufficiently high.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1024

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Superhydrophobic Surface of Surface-Treated Nano-Graphene Structure

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공학부

Surface morphology with superhydrophobicity has attracted extensive interest due to self-cleaning properties, reduced oxidation, and improved efficiency of marine vessels. We report a unique and direct route towards a superhydrophobic graphene surface, which opens up possibilities for transparent flexible graphene-based electrodes with a non-wetting property. Graphene structures were prepared by evenly coating graphene oxide on the surface-treated silica particles followed by reduction of the graphene oxide and etching of silica particles. The contact angle of the transparent film of thermally reduced graphene oxide (rGO) spheres was 125°. After surface treatment with fluorine functional groups, the contact angle reached 157° achieved by further controlling the surface energy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1025

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reversible three-dimensional architectures transformed from the programmed two-dimensional structures

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전북대학교 고분자나노공학과 ¹전북대학교 고분자 나노공학과 ²전북대학교 고분자 나노 공학
과

By controlling the 2D programmed structures, 3D objects can reversibly change their shapes and properties. These 2D structures were first programmed to break their symmetry for structure transformation. Scroll photonic actuators had been first demonstrated by bending the traditional cantilever structure. Both left- and righthanded scrolls and helices with various colours can be achieved by changing the polarity of solvents. Different types of 3D actuators, such as cube, pyramid and phlat ball, were also demonstrated via the folding mechanism. The reversible 3D photonic actuators transformed from the programmed 2D structures via the bending, twisting and folding mechanisms. This work was mainly supported by Converging Research Center Program (2013K000404), and Human Resource Training Project for Regional Innovation funded by the Ministry of Education, Science, and Technology of Korea.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1026

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characteristics of Polymorphic VO₂ Nanoparticles Synthesized by Hydrothermal Method

박희선 정영희 김영일*

부경대학교 화학과

Vanadium dioxide(VO₂) is one of the most extensively studied thermochromic materials. VO₂ has several different polymorphs of VO₂(B), VO₂(M), VO₂(R), VO₂(A), VO₂(C) and VO₂(D). Among them, VO₂(M) has been most attracted because of a reversible phase transition to VO₂(R) at 68°C. By this structural phase transition from monoclinic to rutile VO₂ shows a fully reversible transition from IR-reflective metal to IR-transparent insulator. VO₂(M) was usually synthesized by the polymorphic VO₂ nanoparticles by the hydrothermal reaction of V₂O₅ with oxalic acid. In this study we have synthesized polymorphic VO₂ nanoparticles by the hydrothermal reaction of NH₄VO₃ with several reducing agents. The structural variation of vanadium oxide in these reactions was studied depending on reaction temperature, time and pH, etc.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1027**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphene oxide-assisted production of carbon nitrides using a solution process and their photocatalytic activity

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인하대학교 화학과 ¹한국과학기술원(KAIST) 신소재공학과

Graphitic carbon nitride (g-C₃N₄) and its derivatives are promising candidates as catalysts or supports for photocatalytic applications. Since they are typically produced by polymerization or condensation of monomers under high temperature and high pressure, development of a cost-effective, solution-based, low-temperature method of production is important. Herein, novel hybrid materials composed of g-C₃N₄ and reduced graphene oxide are produced using a simple reaction between graphene oxide and cyanamide using a solution-based process. During the reaction, reduction of graphene oxide and graphene oxide-assisted generation of g-C₃N₄ occurred simultaneously. These hybrids show good photocatalytic performance for the removal of organic dyes under one sun solar light illumination.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1028

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Targeted Fluorescent Carbon Nanodots for Simultaneous Bioimaging and Photodynamic Therapy

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We developed a novel theranostic platform based on FA-conjugated CD loaded with ZnPc in the present study. Targeted delivery of photosensitizer (PS) and therapeutic photodynamic effect are achieved by folic acid (FA) conjugated carbon dot (CD) as a carrier of PS, zinc phthalocyanine (ZnPc). The CDs prepared by thermal decomposition of alpha-cyclodextrin are biocompatible, highly fluorescent and water dispersible. We have successfully demonstrated the targeted delivery of PS via FA-mediated endocytosis of biocompatible CD-PEG-FA/ZnPc and therapeutic photodynamic efficacy by singlet oxygen generation from the internalized ZnPc upon light irradiation. We anticipate that the present CD-based targeted delivery of the PS would offer convenient and effective platform for the enhanced photodynamic therapy to treat cancers in the near future due to its excellent biocompatibility, bioimaging and targeting capability, and therapeutic efficacy.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1029

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Bridgeman's Black (BB) by Using Supercritical Carbon Disulfide (CS₂) and Their Electrochemical Applications

김성복 권영욱*

성균관대학교 화학과

We present the synthesis and electrochemical properties of Bridgeman's Black (BB) coated on various supports (Ketjen black and silica bead). BB is one kind of organic polymer materials composed of carbon and sulfur. Previously, these materials were mainly synthesized via decomposition of CS₂ with high temperature and high pressure. However, structural and electrochemical characterizations of BB have not been reported in reported literatures. In present study, we have focused on synthesis and electrochemical properties of the BB for photocatalysis. Supported BB was synthesized with CS₂ and supports under supercritical condition. In order to prepare optimized BB, various conditions (reaction temperature and time) were considered. The structural properties of the BB were characterized by means of x-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy dispersive x-ray spectroscopy (EDS). Electrochemical properties of the BB were investigated by using rotating disk electrode (RDE) measurements.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1030

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Europium-doped gadolinium sulfide nanocrystals as an agent for T₁-weighted magnetic resonance and photoluminescence imaging

장혜미 정종진 이승재¹ 박자영 박정규^{2,*}

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We developed europium-doped gadolinium sulfide(GdS:Eu³⁺) nanoparticles(NPs) using sonochemical synthesis. This synthetic method allow short reaction times, simple procedures, and mild reaction conditions. The GdS:Eu³⁺ NPs were used as T₁-weighed MR imaging and cell imaging agent due to their photoluminescence and paramagnetic properties. We demonstrated their strong contrast effect from blood vessels and organs of mice. The NPs also have prominent biodistribution, blood half-life and clearance from organs. We showed confocal images of breast cancer cells treated with GdS:Eu³⁺ NPs to assess their photoluminescence properties. The results from the GdS:Eu³⁺ NPs showed their dual-mode imaging capability for various disease-specific imaging.

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발표코드: MAT.P-1031

발표분야: 재료화학

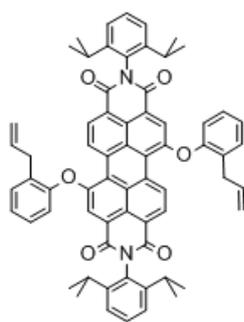
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Perylene Dyes with Substituents at Bay-position as a Colorant for LCD Color Filter

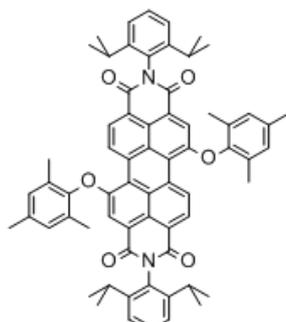
김정윤

서울대학교 재료공학부

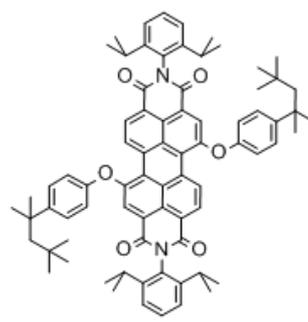
Six red perylene dyes were synthesized to improve the optical performance of LCD color filter. Dyes were designed by mono-substituted form and di-substituted form introducing three substituents to bay-position. To evaluate the dyes for dye-base LCD color filter, spectral properties, solubility to industrial solvent and thermal stability were examined comparing with pigment. Mill base and spin-coated color filter were fabricated with synthesized dyes. Dye aggregation and thermal stability of prepared color filters were investigated using color-difference meter. All of dyes were showed acceptable properties as a colorant for LCD color filter. The prepared color filters exhibited superior spectral properties than pigment-base one due to the smaller particle size of the dyes, which led to less light scattering. And mono-substituted dye were exhibited inferior solubility but superior spectral property and thermal stability than di-substituted dye.



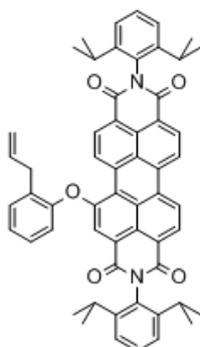
PI2-AP



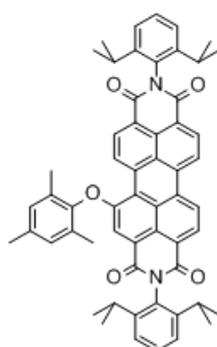
PI2-TMP



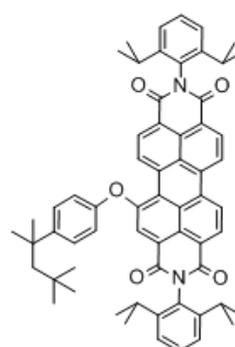
PI2-S2



PI1-AP



PI1-TMP



PI1-S2



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1032

발표분야: 재료화학

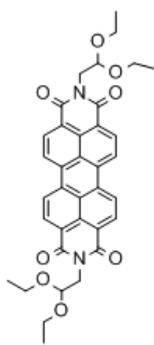
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Some Perylene Red Dyes for Dye-pigment Hybrid LCD Color Filter

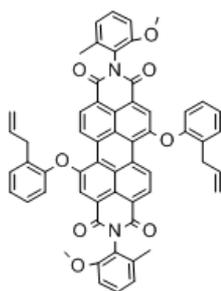
김유현* 김정윤

서울대학교 재료공학부

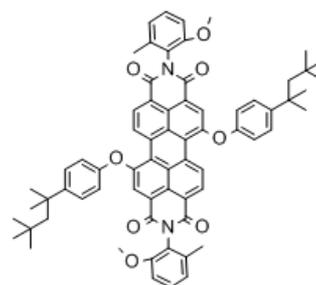
Five novel perylene red dyes were synthesized by introducing new substituents at terminal-position. Absorption spectra, solubility, transmittance and coordinated value of synthesized dyes were investigated to evaluate the dyes for LCD color filter. To fabricate dye-pigment hybrid color filter, the mill bases were consisted with 97% of Pigment Red 177 and 3% of synthesized perylene dye. Then, contrast ratio and luminance of prepared color filters were examined by comparing them with 100% pigment-base one. Dye-pigment hybrid color filters were exhibited lower average particle size than pigment-base color filter. And dye-pigment hybrid color filters were showed higher luminance, lower contrast ratio than pigment-based one.



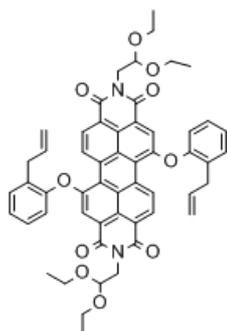
PA



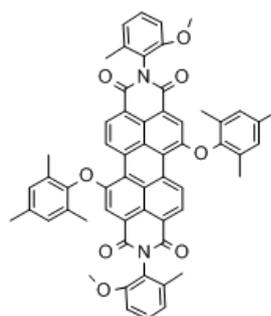
PM-AP



PM-S2



PA-AP



PM-TMP



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1033

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

preperation of superhydrophobic polyacrylated triphenylenes(HATP, HAHTP) surface with nano-micro structures

황지수 안용현*

단국대학교 화학과

The wetting property of a solid surface is important, and is controlled by both the chemical composition and geometrical structure of the surface. A high surface roughness and low surface energy provide high water repellence on a surface. Lotus leaves have nano-/micro-structures and are wax covered. Biomimetic studies of superhydrophobicity in nature have been conducted in the past few years for both academic research and practical applications. Generally, superhydrophobic surfaces have been fabricated using two steps. The first step is to create a nano-/micro-rough surface, and the second step is to modify the rough surface with materials with low surface energies. This poster presents the synthesis of polyacrylated triphenylene derivatives and their application in the fabrication of superhydrophobic surfaces. 2,3,6,7,10,11-Hexaacrylated triphenylene(HATP) was synthesized from hexahydroxytriphenylene, acryloyl chloride and triethylamine. 2,3,6,7,10,11-Hexa(6'-acrylatedhexyl)triphenylene (HAHTP) was synthesized from hexahydroxytriphenylene, Bromohexanol, Potassium carbonate, acryloyl chloride and triethylamine. Nanosilica of an average particle size (200 nm) was mixed with the triphenylene derivatives and a photoinitiator, and then stirred at room temperature for 1 h. After spray-coating, the coated plates were dried at 40 °C and then UV cured. The surface of the coating layer was analyzed using FE-SEM. The setting property of water was studied by measuring the water contact angle on the coated solid surface. The water contact angle on the coated solid surface was found to be 135°. We have synthesized a new functional molecule and successfully used it to fabricate a superhydrophobic surface.

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발표코드: MAT.P-1034

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

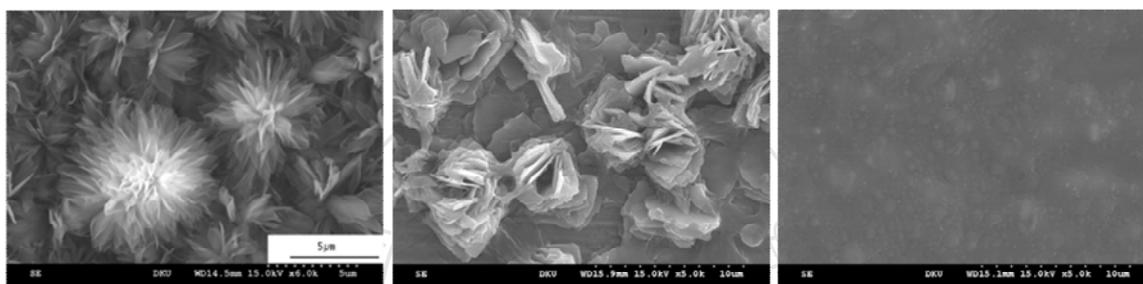
Fabrication of Superhydrophobic Surface with Hierarchical Structure by One Step Immersion Process

김영아 안용현*

단국대학교 화학과

Wettability of a solid surface is one of the most important properties of materials. The wettability is usually determined by measuring the contact angle of a water droplet on a solid surface. When a contact angle of water droplet is larger than 150° , it is considered as superhydrophobic. Such surfaces are self cleaned by enrolling water droplet, therefore, there are many researches to produce superhydrophobic surface by mimicking the nature, like lotus leaf and the legs of water strider. To fabricate a superhydrophobic surface, two factors must be combined. One is the creation of nano-/micro- rough structures on the surface, and the other is coating with low surface materials such as long chain fatty acid, fluorinated alkyl silanes to lower the surface energy of the hierarchical surface of the solid material. Hence, many approaches, such as laser/plasma etching, sol-gel method, electro spinning, chemical vapor deposition, and solution immersion method, have been developed for the fabrication of superhydrophobic surface. Although many methods have been developed, they require numerous steps and expensive instruments. In order to apply to an industry, simple and inexpensive method is needed. In this study, we introduce one step immersion process for the fabrication of superhydrophobic surfaces without any expensive instruments. We fabricate a superhydrophobic surface by dipping metal plates in a solution of fluorinated alkyl silane and alkylphosphonic acid in ethanol. First, we fabricate a superhydrophobic surface with flower-like structures on the Mg plates. Density of the flower-like structures can be controlled by the immersion time and the concentration of alkylphosphonic acid. Also, the purity of the solvent affects the rate of formation of hierarchical structures. After immersing the Mg plates during 24h, Mg plates with a purity of 95% ethanol show superhydrophobic, while with a purity of 99.9% ethanol did not show a superhydrophobic. The resistance of the organic solvent is proved after immersing Mg plates in different organic solvents. All Mg plates dipped in organic solvent has superhydrophobic. The surface

of chemical composition was characterized by X-ray photoelectron spectroscopy (XPS). The spectra show that the modified surface of Mg plate is composed of silicon, fluorine, oxygen, and carbon. It can be concluded that the surface of Mg plate is coated with fluorinated silane and propylphosphonic acid. The composition of coated plate was confirmed by using energy dispersive spectrometry (EDX) analysis. The peaks of C, O, F, Mg, Al, Si, and P are observed in the EDX spectrum of the coated sample. This information confirms that the superhydrophobic Mg plate is coated with polysiloxane and propylphosphonic acid. Second, we fabricate a superhydrophobic surface with plate-like structures on the Cu plates. As the time of immersion was increased, denser nano-/micro structures were formed. The superhydrophobic surface is obtained after immersion at least 12h. The reason why different morphology is obtained is not yet proven, but it thought as the effect of the ion. We also try to fabricate a superhydrophobic surface on Al plate, but it doesn't have superhydrophobic and its morphology is amorphous. In the future, we find out why Cu plates have different morphology and will fabricate superhydrophobic surface on the Al plate.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Seedless Single-step synthesis of Bumpy Ag-nanoshells for SERS-based Cell Tracking *In vivo*

양진경 이현미 이윤식*

서울대학교 화학생물공학부

Silver nanoshells (AgNSs) composed of a dielectric core and a silver shell are of great interest due to excellent SERS sensitivity, and their tunable surface plasmon frequencies in the NIR spectral region, so called biological window (700-900 nm). Previous synthetic approaches to AgNS have not been satisfactory for the effective synthesis under mild conditions. Here, we first report a seedless and single-step synthetic method for bumpy AgNSs and AgNS based NIR-sensitive SERS nanoprobe. The bumpy AgNSs were fabricated in fully extended form without using seed metals under mild condition (1h, 25 °C) and the silver shell thickness could be easily controlled in the range of 32 ~76 nm. In particular, NIR-SER probes, which are consisted of bumpy AgNSs coded with simple aromatic compounds, could generate strong SERS signals from a single particle level (SERS EF of $\sim 6.4 \times 10^5$). The probes were successfully applied to cell tracking in living animals using a portable Raman system.

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장소: 창원CECO

발표코드: MAT.P-1036

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxygen Reduction Reaction on RuSe_x Nanoparticles in Aqueous and Nonaqueous Electrolytes for Application in Li-Air Battery

이은직 권영욱^{1,*}

성균관대학교 나노과학기술협동학부 ¹성균관대학교 화학과

We report the oxygen reduction reaction (ORR) performance of RuSe_x nanoparticles (NPs) in aqueous and nonaqueous electrolytes for application in the fuel cells and Li-air battery. Carbon supported RuSe_x NPs (denoted as RuSe_x/C) were synthesized via supercritical ethanol process (SCE) at 350°C for 1 h. The resultant RuSe_x NPs showed the uniform sized (2.6 nm) and homogeneous elemental composition (Ru:Se = 7:3). Through the structural characterizations of RuSe_x NPs, we confirmed that Se atoms are homogeneously modified on Ru surface. In addition, we also found that this structure could be effective architecture to inhibit the Ru oxidation and enhance the oxygen reduction reaction (ORR) activity by charge transfer from Ru to Se. Rotating disk electrode (RDE) measurements for electrochemical studies showed that RuSe_x NPs have outstanding selectivity to ORR and electrochemical stability than commercial Pt after 3000 potential cycles. Interestingly, the activity trend in 0.1 M LiPF₆ /1, 2-dimethoxyethane (DME) is good agreement with the trend in 0.5 M H₂SO₄. And even RuSe_x NPs showed the higher ORR current than commercial Pt below at ~2.67 V. Based on our finding, we demonstrated that RuSe_x NPs could be potential material for sustainable energy systems.

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장소: 창원CECO

발표코드: **MAT.P-1037**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Superhydrophobic marbles functionalized by fatty acid on particle surface

고승철 안용현*

단국대학교 화학과

Seungcheol Go, Younghyun Ahn*Dept. of Chemistry, Dankook UniversitySurface functionalization of the silica nano particles to obtain a superhydrophobic surface has been issued during many years. A superhydrophobic property is satisfied with a water contact angle of more than 150° and sliding angle of less than 10° . Water-repellent of solid surfaces is controlled by both surface roughness and low surface energy material. Using the nano size marbles to make the surface roughness, the functionalizing fatty acid provides the low surface energy condition. We obtained approximate 700nm silica particles by stober method. Then surface of particles was functionalized in the reaction of the fatty acid. The functionalized particles can create the superhydrophobic surface in a variety of ways and surfaces.

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발표코드: MAT.P-1038

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal and Optical Characterization of PVP-capped Ag nanowires by the times of purification process

오진* 오문비 이효정 김백경

(주)나노픽시스 기술연구소

Silver nanowire (AgNW) transparent electrodes have currently receiving great attention as alternative to indium tin oxide (ITO) for use in many electronic devices. The AgNWs were synthesized by polyol reduction using poly(vinylpyrrolidone) (PVP) as the capping agent. After synthesis, the obtained Ag nanowire solution was purified by precipitation method with acetone and distilled water to remove impurities such as nanoparticles, catalysts, and excess PVP. The impurities have a strong influence on optical and electrical properties of AgNWs. Therefore, in order to investigate the relationship between the properties of AgNWs and the washing process, the times of purification were increased up to 1, 2, and 3. The as-purificated AgNWs were analyzed by thermogravimetric analysis (TGA), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), sheet resistance meter, and haze meter.

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발표코드: **MAT.P-1039**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd_{0.5}Pt_{0.5}-decorated CNTs for electrochemical oxidation of methanol

이슬기 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have drawn particular attention on account of both their scientific interest and their potential for technological applications. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO₂) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and hydrodehalogenation. In this work, we prepared the Pd_{0.5}Pt_{0.5}-decorated carbon nanotubes by thiol-functionalized CNTs. The obtained samples are characterized by transmission electron microscopy, X-ray photoelectron spectroscopy, cyclic voltammetry. For the methanol oxidation the Pd_{0.5}Pt_{0.5}-decorated CNTs exhibits higher electrochemical activity than thiolate CNTs.

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장소: 창원CECO

발표코드: **MAT.P-1040**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic properties of CNT-TiO₂

김성필 최현철*

전남대학교 화학과

Recently, photocatalysis has played an important role in the environmental procedures such as air purification, water disinfection and purification. Among them, titanium oxide (TiO₂) has been extensively studied due to its low cost, non-toxicity, outstanding stability, and high efficiency. The photocatalytic efficiency of TiO₂ is greatly influenced by crystal structure, particle size, surface area and porosity. One of the methods to improve the photocatalytic efficiency is to increase the surface area of the catalyst. In this study, We was manufactured CNT-TiO₂ using multi-walled carbon nanotubes as a supporting material and titanium n-tetra butoxide as titanium source. The obtained CNT-TiO₂ were calcined at various temperatures and characterized by using X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photoactivity of the manufactured materials was estimated by the conversion of methylene blue in aqueous solution under UV irradiation.

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발표코드: MAT.P-1041

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Self-assembled TiO₂ Nanorods for Colloidal Quantum Dot Solar Cells

이지한 박수진*

인하대학교 화학과

In this work, TiO₂ nanorods on FTO-glass were prepared by bottom-up process to apply for colloidal quantum dot solar cell. This process begins with a ZnO scaffold and that converts it to TiO₂ which retain the morphology of the original structure. It is known that the growth mode of ZnO nanorods provides the most morphologically optimal template; but the TiO₂ nanorods show better electronic surface behavior. We made an attempt to control the size, density, length of nanorods by changing the growth time, temperatures, solution concentration, etc. The crystalline and structural features were investigated by X-ray diffraction (XRD). The morphology of the ZnO and TiO₂ nanorods were characterized by Scanning electron microscopy (SEM).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1042**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

CNT-Pd catalyst for efficient Hiyama-coupling reaction

김성필 최현철*

전남대학교 화학과

One of the most important issues in current organic synthesis is the development of new efficient carbon-carbon forming reactions. In this regard, transition metal-based catalysts have generally been used for these reactions. Among them, Palladium is an attractive catalyst for the hydrodehalogenation reaction because it enhances the division of carbon-halogen bonds and facilitates hydrogenation. In this study, we manufactured CNT-Pd by modifying amine groups on CNTs surfaces. Amine groups were utilized as linkers to secure the Pd nanoparticles without aggregation. The catalytic effect of CNT-Pd was investigated about Hiyama-coupling reaction of 4-iodotoluene with trimethoxy phenyl silane in p-xylene. The morphology and structure of prepared surfaces are also examined by transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1043

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical reduction of H₂O₂ on bimetal (Pd, Pt) nanoparticles decorated carbon nanotubes

이슬기 최현철*

전남대학교 화학과

Carbon nanotube (CNT) have received a considerable amount of attention due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. These properties allow them to be applied for a wide range of promising applications in nanoelectronic devices, composite materials and sensors. Recently, carbon nanotube has extensively studied as catalyst supports in both heterogeneous catalysis and electrocatalysis. In this work, we prepared the bimetal (Pd and Pt) - decorated CNTs and studied its application for the electrochemical catalyst of H₂O₂ reduction using cyclic voltammetry and amperometric measurements.

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장소: 창원CECO

발표코드: **MAT.P-1044**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conductive Polymer and Catechol-Containing Graphene Oxide Composites for Supercapacitors

차인환 송창식* 최은정 이해경

성균관대학교 화학과

Supercapacitors have been highlighted as the next generation energy storage device due to fast charge/discharge rate, high efficiency, and semi-permanent characteristics. When conductive polymers are used as electrode materials, there are advantages differentiated from inorganic materials such as flexible, eco-friendly, safety and low cost. We report a new nanocomposite based on polydopamine-capped graphene oxide (PDA-GO) and poly(3,4-ethylenedioxythiophene) (PEDOT). PDA-GO/PEDOT nanocomposites were prepared from one-step coelectrodeposition method. During the process of electrochemical polymerization, the anionic PDA-GO acted as a weak electrolyte and was entrapped in the PEDOT nanocomposites. We investigated electrochemical properties, capacitance and charge/discharge of PDA-GO/PEDOT nanocomposite, and also compared with those of graphene oxide/PEDOT, and PEDOT only.

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발표코드: MAT.P-1045

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Humidity-dependent various morphologies of iron oxide films for ultra-high performance supercapacitor

Jingling Liu 권영욱^{1,*}

성균관대학교 나노과학기술학부 ¹성균관대학교 화학과

Iron oxide thin film with various nanostructured morphologies was synthesized by self-assembly via PEO-PPO-PEO tri-block copolymer (F127) as a directing agent. The relative humidity (RH) during the aging process has been found to be an important role in achieving various nanostructured morphologies. Uniform iron oxide nanowires with 5 nm in diameter were obtained under relative high humidity aging condition, while under relative low humidity aging condition, mesoporous iron oxide with 8 nm in pore size was obtained, and the prospective mechanism was discussed in detail. More importantly, electrochemical properties were also investigated based on nanowire and mesoporous iron oxide thin films. The maximum capacitance of 411.9, 353.6 F/g for the nanowires and mesoporous at 2 A/g current density was achieved, which can be attributed to their unique nanostructures, ultra high surface areas, and abundance of surface active sites.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1046

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of gold nanoparticles with N-heterocyclic carbene-incorporated π -conjugated polymers: disproportionation and concomitant oxidative polymerization

송선구 이해경 양기석 송창식*

성균관대학교 화학과

We synthesized gold nanoparticles decorated with N-heterocyclic carbene-containing conjugated polymers (NHC-CP) by disproportionation of Au(I). In our system, Au(I) was coordinated to NHC with bis-bithiophenes that are oxidatively polymerizable. The three Au(I) were disproportionated to two Au(0) and one Au(III); Au(0) formed nanoparticles and Au(III) oxidized bithiophenes to produce NHC-CP that could stabilize the gold nanoparticles. We examined UV, XRD, SEM and TEM to figure out the size and morphology of gold nanoparticle and NHC-CP complexes. These complexes could be used in water splitting application.

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발표코드: MAT.P-1047

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly CO-Poisoning-Tolerance in Methanol Oxidation Reaction on Ternary PtRuFe Nanoparticles Synthesized by One-Step Sonochemical Approach

Matin Md Abdul 권영욱* 이은직¹

성균관대학교 화학과 ¹성균관대학교 나노과학기술협동학부

In this work, the ternary nanoparticles (NPs) were synthesized by the sonochemical treatment in presence of Pt(acac)₂, Ru(acac)₃, and Fe(acac)₃ in a solvent of Ethylene glycol. The ternary NPs of Pt_xRu_xFe_{100-x} (x = 28, 31, 33, and 35) supported on carbon are characterized by XRD, TEM, and ICP-AES for particle size, morphology, and compositions. The core-shell (Fe in the core, and PtRu-alloy in the shell) structure has been confirmed by STEM-EDS. The NPs were applied to the electrocatalysis for methanol oxidation reaction (MOR). The ternary NPs of Pt₂₈Ru₂₈Fe₄₄, Pt₃₁Ru₃₁Fe₃₈, Pt₃₃Ru₃₃Fe₃₄, and Pt₃₅Ru₃₅Fe₃₀ have demonstrated combative electrocatalytic activity to withstand CO-poisoning in MOR than does the commercial PtRu/C alloy. Among catalysts, Pt₃₅Ru₃₅Fe₃₀ shows a bit higher activity than others three in MOR. Moreover, the origin of the tremendous CO-poisoning-resistance on the ternary NPs surface was investigated by CO-stripping. The earlier onsets and low charge calculated from CO-oxidation peaks are found on Pt_xRu_xFe_{100-x} than that of PtRu/C due to the weakness of Pt-CO bond by the charge transfer from Fe-core to PtRu-alloy in the shell. The stability test performed by chronoamperometry on all Pt_xRu_xFe_{100-x} catalysts has been improved in comparison with PtRu/C. Overall, the experimental results has pointed out a simple route for finding the combative-ability catalysts against CO-poisoning, and the low usage of Pt and Ru for the fuel cell applications.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1048**

발표분야: 재료화학

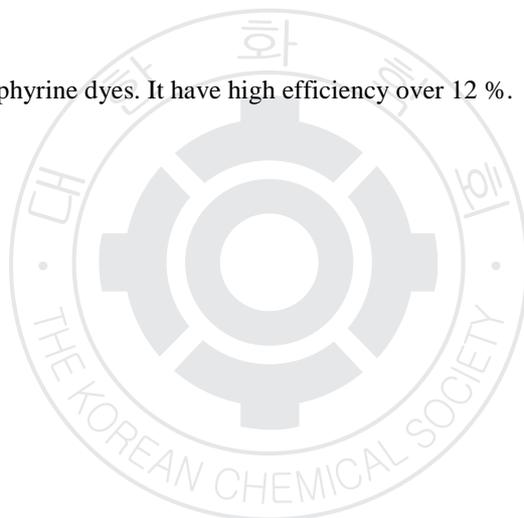
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly efficient porphyrine based DSSCs over 12 %

이춘영 천철홍*

고려대학교 화학과

We synthesized two Zn-porphyrine dyes. It have high efficiency over 12 %.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1049**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and structure of $\text{Na}_{3.8}\text{Rb}_{0.2}\text{Ni}_7\text{P}_6\text{O}_{24}$

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아주대학교 에너지시스템학부 응용화학과 ¹아주대학교 화학과

The new single-crystalline mixed alkali metal phosphate, $\text{Na}_{3.8}\text{Rb}_{0.2}\text{Ni}_7\text{P}_6\text{O}_{24}$, has been prepared with the use of the metal halide, eutectic mixture of NaCl and RbCl as a reactive flux. This compound has been structurally characterized by single-crystal X-ray diffraction techniques. The title compound is crystallized in the space group C2/m of the monoclinic system. The ${}^3_{\infty}[\text{Ni}_7\text{P}_6\text{O}_{24}^{4-}]$ framework is composed of layers formed by edge-sharing of NiO_6 octahedra and PO_4 tetrahedra connecting these layers. This framework was found in the previously reported $\text{Na}_4\text{Ni}_7\text{P}_6\text{O}_{24}$. While previous material have three Na^+ sites at tunnel formed between layers, the title compound have two site fully occupied by Na^+ and one site disordered by Na^+ and Rb^+ . The classical charge valence of the title compound can be represented by $[\text{Na}^+]_{3.8}[\text{Rb}^+]_{0.2}[\text{Ni}^{2+}]_7[\text{P}^{5+}]_6[\text{O}^{2-}]_{24}$.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1050

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymorphism of $\text{Cs}_2\text{FeGe}_3\text{Se}_8$

윤우진 윤호섭^{1,*}

아주대학교 에너지시스템학부 응용화학과 ¹아주대학교 화학과

Two new two-dimensional selenogermanates, α -, and β - $\text{Cs}_2\text{FeGe}_3\text{Se}_8$ have been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. The α form crystallizes in the space group P-1 of the triclinic system with two formula units in a cell dimensions, $a=7.5940(9)$ Å, $b=7.6718(9)$ Å, $c=15.0907(18)$ Å, $\alpha=90.6549(39)^\circ$, $\beta=92.4327(37)^\circ$, $\gamma=105.5575(32)^\circ$, and $V=845.97(17)$ Å³. The β form crystallizes in the space group $P2_12_12_1$ of the orthorhombic system with four formula units in a cell dimensions, $a=7.5961(2)$ Å, $b=12.5833(4)$ Å, $c=17.7332(4)$ Å, and $V=1695.02(8)$ Å³. Both phases share common structural features. Fe and Ge atoms are surrounded by four selenium atoms in a tetrahedral fashion and the tetrahedra share Se atoms to form two-dimensional infinite layers, ${}^2_\infty[\text{FeGe}_3\text{Se}_8^{2-}]$. Polymorphism has been induced due to the different arrangement of Ge and Fe tetrahedra. The classical charge valence of both α form and β form can be described as $[\text{Cs}^+]_2[\text{Fe}^{2+}][\text{Ge}^{4+}]_3[\text{Se}^{2-}]_8$. In this presentation, structural difference will be discussed as will the synthetic conditions of the related compounds.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1051**

발표분야: 재료화학

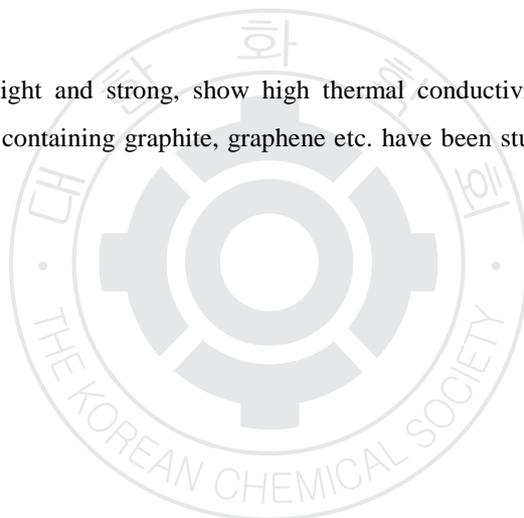
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of thermal conductivity of carbon with the addition of metals

오영희* 현일환 이은경 김윤미 장영환

동의대학교 화학과

Carbon sheets which are light and strong, show high thermal conductivity. The thermal conducting properties of carbon sheets containing graphite, graphene etc. have been studied through the addition of aluminum, iron, or copper.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1052

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses and structure studies of A new disordered cubic CsPdPS₄ related phase

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In the middle of searching for new soluble inorganic polymers using the reactive halide-flux technique, we have found new phase related with CsPdPS₄. The crystal structure and composition of the compound was determined by single-crystal X-ray diffraction. While CsPdPS₄ have one-dimensional ¹_∞[PdPS₄] chain, title compound consist of three-dimensional framework. The framework found in the cubic system is composed of square planar PdS₄ and tetrahedral PS₄ and this framework have already been found in the previously reported RbPdPS₄{Rb_{0.33}P_{0.4}S_{2.23}O_x}. In this compound, the three-dimensional framework have tunnels including Cs⁺ ions and peaks guessed as Cl⁻ ions. The classical charge balance of the compound can be represented as [Cs⁺]_{1.23}[Pd²⁺][P⁵⁺]_{1.09}[S²⁻]₄[Cl⁻]_{0.76}.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1053

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis and Characterization of the Mixed Group 5 Metal Thiophosphate, $\text{Cs}_{0.46}(\text{Nb}_{0.76}\text{Ta}_{0.24})\text{PS}_6$

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The mixed-metal thiophosphate, $\text{Cs}_{0.46}(\text{Nb}_{0.76}\text{Ta}_{0.24})\text{PS}_6$ has been synthesized by using reactive alkali metal halide fluxes and structurally characterized by single-crystal X-ray diffraction techniques. The title compound is made up of the bicapped trigonal bipyramidal $[\text{M}_2\text{S}_{12}]$ units and the tetrahedral $[\text{PS}_4]$ groups. The $[\text{M}_2\text{S}_{12}]$ units linked by the $[\text{PS}_4]$ tetrahedra form infinite chains, yielding a 3-dimensional open framework anions, $[\text{MPS}_6]^{0.46-}$ ($\text{M} = \text{Nb}/\text{Ta}$) with rather large van der Waals space along the c axis in which the disordered Cs^+ ions reside. The intermetallic bond can be strengthened gradually by the amount of the alkali metals. The classical charge balance of the compound is represented by $[\text{Cs}^+]_{0.46}[(\text{Nb}/\text{Ta})^{4.54+}][\text{P}^{5+}][\text{S}_2^{2-}][\text{S}^{2-}]_4$. The UV/Vis spectrum of the compound shows that the title compound is semiconducting and the band gap, E_g is estimated to be 2.62 eV.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1054**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of transparent and colortunable nanocomposite polymer films reinforced by luminescent nanofillers

이병일 변송호*

경희대학교 응용화학과

Organic/inorganic hybrid composites are increasingly developed for use in applications such as flame retardant materials, gene and drug delivery, catalyst carriers and, possibly most importantly, flexible substrates because they show outstanding flexibility and optical clarity. We demonstrate here that inorganic/polymer hybrid films formed by calcined layered gadolinium hydroxide nanosheets (c-LGdH NSs) and polyvinyl alcohol (PVA) exhibit highly reinforced mechanical strength without loss of optical transparency, and also can display versatile photoluminescence (PL) features at rolled or folded shapes.

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장소: 창원CECO

발표코드: **MAT.P-1055**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of layered polymorph of $\text{Re}(\text{OH})_3$ (Re = Sm-Er, and Y)

정희진 변송호*

경희대학교 응용화학과

A layered polymorph series of $\text{Re}(\text{OH})_3$ (Re = Sm-Er, and Y) has been developed by conversion interlayer anions (e.g. Cl^-) of layered rare-earth hydroxychloride (LReH-Cl) to OH^- anions in basic aqueous solutions (pH 13-14). The irreversible conversion led to formation of layered $\text{Re}(\text{OH})_3$ at pH 13 (for Re = Sm-Tb) and at pH 14 (for Re = Dy-Er and Y). The structural difference between layered $\text{Re}(\text{OH})_3$ and typical hexagonal $\text{Re}(\text{OH})_3$ was confirmed through X-ray diffraction (XRD), electron diffraction (ED), infrared (IR), and thermogravimetric (TG) analyses. Slurry containing layered $\text{Re}(\text{OH})_3$ was readily dispersed in water by shaking vigorously. A 1.0 g/L colloidal solution of $\text{Re}(\text{OH})_3$ was stable for more than one month. This new polymorph series for $\text{Re}(\text{OH})_3$ would provide simple, low-cost, large-scale, and reproducible production of $\text{Re}(\text{OH})_3$ colloidal solution, which is useful for biomedical and optoelectronic applications such as imaging agents or thin films.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1056

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective luminescence enhancement of (Eu, Tb)-doped layered (Y, Gd) hydroxides induced by antenna effect of metalate anions

이기룡 이병일 정희진 변송호*

경희대학교 응용화학과

A selective energy transfer from metalate anions to (Eu, Tb)-doped layered rare-earth hydroxides (LReH-A, where Re = Y, Gd and A = Cl⁻, NO₃⁻) has been investigated. The energy transfer, so-called 'antenna effects', was simply induced by adsorbing metalate anions on the surface of LReHs within a few minutes. To find sets exhibiting an efficient energy transfer between various metalate anions and varied LReH compounds, we prepared varied LReHs compounds, which are composed of different host/activator rare-earth metals and interlayer anions, and various metalate anions were used such as metavanadate (VO₃⁻), orthovanadate (VO₄³⁻), molybdate (MoO₄²⁻), tungstate (WO₄²⁻), and chromate (CrO₄²⁻). In case of Eu doped LReH-A (Re = Gd, Y, and A = Cl⁻, NO₃⁻), the enhanced red emission have observed by adsorption of meta/ortho-vanadate, molybdate, and tungstate anions, but in case of Tb doped LReH-A (Re = Gd, Y, and A = NO₃⁻), the enhanced green emission have only observed by adsorption of tungstate anions. In adsorption of chromate anions, all transitions resulted from LReHs have quenched.

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장소: 창원CECO

발표코드: MAT.P-1057

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution-processed MoS₂ As Counter Electrode for Scalable and Efficient Dye Sensitized Solar Cells

수프리야 한성환*

한양대학교 화학과

Abstract Molybdenum disulfide (MoS₂) has recently become one of the most interesting materials for semiconductor device applications due to its two-dimensional and layered structures. However, the ongoing synthesis methods require insensitive environments and high synthesis temperatures. We report here synthesis of MoS₂ (2.5 x 10 cm²) at an ambient temperature using a simple chemical bath deposition method (solutions-process) and used as a counter electrode for dye-sensitized solar cells (DSSCs) alternative to expensive platinum, which is commonly preferred. As-prepared MoS₂ counter electrode is characterized for its structural, morphological, elemental analysis and electrochemical studies by means of X-ray diffraction (XRD), Raman, scanning electron microscopy (SEM), X-ray photoemission spectroscopy (XPS), transmission electron microscopy (TEM) and cyclic-voltammetry (CV) measurements, respectively. Extensive cyclic voltammograms confirm the cathodic current density. Moreover, the peak current densities confirm no sign of degradation after consecutive hundred cyclic scans, suggesting the duration potentiality of the MoS₂ counter electrode. An impressive low charge transfer resistance compared to platinum for I³⁻ reduction is beneficial. The DSSCs performance is measured with MoS₂ and platinum (Pt), wherein cell with MoS₂ counter electrode demonstrated a power conversion efficiency of 7.01% which is comparable to the DSSCs with Pt (7.31%) indicating significance of solution-processed MoS₂ in DSSCs application

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1058**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New indolocarbazole derivative small molecule for solution-processed organic solar cell

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한양대학교 화학과

Solution processable organic semiconductors based on indolocarbazole derivative was synthesized, and it is applied to bulk-heterojunction organic solar cells (BHSCs) as an p-type donor material. The optical and electronical properties were characterized by UV-vis absorption spectroscopy and cyclic voltammetry. This small molecule has good solubility in common organic solvents due to long alkyl chain. Photophysical and electrochemical studies indicate that new p-type semiconductor have 2.45 eV optical band gaps and its HOMO/LUMO energy levels are aligned with the PC60BM electron acceptors. The device structure of BHJ photovoltaic cells is ITO/PEDOT:PSS/small molecule:PC60BM/Al were evaluated and compared as different blending ratio of C12-BBICZ : PC60BM. The small molecule shows the best power conversion efficiency of 1.26 % when processing the active layer consisted of the 1:1 blending ratio with PC60BM.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1059

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Exfoliation of dion-jacobson type perovskite into colloidal nanosheets

이원재 백승민^{1,*}

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Recently, perovskite-type compounds have highly attracted research interests because of their potential applications in the industrial and scientific fields such as photocatalysis, energy storage, ferroelectricity. In this study, a tantalum-based layered perovskite with Dion-Jacobson phase, RbLaTa₂O₇, was successfully exfoliated into nanosheets via ion-exchange and two-step intercalation reaction. First of all, the pristine RbLaTa₂O₇ was prepared by ordinary solid-state reaction, and then, the rubidium cations in the interlayer spaces were ion-exchanged with hydronium cations to synthesize a proton-intercalated perovskite. The obtained proton-exchanged perovskite was reacted with ethylamine to expand the interlayer spaces for further intercalation reaction. Finally, the ethylammonium-intercalated perovskite was exfoliated into colloidal nanosheets through an intercalation of bulky tetrabutylammonium(TBA) cations. X-ray diffraction analysis showed that the TBA-intercalated perovskite had an increased interlayer spacing of 2.06 nm in comparison with that of RbLaTa₂O₇. Transmission electron microscopic image of exfoliated perovskite revealed that the present exfoliated perovskites were composed of very thin layers. This exfoliated perovskite nanoplatelets could be used as host material for fabricating new functional nanocomposites.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1060**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

EMI Shielding Behaviors of Ni-coated MWCNTs-filled Epoxy Matrix Nanocomposites

배경민 박수진*

인하대학교 화학과

Multi-walled carbon nanotubes (MWCNT) were nickel (Ni)-plated chemically to enhance the electrical performance, resulting in an increase in the electromagnetic interference (EMI) shielding efficiency (SE) of the Ni-MWCNTs-reinforced epoxy matrix nanocomposites. The micro-structural and morphological properties of the Ni-MWCNTs were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM), respectively. The surface characteristics of the Ni-MWCNTs and the EMI SE of the Ni-MWCNTs/EP composites were examined by X-ray photoelectron spectroscopy (XPS). From these results, the addition of the MWCNTs in the EP matrix led to an increase in the EMI SE of the composites. The higher Ni content on the MWCNTs of the Ni-MWCNTs/EP composites showed a better EMI SE. This indicates that the presence of Ni on the MWCNTs can lead a good EMI SE due to the EMI adsorption behavior of the metal particles.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1061

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation on etch characteristics of magnetic materials using solution-based etch methods

이원재 김유정¹ 백승민^{1,*} 이홍인^{1,*} 정종화^{1,*}

경북대학교 자연과학대학/화학과 ¹경북대학교 화학과

Magnetoresistive random access memory (MRAM) has been extensively investigated in recent years owing to its potential importance in data storage systems. Among those, spin transfer torque MRAM (STT-MRAM) is considered as a next generation universal memory because it can operate in sub-nanometer scale. Though a conventional etch method to fabricate magnetic stacks, which constitutes STT-MRAM, with high degree of integration is a plasma-based one, it has several inherent limitations in terms of undesirable byproducts. In this study, to circumvent such drawbacks, magnetic stacks on Si wafer were chemically treated by various etchants. According to scanning electron microscope measurements, etch profiles of the magnetic stacks could be controlled by using the present solution-based method. Energy-dispersive X-ray spectroscopic results suggested that the composition of magnetic stacks was changed upon the chemical treatment of etchants. This process is potentially applicable to the efficient etching of magnetic stacks in STT-MRAM.

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장소: 창원CECO

발표코드: MAT.P-1062

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Sulfur-containing Functional Groups on Elemental Mercury Adsorption Behaviors of Porous Carbons

배경민 박수진*

인하대학교 화학과

In this work, sulfur-containing functional porous carbons based hybrid materials were prepared by heterogeneous and homogeneous methods. Their structures were characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), porous structure analysis and elemental analysis. The results showed that higher degree of functionalization was obtained by the heterogeneous method than the homogeneous method. Higher content of functional groups was found in heterogeneously prepared adsorbent than the homogeneously prepared one. Both sulfur and amidoxime in the two adsorbents took part in the coordination with Hg(II), forming chelating complexes. The sulfur-containing functional porous carbons could be promising adsorbents for removing elemental mercury.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1063

발표분야: 재료화학

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Significant enhancement of hybrid solar cells by wide-range photon absorption and well-assembled charge transfer networks with PbS_xSe_{1-x} quantum dots and nanorods

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We suppose a new device architecture of hybrid bulk heterojunction solar cells using a novel donor-acceptor combination (D-A combination) of poly[2,6-(4,40-bis-(2-ethylhexyl)dithieno[3,2-b:20,30-d]silole)-alt-4,7(2,1,3-benzothiadiazole)] (PSBTBT) and a PbS_xSe_{1-x} inorganic semiconductor. The hybrid nanocomposit layers of with PbS_xSe_{1-x} quantum dots (QDs) and nanorods (NRs) in the polymer matrix formed by post-ethanedithiol chemical treatment. The performance enhancement was mainly straight pathways for photogenerated carriers within NRs that are conductively interconnected by spherical QDs. We could fabricate efficient photovoltaic cells having an overall energy conversion efficiency (PCE) of 3.4% with a PbS_{0.7}Se_{0.3} QD : NR blending ratio of 0.3 : 0.7 (wt/wt) under 1.5(AM) sun illumination, Voc of 0.43V, Jsc of 14.87 mA/cm², and F²F of 0.53.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of the Mixed-metallic Phosphates, $\text{Li}_2\text{Ti}_{1.81}\text{V}_{0.19}(\text{PO}_4)_3$

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Li metal phosphates, $\text{Li}_3\text{M}_2(\text{PO}_4)_3$, have been widely investigated for secondary Li batteries. The positions and stoichiometries of Li ions in this phase play crucial roles to determine the efficiency of the system. In our group we have focused on the systematic approach toward the synthesis of new members of this family via partial substitution of metal sites with different oxidation states. As a result of our effort, we report here the synthesis and structural characterization of the mixed-metal phosphates, $\text{Li}_x(\text{Ti}/\text{V})_2(\text{PO}_4)_3$. Although they have various Li contents and positions, they share the common framework structure. The framework is comprised of (V/Ti)-centered octahedra and P-centered tetrahedra. The metal sites are occupied by statistically disordered V and Ti atoms. These polyhedra are sharing O atoms to form a three-dimensional framework with huge empty space. The stoichiometry of Li ions in this space can be controlled by the sum of the oxidation states of each metal. The classical charge balance of the title compounds can be represented as $[\text{Li}^+]_x[\text{V}^{3+}]_{2-y}[\text{Ti}^{3.5+}]_y[\text{P}^{5+}]_3[\text{O}^{2-}]_{12}$.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct Synthesis of Gold-graphene Nanocomposites with Polyethylene Glycol (PEG)

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We report on the direct synthesis of gold-graphene nanocomposites from graphite using polyethylene glycol (PEG). In this method, gold nanoparticles photo-synthesized by white-light and it simultaneously intercalated in graphene layers. The product was characterized by x-ray diffraction analysis (XRD), transmission electron microscopy (TEM) and atomic force microscopy (AFM). As a result, gold-graphene nanocomposites are composed of graphene layers (It has 7 nm thickness) and two different size of gold nanoparticles (about 10 nm and 2nm). We also observed their catalytic activity through reduction reaction of 4-nitrophenol to 4-aminophenol.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Virus nanostructure based novel photonic device for full color display

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Reflective displays have attracted a lot of attention because of their low power consumption, simpler manufacturing process, without the backlighting source. Many researchers have presented various types of reflective displays. such as cholesteric liquid crystal displays, bistable nematic liquid crystal displays, zenithal bistable displays with bistability, electrophoretic displays (EPD), and interferometric modulator displays. Among these, nowadays reflective liquid crystal displays (LCDs) have been studied mainly for use in mobile devices, outdoor signboard applications, and e-books. Recently, we reported that virus can act like liquid crystal materials. In particular, because of virus's unique properties such as self-evolve, self-amplification, and self-assembly, it can be used for various applications. Here, we developed novel reflective display device for full color display using selfassembled virus (M-13 bacteriophage). We fabricated structural color matrix using simple pulling method. When light is incident on the virus based nanostructure with appropriate periodicity, desired colors were preferentially reflected. This structural color can be changed at different temperature through structure modulation. We designed the 7-digits display device with patterned micro-heater, which can be used to control the temperature. We expect that virus based color display device will be used for next generation full-color displays.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Simple and Novel Approach to the Synthesis of a Variety of Shaped Silver Nanoparticles

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조선대학교 화학과

Noble metal nanoparticles are very useful materials that can be used in many different areas such as therapeutics, catalysis, sensing, electronics and plasmonics. At present, a variety of synthetic methods have been developed and one can control the size and shape of gold, silver, even multimetallic nanoparticles. Usually, the growth of nanoparticles is explained by either "Ostwald Ripening (OR)" or "Oriented Attachment (OA)", however, the vast majority of work has focused on OR. In this study, we drove growth conditions for OA to be favored and synthesized peculiar shaped silver (Ag) nanoparticles.

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One-pot Synthesis of Silver Nanowires

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Since silver (Ag) nanowires have shown a lot of potential in a variety of fields (e.g. plasmonic waveguiding, surface-enhanced Raman spectroscopy, catalysis, sensing), amount of research on Ag nanowires have been conducted. Especially, Ag nanowires have attracted increasing attention at present, because they can be used as the conducting materials for flexible display. Ag nanowires have been prepared using either template-based method or templateless approaches. Usually, templateless approaches are performed in several steps by adding seeds solutions into the growth solutions with shape-directing capping agents. In this presentation, we introduced a novel method to synthesize Ag nanowires. This reaction is very simple and efficient. All reactions are performed in one pot with yield of 100%.

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발표코드: MAT.P-1069

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Neutron diffraction study of defect perovskite oxynitride



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Ammonolysis of layered perovskite $\text{Sr}_2\text{Ta}_2\text{O}_7$, in the presence of Li_2CO_3 , induces cooperative Li^+ insertion and the charge-balancing $\text{O}^{2-}/\text{N}^{3-}$ exchange, leading to perovskites with vacancy defects both on the cation and anion sites. Single phase products could be obtained from the compositional range of $[\text{Li}]:[\text{Ta}] = 0\sim 0.4$. Here we carried out detailed characterization of a phase with the composition $\text{Sr}_{0.7}\text{Li}_{0.3}\text{Ta}_{0.7}\text{O}_{2.6-3y}\text{N}_{2y}$. Inductively coupled plasma spectroscopy and combustion analysis were employed to estimate the Li and N contents. Rietveld refinement of neutron powder diffraction pattern indicated that Li occupied the octahedral site without any ordering with Ta. By heat treatment in air, $\text{Sr}_{0.7}\text{Li}_{0.3}\text{Ta}_{0.7}\text{O}_{2.6-3y}\text{N}_{2y}$ could be further transformed to an oxide-type defect perovskite $\text{Sr}_{0.7}\text{Li}_{0.3}\text{Ta}_{0.7}\text{O}_{2.6}$. Ionic conductivities of $\text{Sr}_{0.7}\text{Li}_{0.3}\text{Ta}_{0.7}\text{O}_{2.6-3y}\text{N}_{2y}$ and $\text{Sr}_{0.7}\text{Li}_{0.3}\text{Ta}_{0.7}\text{O}_{2.6}$ are being examined by ac impedance spectroscopy.

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발표코드: **MAT.P-1070**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The Role of Bis(p-sulfonatophenyl)phenylphosphine dihydrate dipotassium salt for the Synthesis of Silver Nanoprisms

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Triangular silver (Ag) nanoprisms can be simply synthesized through Mirkin's photomediated synthesis. This method is highly controllable with tuning the edge length of Ag nanoprisms, and efficiently transforms a sphere to prism with yield of 100%, however, the reaction mechanism has not been revealed yet. Several mechanisms suggest that bis(p-sulfonatophenyl)phenylphosphine dihydrate dipotassium salt (BSPP) plays an important role to control the reaction rate for the synthesis of nanoprisms. In this research, we studied the role of BSPP in photomediated synthesis of Ag nanoprisms, and especially, focused on how BSPP can control the reaction rate.

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발표코드: MAT.P-1071

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The effects of counter electrodes on the Quantum dot sensitized solar cells

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공학

다중 여기자 생성(Multiple Exciton Generation, MEG), 높은 광 흡수율, 크기에 따른 밴드갭 조절이 가능한 양자점을 이용하는 양자점 감응형 태양전지(Quantum dot-sensitized solar cell, QDSSC)는 차세대 태양전지로 주목을 받고 있다. 특히 상대전극(Counter electrode)은 전해질 산화 환원반응 속도를 조절해서 광 전류(Jsc) 향상에 중요한 요소로서 작용한다. 기존 DSSC 에서 상대전극(Counter electrode, CE)으로 이용되던 백금(Pt)은 양자점 감응형 태양전지의 전해질로 이용되는 Polysulfide 와의 반응성이 좋지않아 산화환원반응 속도를 저하시킨다고 보고되고 있다. 이에 본 연구에서는 Polysulfide 전해질과 호환성이 좋은 Cu₂S 나노입자를 합성하고 태양전지 효율에 미치는 나노입자의 크기에 대한 영향을 조사하였으며, 또한 무기물로 치환된 Cu₂S 나노입자 및 환원된 그래핀(reduced graphen oxide)과의 혼합물을 형성하여 양자점 감응형 태양전지 효율 향상에 미치는 영향등을 조사하였다.

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발표코드: MAT.P-1072

발표분야: 재료화학

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Orthorhombic-to-tetragonal phase transition of tungsten-bronze β - SrTa_2O_6 induced by lithium insertion

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영남대학교 화학과

Tungsten-bronze (TB) type solids contain three different crystallographic sites for cation, but two of them are partially or completely vacant, giving promises as a host for insertion reactions. In this regard, we attempted to incorporate Li^+ ion into the TB-type lattice, where an orthorhombic TB-phase β - SrTa_2O_6 was reacted with Li_2CO_3 in the ratios of $[\text{Li}]:[\text{Sr}] = 0\sim 0.7$. According to the powder X-ray diffraction, single phase products could be obtained when $[\text{Li}]:[\text{Sr}] = 0.2\sim 0.5$. The Li-insertion into β - SrTa_2O_6 caused a volume contraction and an evolution of crystal symmetry from orthorhombic to tetragonal. The resulting $\text{Li}_x\text{SrTa}_2\text{O}_6$ phases have significantly smaller lattice constants than those of the tetragonal β' - SrTa_2O_6 . As studied by ac impedance spectroscopy, $\text{Li}_{0.4}\text{SrTa}_2\text{O}_6$ possesses an ionic conductivity of $\sim 10^{-7} \text{ S/cm}$ at 290 K. Spectroscopic investigations by solid-state Li-7 nuclear magnetic resonance and infrared will be also presented.

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Energy storage application of SnO₂-MoS₂ hybrids

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The SnO₂ nanoparticles were successfully randomly hybridized with MoS₂ via exfoliation and subsequent reassembling reaction. The structure and physico-chemical properties of SnO₂-MoS₂ hybrid were characterized by X-ray diffraction, scanning electron microscopy, nitrogen adsorption-desorption measurements, transmission electron microscopy analyses and electrochemical measurements. Because nanoporous characteristics of the present hybrids could result in the enhancement of energy storage properties, we examined the charge-discharge profiles of hybrid materials. Compared with the specific capacity of the pristine MoS₂, the hybrid material exhibited much higher specific capacity of 500 mA h/g even after 30 charge-discharge cycles. Such results indicated that the present synthetic method was effective for improving the energy storage properties of electrode materials in lithium ion batteries.

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은 입자 생성 과정을 응용하여 여러 형태를 가지는 은 입자의 제조

도희진 최송이 송재희^{1,*}

순천대학교 기초의화학부 ¹순천대학교 화학과

금속 나노 입자는 입자의 크기 및 형태에 따라 입자 표면의 국부 플라즈몬 공명현상(Localized Surface Plasmon Resonance, LSPR)에 의해 광학적 특성이 달라진다. 이로 인하여 센서, SERS(Surface-Enhanced Raman Spectroscopy) 등 우리 실생활에 전반적으로 많은 분야에서 활용되고 있으며 아직까지도 활발한 연구를 진행 중이다. 본 연구에서는 수소화붕소나트륨(NaBH_4)에 의해 질산염(AgNO_3)의 화학적 환원으로 은 입자를 만들고 다양한 $\text{AgNO}_3/\text{NaBH}_4$ molar ratio 를 통해 나노결정의 크기분포를 알 수 있고 다양한 형태를 만들어 낼 수 있었다. $\text{AgNO}_3/\text{NaBH}_4$ molar ratio 가 증가할수록 단파장(blue shift)으로 이동했다. Ag colloidal nanorings 은 trisodium citrate($\text{C}_6\text{H}_5\text{Na}_3\text{OH}_7 \cdot 2\text{H}_2\text{O}$) 용액에 NaBH_4 를 첨가하여 은 이온이 환원되어 합성됐다. pH 를 조절하여 환원반응 속도를 빠르게 하여 반응시켰다. 또 다른 형태로는 시드 성장법(seed-mediated growth method)을 응용하여 citrate 로 안정시킨 프리즘 형태의 은 입자를 제조하였다. 이때 시드(seed)의 농도를 조절하여 입자의 크기를 제어할 수 있었다. 시드의 농도가 증가할수록 입자의 크기는 작아졌고 blue shift 하였다. Ag nanorings 은 UV-Vis 흡수띠가 약 400nm 근처와 그리고 600~700nm 사이에서 두 개의 peak 이 나타난다. 다른 형태인 Ag nanoprisms 은 UV-Vis 흡수띠가 약 400nm 근처와 550~700nm 사이에서 두 개의 흡수밴드를 보인다. 입자들은 TEM(Transmission Electron Microscopy)과 UV-Vis spectrum 으로 분석했다.

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발표코드: MAT.P-1075

발표분야: 재료화학

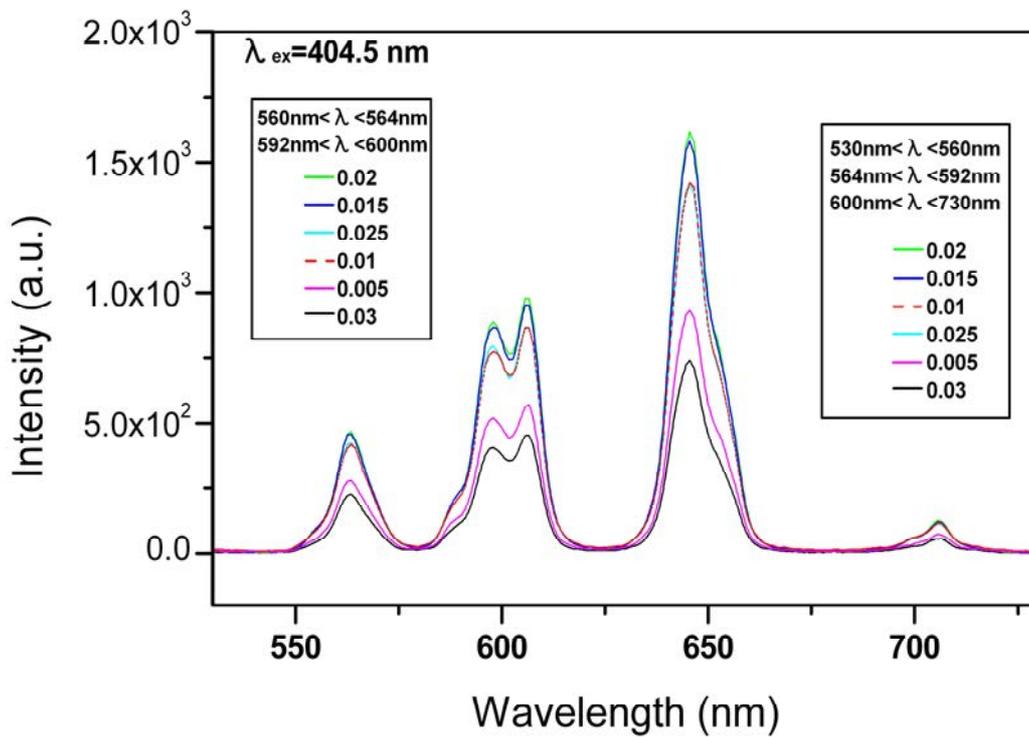
발표종류: 포스터, 발표일시: 수 16:00~19:00

Sm 함유량 x 와 점 결함 차이에 따른 적색형광체 $\text{CaWO}_4:\text{Sm}_x$ 와 $\text{CaWO}_4:\text{Sm}_x,\text{Na}_x$ 분말의 발광특성

백경래 이승한 조선욱*

신라대학교 신소재공학과

두 가지 종류 적색형광체 $\text{CaWO}_4:\text{Sm}^{3+}$ 와 $\text{CaWO}_4:\text{Sm}^{3+},\text{Na}^+$ 를 고상반응법을 이용하여 합성하였다. XRD 를 이용하여 구조를 결정하고, 발광 특성을 측정하였다. +3 가인 Sm 이온이 +2 가인 Ca 이온 자리에 치환되면서 앞의 두 가지 형광체는 구조적으로 차이가 있다. $\text{CaWO}_4:\text{Sm}^{3+}$ 는 치환과 함께 빈자리(vacancy)를 만들지만, $\text{CaWO}_4:\text{Sm}^{3+},\text{Na}^+$ 에서는 오직 치환 점 결함만 만들어진다. XRD 피크의 위치가 모재에 활성제를 도핑하기 전후에 변화를 보이지 않는다는 것은 빈자리가 나름대로 사이즈를 가진다는 것을 의미한다. Vegard 법칙으로부터 벗어나는 행동의 요인은 원자간 또는 이온 간의 인력이 원자 또는 이온의 사이즈 효과 보다 크게 작용하기 때문이다. 이런 구조 차이에 기인하는 발광특성의 차이를 확인하였다. 또한, 적외선 분광기와 라만 분광기를 이용한 점 결함의 차이도 확인하였다.*Corresponding author (S. -W. Cho, Silla University)



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Synthesis of Ni/graphene hybrids via electron beam irradiation

민영제 백승민*

경북대학교 화학과

Graphene-based materials can be used for energy storage applications because graphene has a chemical stability, a large specific surface area and a good electric conductivity. When graphene was used as a new energy storage material, it is important to meet the increasing demand for energy storage property with higher energy density. At first, we prepared nickel-graphene oxide (Ni/GO) hybrids with flexible delaminated structure. And then, the obtained Ni/GO hybrids were reduced by facile synthetic method via electron beam irradiation. According to X-ray diffraction and X-ray absorption spectroscopic analysis, nickel nanoparticles were homogeneously distributed on graphene nanosheets. Transmission electron microscopy images of these hybrids showed several defects induced by electron beam irradiation, which could improve electrochemical properties for energy storage. Nitrogen adsorption-desorption isotherms shows that specific surface area of these hybrids increased due to the void spaces developed by random hybridization. The present hybrids exhibited higher energy storage properties than those of starting materials.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bi³⁺,Eu³⁺ 치환된 옥시플로라이드 합성 및 광학특성 연구

노민희 박상문*

신라대학교 에너지융용화학과

Bi³⁺와 Eu³⁺를 옥시플로라이드인 Sr₃AlO₄F 모체에 고상법으로 성공적으로 합성하였다. X 선 회절방법으로 단일상을 확인하였으며, 여기 발광 PL 스펙트럼으로 광학적 특성을 연구하였으며, 활성체의 농도에 따른 농도 소광현상을 모니터링 하였다. Bi³⁺가 치환된 옥시플로라이드는 푸른색 발광을 보였으며, Eu³⁺가 공동 치환되면서 보라색과 붉은색으로 발광 변화를 보였다. 한편 Bi³⁺와 Eu³⁺를 옥시플로라이드에 공동 치환하여 CIE 와 energy transfer 등의 광학 특성을 비교 분석하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1078**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd Nanoparticles Decorated Polymer Nanocapsule

윤경원 Zahid Hassan¹ 김지홍 김기문*

포항공과대학교 화학과 ¹한국기초과학지원연구원 복잡계자기조립연구단

Metal nanoparticles are important for a wide range of applications including catalysis, photonics, electronics, and biomedical sensing. Protecting agents such as surfactants, dendrimers and polymers are needed to stabilize the nanoparticles (NPs) from self aggregation. However, these protecting agents have strong affinity towards the surface of NPs and restrict the chemical activity of NPs. We synthesized a novel polymer nanocapsule, which not only stabilized the NPs, but also provided a uniform distribution of NPs over the surface of the nanocapsule. Polymer nanocapsules were synthesized via polymerization of (allyloxy)₁₂cucurbit[6]uril which has a rigid core and multiple polymerizable allyl groups at the periphery. Recently, we developed Pd nanoparticles decorated polymer nanocapsules (Pd-PNs) and they showed excellent regio-, chemo- and sequential selectivities in carbon-carbon bond formation of multihalogenated arenes and hetarenes. Furthermore, the Pd-PNs were also successful in carbon-nitrogen bond formation reactions as well. Details of the synthesis, characterization and applications of the NPs on nanocapsule will be presented.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1079**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design of phosphorus-nitrogen dual doped ordered mesoporous carbons for non Pt electrocatalyst

정헌종 김지만*

성균관대학교 화학과

Among the various types of fuel cells, polymer electrolyte membrane fuel cells (PEMFC) is being in the vanguard, and have recently drawn lots of attention in both fundamental and application. carbon-supported platinum or platinum alloys are commonly used as electrocatalysts to enhance the oxygen reduction reaction (ORR). However, it's difficult to commercialize PEMFCs due to the cost of platinum. So, many research groups have suggested alternatives. Especially, N-doped carbon-based catalysts have attracted attention because of its much better electrocatalytic activity, tolerance to crossover effect, long-term operation stability than platinum for ORR in alkaline fuel cells. However, In acidic media, N-doped carbon shows a lower ORR activity than Pt catalysts. For enhancing the oxygen reduction reaction (ORR) activity, we synthesized Phosphorus-nitrogen dual doped carbon. The P,N-doped carbon is prepared via pyrolysis of mixture composed of 1,10-phenanthroline, 9,10-Dihydro-9-oxa-10-phosphaphenanthrene 10-oxide, iron chloride at 900oC under an N₂ atmosphere. The physical properties of the prepered doped OMC were examined via X-ray diffraction (XRD), Raman spectroscopy, Brunauer-Emmett-Emmett-Teller(BET) surface area analyses, X-ray photoelectron spectroscopy (XPS).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1080**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mechanochemical Synthesis of Organic and Inorganic Materials

이규형 이주희 박규리 허남희*

서강대학교 화학과

We report a novel method that can synthesize organic and inorganic materials through a mechanochemical method, which is based on nontoxic solid hydrazine ($\text{H}_3\text{N}+\text{NHCO}_2^-$). Azines, pyrazoles, and pyridazinones were prepared as the sole products in high yields simply by grinding solid hydrazine with di-carbonyl compounds. Typically, complete conversions were achieved within a day at ambient temperature without using catalysts. Reaction rates were generally enhanced upon increasing the reaction temperature. The solid-state reactions did not produce any wastes besides water and carbon dioxide. In a similar manner, we were able to synthesize various inorganic materials by grinding solid hydrazine with corresponding precursors. The mechanochemical method is environmentally benign and readily scalable, which allows for highly selective synthesis of a wide range of materials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1081

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Er³⁺, Yb³⁺ 치환된 Ba₂Y₂Si₂O₁₀ 합성 및 광학 특성 연구

최슬기 박상문*

신라대학교 에너지융용화학과

Er³⁺, Yb³⁺의 활성체가 치환된 Ba₂Y₂Si₂O₁₀ 형광체를 고상법으로 성공적으로 합성시켰다. Er³⁺를 모체인 Ba₂Y₂Si₂O₁₀에 치환 하였으며 Er³⁺ 농도 변화에 따른 광 변화를 관찰 하였으며, Yb³⁺의 공동 치환을 통해 Er³⁺과 Yb³⁺ 농도에 따른 광학적 특성 변화를 모니터링 하였다. 하향변환과 상향변환의 관계를 비교 관찰 하였으며, NUV의 영역의 빛과 980 nm IR 레이저를 이용한 광 특성을 비교 연구를 하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1082**

발표분야: 재료화학

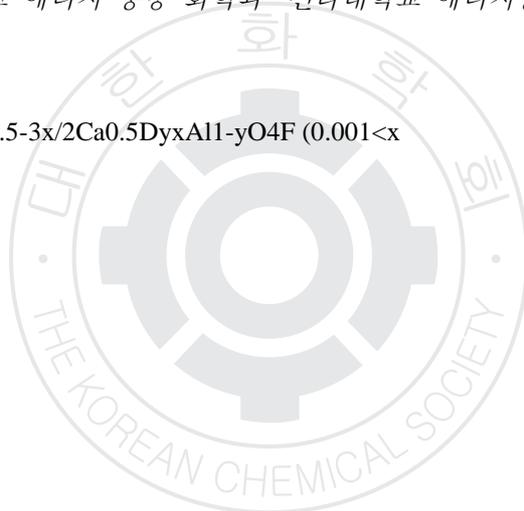
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dy³⁺ 치환과 결합 유도된 옥시플로라이드의 합성과 특성 연구

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신라대학교 에너지 응용 화학과 ¹신라대학교 에너지응용화학과

Dy³⁺ 이온이 치환된 Sr_{2.5-3x/2}Ca_{0.5}Dy_xAl_{1-y}O₄F (0.001<x



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1083

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Efficient Visible Light-Active Photocatalysts: A Linker Mediated Mesoporous Nanohybrids of CdS and Zn-Cr-Layered Double Hydroxide

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We are successful in hybridizing isocharged nanospecies of cationic CdS quantum dots (QD) and cationic Zn-Cr-layered double hydroxide (Zn-Cr-LDH) nanosheets using inorganic anion as a linker. Powder X-ray diffraction and X-ray absorption spectroscopy clearly demonstrate the maintenance of the original crystal structures of Zn-Cr-LDH and CdS upon hybridization. A strong electronic coupling between the two components is evidenced by diffuse reflectance UV-vis spectroscopy and photoluminescence spectroscopy. The present nanohybrids display high efficient photocatalytic activity for visible light-induced H₂ production (~2.1 mmol/h·g), which is much superior to that of the pristine CdS (~0.3 mmol/h·g). The observed improvement of photocatalytic activity is attributable to the depression of electron—hole recombination in the CdS QD via the strong coupling between the two components. The present findings underscore not only the usefulness of the CdS-Zn-Cr-LDH nanohybrids as efficient photocatalyst for H₂ production but also the effectiveness of the anionic linker in hybridizing two kinds of isocharged nanomaterials.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1084

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Doping Effect of $\text{NaNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ for Enhanced Electrochemical Properties

배은경 표명호*

순천대학교 화학과

$\text{NaNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ (NNMO), which has a layered structure, is a promising cathode material for sodium ion batteries. It is well known that the substitution of Mn with Ni in $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$, renders Li^+ ion diffusion kinetics better. In a layered structure of $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$, the stack of $\text{Mn}(\text{Ni})\text{O}_2$ slabs, which are composed of edge-shared $\text{Mn}(\text{Ni})\text{O}_6$ octahedra, form the metal-occupied octahedral sites and the empty tetrahedral sites. The octahedral sites in Li slabs are also occupied by Li^+ ions, which are sandwiched by edge-sharing with $\text{Mn}(\text{Ni})\text{O}_2$ slabs. Li^+ ions move from one octahedral site to another by passing through the empty tetrahedral sites within a Li slab. During this process, Li^+ ions are strongly repelled from a nearby transition-metal cations (Mn^{4+} , Ni^{2+}) of octahedral sites. The activation energy is rapidly increased at this moment, which aggravates Li^+ ion diffusion kinetics. By using rare earth metals (Gd, Tb), the activation energy and the repulsive force could be decreased, leading to substantial improvement of the Li^+ diffusion kinetics and, thereby, charge-discharge rates. Expecting that the same rule can be applied to Na^+ , we are currently focusing on the synthesis of phase-pure Tb-doped NNMO and the comparison of electrochemical properties of pertinent Tb-doped NNMO cathodes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1085

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Single-Crystal Poly(3,4-ethylenedioxythiophene) Nanowires with High Conductivity

조보람 성명모*

한양대학교 화학과

We developed single-crystal poly(3,4-ethylenedioxythiophene) (PEDOT) nanowires with ultra-high conductivity using liquid-bridge-mediated nanotransfer printing via vapor phase polymerization. The single-crystal PEDOT nanowires are formed from ethylenedioxythiophene (EDOT) monomers that are self-assembled and crystallized during vapor phase polymerization process within nanoscale channels of a mold having FeCl₃ catalysts. These PEDOT nanowires, aligned according to the pattern in the mold, are then directly transferred to specific positions on a substrate to generate a nanowire array by a direct printing process. This direct printing method in combination with vapor phase polymerization simultaneously enables the synthesis, alignment and patterning of single-crystal PEDOT nanowires. The conductivity of the single-crystal PEDOT nanowires is an average of 7619 S/cm which remarkably exceeds literature values of PEDOT nanostructures/thin films. To demonstrate usefulness of single-crystal PEDOT nanowires, we fabricated an organic nanowire field-effect transistor array contacting the ultra-high conductive PEDOT nanowires as metal electrodes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1086

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Bond Covalency on the Band Structure and Photocatalytic Activity of Silver Oxosalts

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The effects of the bond covalency of oxosalt group on the electronic structure, surface property, and photocatalytic activity of silver oxosalts, $\text{Ag}_x(\text{XO}_y)_z$, are systematically investigated with comparative experiments and theoretical calculation. The covalency of (X-O) bond is sensitive to the charge-to-size (Z/r) ratio of central atom (X). The increase of the Z/r ratio causes the enhancement of the bond covalency of (X-O) and in turn the decrease of the covalent character of neighboring (Ag-O) bond via bond competition effect. The resulting narrowing of band width induces the enlargement of bandgap separation. A useful empirical formula about the linear relationship between the Z/r ratio of the central atom of oxosalt group and the ΔE of silver oxosalts is obtained from the experimental data of several silver oxosalt compounds. The relationship between the Z/r ratio of central atom and photocatalyst performance is well-confirmed by experimental studies on a series of silver oxosalts, Ag_2CO_3 , Ag_3PO_4 , Ag_3AsO_4 , and Ag_2SO_4 . On the basis of the theoretical conjecture, Ag_2SeO_4 is newly found to exhibit promising visible light photocatalytic activity. The present results clearly demonstrate that the Z/r ratio of central atom has profound influence on the photocatalyst performance and band structure of silver oxosalts.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1087

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of high functional polymer on the wettability of hydrogel soft ophthalmic lenses

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세한대학교 안경광학과

For the preparation of high functional hydrogel ophthalmic lens, the copolymer containing 2-chloropyridine-4-carboxylic acid as additives were manufactured and also the physical properties of the produced hydrogel ophthalmic lenses were measured. In this study, 2-chloropyridine-4-carboxylic acid with, EGDMA (ethylene glycol dimethacrylate), HEMA (2-hydroxyethyl methacrylate), MMA (methyl methacrylate), AA (Acrylic acid) and the initiator AIBN (azobisisobutyronitrile) were used for thermal copolymerization. The mixture was heated at 115 °C for 40 mins to produce the hydrogel soft contact lens by cast mould method. The measurements of water content, refractive index and visible transmittance were in the range of 36.00 ~ 35.74%, 1.4348 ~ 1.4360 and 91.4 ~ 92.0%, respectively. Also, the transmissibility of UV-A and UV-B decreased slightly from 88.8 to 87.0% and 84.4 to 80.0%, respectively. The tensile strength of sample was in the range of 0.2674 ~ 0.3190 kgf. Also, the results of these measurements showed that the refractive index increased as the ratio of 2-chloropyridine-4-carboxylic acid increased. The contact angle of ophthalmic lens sample containing 2-chloropyridine-4-carboxylic acid was in the range of 66.38~72.52°. Based on the results of this study, the produced copolymer is suitable for hydrogel soft ophthalmic lenses with high wettability.

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장소: 창원CECO

발표코드: **MAT.P-1088**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the UV-block Material for Hydrogel Lens Polymer

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세한대학교 안경광학과

The physical and optical characteristics of hydrophilic contact lens polymerized with addition of 2,5-difluoroaniline in the basic hydrogel contact lens material were evaluated, and in particular, the utility of 2,5-difluoroaniline as a UV-blocking material for ophthalmologic devices by measuring the UV transmittance was investigated. In this study, 2,5-difluoroaniline was added to the cross-linker EGDMA (ethylene glycol dimethacrylate), HEMA (2-hydroxyethyl methacrylate), NVP(N - vinyl pyrrolidone), MA (methacrylic acid) and the initiator AIBN (azobisisobutyronitrile) in various concentrations. The results showed that water content, refractive index, contact angle and tensile strength were in the range of 37~38%, 1.434~1.438, 59~64° and 0.210~0.330 kgf independently. The transmittance of visible light decreased from 91% to 90% as the increase of 2,5-difluoroaniline. Also, the transmittance of UV-A and UV-B decreased from 86% to 79% and from 77% to 47%, independently. The material containing 2,5-difluoroaniline is expected to be used usefully as a material for UV-block hydrogel contact lens without affecting the water content and wettability.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1089

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Characterization of Solid Cap and Photo-protected Silica Nanotubes (SNTs) using Polydimethylsiloxane (PDMS) filling method

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경원대학교 바이오테크놀로지학과¹ 경원대학교 바이오테크놀로지학과

Silica nanotubes (SNTs) can store and transport nano-materials such as organic molecules and nanoparticles as a nano-sized carrier. In this study, we developed a facile method for fabrication of photostable fluorescent silica nanotubes (SNTs) based on polydimethylsiloxane (PDMS) filling technique. In addition, Ar plasma treatment was turned out to be necessary to prevent dye leakage from the SNTs by forming solid cap in the open ends of the SNTs. The photostability of various SNTs was confirmed by photobleaching test. Compared with bare SNTs embedded dyes, the SNTs filled with PDMS-dyes mixture showed better photostability. In order to confirm that Ar plasma treatment is an essential process to protect dye molecules from being release from the SNTs, dye release tests was performed with the SNTs with and without Ar plasma treatment. The TEM analysis revealed that a solid dense layer was formed after the plasma treatment, which enables the lower dye leakage. The PDMS-filled and welded SNTs are useful for bioanalysis such as cell or antigen targeting as probes because of low level of leakage and high photostability of the silica naotubes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: MAT.P-1090

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrophobic end-gated silica nanotubes for intracellular glutathione-stimulated drug delivery in drug-resistant cancer cells

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경원대학교 Bionano ¹경원대학교 바이오나노대학

Silica nanomaterials have been used in potential drug delivery because of their unique structures, large surface areas, tunable sizes, and good biocompatibility. The void structures and biocompatibility of silica nanotube (SNT)-based drug delivery systems (DDSs) make them important tools for enhancing the efficacy of chemotherapeutics. Surface-functionalized, end capped porous silica nanomaterials have been used to fabricate stimuli-responsive carriers for controlled drug delivery. Glutathione (GSH), the most abundant thiol species at a concentration range of 1-10 nM in the cytoplasm has been used as an in situ released reagent in living cells due to its major reducing capability in biochemical process. A gold nanoring was fabricating specifically only at the open end of SNT via a seed-mediated gold growth reaction. Then, 1-octadecanethiol (C18-SH) was modified on the surface of the gold nanoring to encapsulate doxorubicin (DOX) inside SNTs. The C18-SH anchored on the gold ring surface can act as a chemical labile hydrophobic cap at the open ends of SNTs and later will be detached by naturally existing GSH triggers in a cell. In this work, GSH-triggered conversion from hydrophobic to hydrophilic end capping at the pores of SNTs was demonstrated to achieve improved efficacies in drug resistant and overcome the drug resistance of MCF-7/ADR cells and in vivo experiment via injection into MCF-7/ADR xenografted mice.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1091**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal-Support Interactions of Pt-Mesoporous Gallium Oxide Thin Films Composite with CO Tolerance in Methanol Oxidation Reaction

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성균관대학교 나노과학기술학과 ¹성균관대학교 화학과

We have developed a facile synthesis of MGTf with wormlike structure by using a F-127 as a SDA and a highly improved kinetics with superior CO tolerance in an electrocatalytic methanol oxidation reaction (MOR) on platinum-mesoporous gallium oxide composite thin films (Pt-MGTfs). We prepared Pt-MGTfs by electrochemical depositing Pt into the pores of MGTfs. The MGTfs' properties were characterized by means of scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). From those analyses we could confirm that strong metal support interaction (SMSI) between Pt and MGTfs in Pt-MGTfs samples and significant changes of the electronic properties of the metals, Pt herein. Pt-MGTfs exhibited not only negatively shifted onset potential by 0.2 V vs. Pt replica but also remarkable CO tolerance property. It is the first attempt to use gallium oxide for the enhancement of MOR via CO tolerant property and SMSI and these Pt-MGTfs suggest a new manner to construct exceedingly active and durable electrocatalyst.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **MAT.P-1092**

발표분야: 재료화학

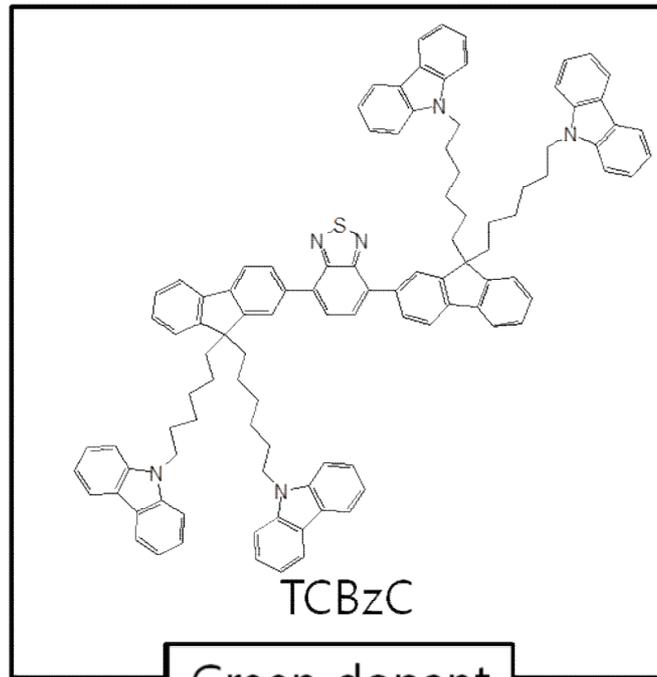
발표종류: 포스터, 발표일시: 수 16:00~19:00

Three Color White OLEDs Using Highly Efficient Green Dopant based on Solution Process

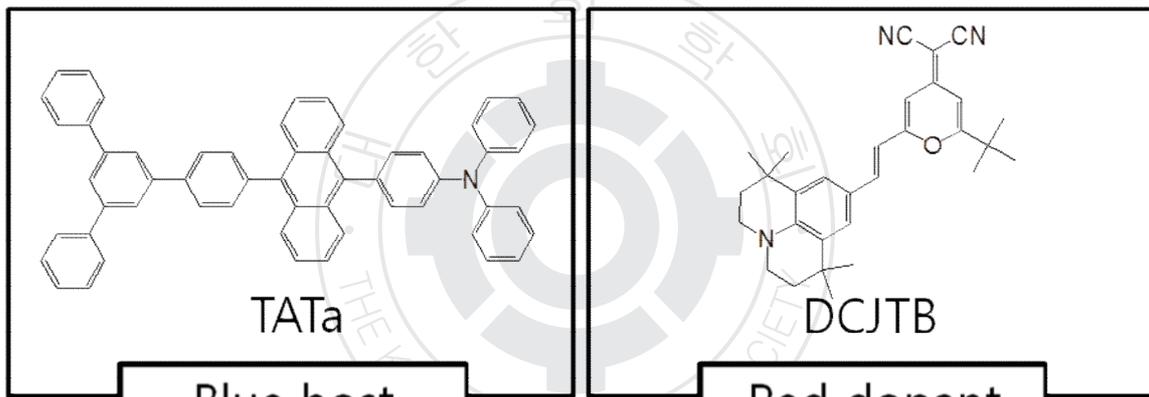
이재현 김승호 박종욱*

가톨릭대학교 화학과

new green dopant of TCBzC substituted carbazole units was investigated in solution process WOLED device. 4-(10-(3',5'-diphenyl-biphenyl-4-yl)anthracen-9-yl)-N,N-diphenyl-aniline (TATa) and 4-(dicyanomethylene-4)-2-t-butyl-6(1,1,7,7-tetramethyljulolidyl-9-enyl)-4H-pyran (DCJTB) were used for the blue host and red dopant. A structure of the device was fabricated as ITO / PEDOT (40 nm) / PVK (14nm) / EML: TATa + TCBzC: 3.0wt% + DCJTB: 0.08wt% (50 nm) / TPBi (20 nm) / LiF (1 nm) / Al. As a result, TCBzC device of 1.44 cd/A was obtained. CIE value of TCBzC device was (0.26, 0.41). More device performance data will be discussed.



Green dopant



Blue host

Red dopant

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발표코드: **MAT.P-1093**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Various Core-shell Nanoparticles with Dielectric Interlayers

백연경

재료연구소 분말 세라믹 세부

Core-shell Nanoparticles continue to attract strong interest on account of their fascinating properties and potential applications in optical sensing, optoelectronics, biomedicine, imaging and catalysis applications. Especially, Ag, Au, Pt and Pd nanoparticles have been widely used as light absorbers with specific wavelength regions due to their remarkable surface plasmon characteristics. The incorporation of two different metals in a core-shell nanoparticle has been widely synthesized for various applications. However, the direct contact between core and shell metal component leads to the incorporation two plasmonic scattering, resulting in a single absorption characteristic peak. Herein, we have conducted the facile fabrication method of various core-shell nanoparticles with dielectric interlayers. Our strategy using silica interlayers can enables to obtain core-shell nanoparticles showing the two different absorption peaks together, which can pave the way for plasmonic application requiring the broad light absorption.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Incorporation of Ligand-Assisted Plasmonic Nanoparticles for Enhanced Performance of Polymer Solar cells

백연경

재료연구소 분말 세라믹 세부

Enhancement of light absorption of solar cells using nanoscale structures and novel physical effects has attracted a great deal of attention in recent years. Especially, utilizing plasmonic nanoparticles (NPs) such as Au and Ag NPs is considered as one of the promising methods for significant enhancement of local electromagnetic fields and thus improves the optical properties of the nanostructure devices. In addition, the incident photons can be scattered over a longer propagation path in the active layer by metallic nanostructures. These features can potentially benefit the light absorption and photocurrent generation of polymer solar cells. Thus, the incorporation of metallic NPs in organic solar cells has been conducted for improving photovoltaic performances. Especially, recent studies has been devoted to adding plasmonic nanoparticles into bulk heterojunction (BHJ) polymer because the method enhances the overall performance of the cell; reduction of the device resistance and efficient increase in the optical path length in the polymer. However, most metal nanoparticles utilized were prepared in aqueous media, which means the nanoparticles have incompatible surface to organic solvent containing BHJ polymer. Here, we examined the effects of various organic based ligands on dispersion of plasmonic metal nanoparticles in P3HT/PCBM layer and the performance of organic solar cells. The strategy employing optimum ligands to disperse metal nanoparticles in BHJ layer would provide improvement in optical properties and performance of polymer solar cells.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Porous Structured NiO Nanotubes on Carbon Fiber Paper as Electrode Materials of Pseudo-capacitors

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A wide variety of transition metal oxides have long been at the center of the research of pseudocapacitor electrodes. NiO has in particular received great interest as one of the promising electrode materials for pseudocapacitors because of its high theoretical specific capacitance, excellent chemical and thermal stability, and low cost . However, NiO often suffers from low electrical conductivity and poor long-term durability. To address these hurdles, conductive additives such as activated carbon, carbon nanotubes, or graphene have been used. However, the use of a binder and non-homogeneous mixing with the carbon additives hinders the full utilization of NiO. In this work, we synthesized porous NiO nanotubes array on carbon fiber paper via a simple template method. The unique nanostructure of our NiO electrode led to the increase in contact area between electrolyte and electrode material, facilitated ion transport, and relieved strain induced during charge/discharge cycling. As a result, the NiO nanotubes integrated on carbon fiber paper exhibited a superior performance and long-term stability.

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발표코드: **MAT.P-1096**

발표분야: 재료화학

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Emerging Strategy for InfoHybrid System

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We briefly address the recent challenges and strategies to “infohybrids” that combines hybrid science and information technology. The aspects of the infohybrid system will be discussed in terms of materials and devices used in the design and application of infohybrid systems. Furthermore, we will describe how we have innovatively approached the design and development of a systematic diagram of the infohybrid for its potential use in barcoded molecular sensing, steganographic nanoforensics, item-level tagging identification, data storage, and even communication. In our study, chemically well-defined Bio Core@Inorganic Shell nanohybrid, which consists of rational DNA molecules core with a size of 100 nm and spherical inorganic nanoshell with wall thickness of 10 nm reassembled with exfoliated layered double hydroxide (LDH nanosheets), is prepared. The encapsulation of information DNA and its release, due to the pH dependent solubility of LDH nanoshell, plays a crucial role in maximizing the stability of base sequence-manipulated and probes-functionalized DNA molecules with designed information. Furthermore, the DNA@LDH materials applied to the infohybrid system, as a newly adopted integrative concept combining Nano-Bio-Info-Congo technologies.

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발표코드: MAT.P-1097

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Band Gap Engineering of Ordered Mesoporous $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ Ternary Compound Semiconductors for Photocatalysis

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II-VI compound semiconductors, such as ZnE and CdE ($E = \text{S}, \text{Se}, \text{and Te}$), are known as most important semiconductors due to their unique optical and semiconducting properties. Due to the physicochemically and optically unique properties, plenty of the papers were reported in the fields of syntheses and applications of the II-VI semiconductor materials with various morphologies such as spheres, nanorods, tetrapods, nanowires, or any other nano-structures. Notably, metal chalcogenides have excellent properties in that the band gap corresponds well to the spectrum of sunlight, and the conduction band edge is more negative than the $\text{H}_2\text{O}/\text{H}_2$ redox potential. Although successful photocatalytic systems have yet to be achieved, these semiconductors are attractive as visible light driven catalysts once the stability is improved. As a typical alloyed chalcogenides, recently, $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ has been intensively studied because of its high density optical recording, blue or even UV laser diodes. These studies have revealed that $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ has good and tunable absorption properties in the visible zone of the solar spectrum resulting from the regulable band gap between CdS and ZnS materials. As a response to their sufficiently negative flat band potentials, $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ alloys are excellent candidates as visible light driven photocatalysis. Herein, we report on the band gap engineering of the ordered mesoporous $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ materials, and the synthesized materials were characterized by X-ray diffraction, N_2 -sorption isotherms, electron microscopy, and diffuse reflectance UV-visible spectroscopy. The photocatalytic activities of materials were also investigated.

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발표코드: MAT.P-1098

발표분야: 재료화학

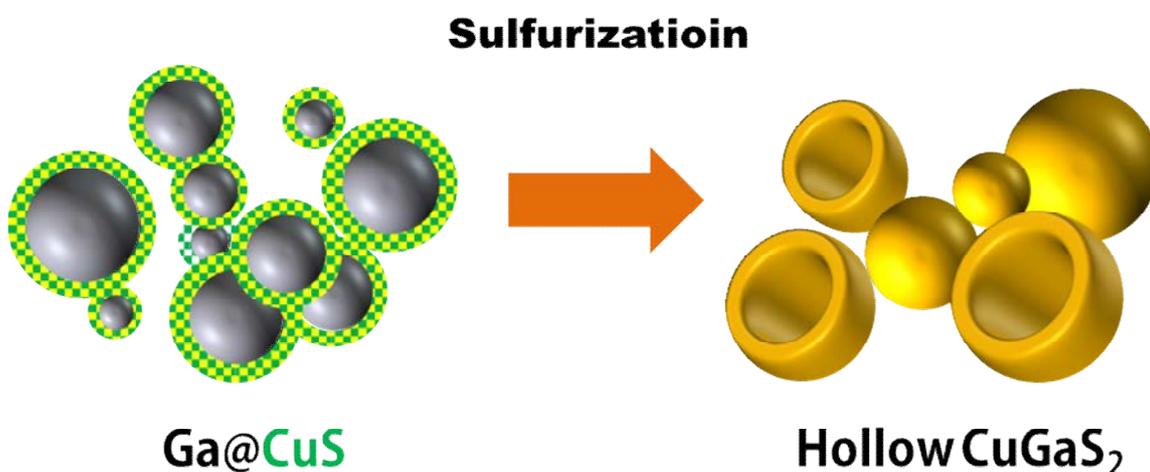
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasonic Synthesis of Ga@CuS Core-Shell Nanoparticles and Transformation to Hollow Sphere CuGaS₂ Compounds

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성균관대학교 화학과 ¹성균관대학교 화학

Core shell nanoparticles of Ga@CuS were successfully synthesized by ultrasound process in liquid medium. The Ga@CuS nanoparticles were obtained by using Ga metal nanoparticles as the template, which were prepared by ultrasound irradiation of the system in ethylene glycol medium, and then CuS shell on Ga nanoparticles was directly obtained by sonochemical reaction. Structural characterization indicates that core and shell of the products are composed of amorphous Ga metal and covellite structure CuS. Ga@CuS core shell particles were transformed into well-crystallized CuGaS₂ hollow sphere after sulfurization at 450°C, as confirmed by X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray fluorescence (XRF), diffuse reflectance UV-vis spectroscopy (DRS-UV) and Raman spectroscopy. The formation of hollow nanostructure was explained by a Kirkendall mechanism, in which Ga metal nanoparticles play a important roles as reactive template.



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발표코드: **MAT.P-1099**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

UV-blocking Property of Mesoporous TiO₂ containing Bemotrizinol

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성균관대학교 화학과

Titanium dioxide (TiO₂) is one of the most important semiconducting materials for UV-blocking materials, photocatalysis, dye-sensitized solar cell, gas sensing, etc. TiO₂ has several advantages; high band gap energy (~3.2 eV), high oxidative ability, high stability, strong catalytic activity, non-toxicity, and low cost. Especially, in cosmetics, TiO₂ is widely studied as a sun screening materials due to its high UV absorbing or blocking ability, and high stability. However, TiO₂ only could absorb or block the UVB region, it could not handle UVA region which gives critical injuries to the corium. Thus, it is necessary to take advantage of UVA adsorb-materials. In this study, we have synthesized mesoporous TiO₂ with high surface area. For UVA and UVB blocking materials, we have studied to synthesize mesoporous TiO₂ impregnated with Bemotrizino which could block UVA light. Synthesized materials were characterized by X-ray diffraction, N₂-sorption analysis, scanning electron microscopy, transmission electron microscopy, and UV-visible diffuse reflectance spectroscopy.

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발표코드: MAT.P-1100

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Methylene Blue Embedded Gold Nanorod@SiOH₂ Core@Shell Nanoparticles as the New Theragnostic Agent for Cancer

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금오공과대학교 응용화학과

Early diagnosis of cancer plays a crucial role in increasing chance of survival from cancer death and molecular imaging technology has emerged as a new paradigm for cancer management. For that reason, the recent rapid evolution of nanoscience and nanotechnology has propelled the development of various multifunctional solid nanoparticles with unique chemical and physical properties for biomedical applications as multimodal molecular imaging probes. In many cases, however, the chemical toxicity of the metal ions, dissolved by the metabolic process, restricts the use of these species (e.g., CdSe quantum dots) to clinical applications. Thus, biocompatible materials such as gold, iron oxide, and silica nanoparticles are becoming choice of materials for biomedical applications. Among them, gold nanorods (GNRs) grown anisotropically along the [001] direction have been extensively studied during the past decade because of their biocompatibility and excellent plasmonic responses. In particular, longitudinal surface plasmon resonance (LSPR) along the elongated axis of the GNR strongly exhibits around the near infrared (NIR) wavelength region depending on aspect ratio that well defined plasmonic property of the GNR provides the new challenge in nanomedicine area such as photothermal theragnostics, SERS (surface enhanced Raman scattering) molecular imaging, and photoacoustic tomography. Herein, methylene blue (MB) was incorporated into the mesoporous silica coated GNR as not only Raman active dye but also photosensitizer. The resulting MB embedded GNR@SiO₂ nanocomposites show excellent SERS efficiency and cancer killing effect combining photothermal and photodynamic therapy (PDT). Therefore, the MB-Au NR@SiO₂ nanoparticles could allow us to explore the new theragnostic agent for cancer and it would be considerable advances in predictive and personalized nano-medicine.

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발표코드: MAT.P-1101

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Single-Step Synthesis of Ag Nanoshells onto Silica Nanosphere for Surface Enhanced Raman Scattering and Pesticides Detection

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서울대학교 화학생물공학부

Metal nanoshells (NSs), which consist of metallic shell and dielectric core, have drawn a lot of interest due to their tunable optical properties. Although there have been many efforts to synthesize uniform, reproducible, and controllable Ag-NSs, previously reported synthetic methods suffer from complex synthetic steps and difficulty in controlling the thickness. In this paper, we demonstrate a seedless single-step synthesis of Ag-NSs at room temperature. The size and thickness of Ag-NSs can be tuned by controlling the relative concentration of silica nanoparticles (NPs). The key of synthetic step was stabilization of Ag^+ ions by ethylene glycol and subsequent rapid reduction of Ag^+ ions by octylamine, which led to burst nucleation and growth of silver shell layer on silica NPs. As-prepared Ag-NSs gave strong surface-enhanced Raman scattering (SERS) and afforded SERS-active substrate for direct on-site detection of pesticide residues.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and structure analysis of nitrodo-oxo-phosphate



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아주대학교 에너지시스템학부

Sodium-nickel-nitrodo phosphate, $\text{Na}_2\text{Ni}_2(\text{PO}_3)_3\text{N}$ were synthesized by solid state reaction of stoichiometric mixture of NaPO_3 , $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and $\text{NH}_4\text{H}_2\text{PO}_4$ under ammonia gas flow. The crystal structure of $\text{Na}_2\text{Ni}_2(\text{PO}_3)_3\text{N}$ was determined from X-ray powder diffraction data and investigated by means of Rietveld refinement method. The diffraction pattern showed the cubic symmetry with space group of $P2_13$ ($Z=4$) and lattice parameters $a = 9.1749(1)\text{\AA}$. In the structure of $\text{Na}_2\text{Ni}_2(\text{PO}_3)_3\text{N}$, phosphorous atom is coordinated to three oxygen atoms and one nitrogen atom to form a PO_3N tetrahedron. The $(\text{PO}_3)_3\text{N}$ entity is formed by three PO_3N tetrahedra sharing a common corner occupied by nitrogen atom. A nickel atom is coordinated to six oxygen atoms to form an octahedron and the six oxygen atoms are connected to the three $(\text{PO}_3)_3\text{N}$ groups. Na, Ni and N atoms are arranged along $[111]$ direction in the sequence of Ni1-Ni2-N-Na1-Na2-Ni1-Ni2- The $\text{Ni}1\text{O}_6$ octahedron is connected to $\text{Ni}2\text{O}_6$ octahedron with face-sharing.

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발표코드: MAT.P-1103

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of New Lithium Ionic Conductor

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Li_5AlS_4 was synthesized by solid state reaction. The starting materials Li_2S and Al_2S_3 were weighed in appropriate molar ratios in argon filled glove box, put into a quartz tube and heated at a 650°C for 10hrs. Because Li_5AlS_4 is very unstable and uptake moisture from atmosphere all synthetic procedures should be performed in glove box. The crystal structure of Li_5AlS_4 was investigated by means of Ab initio structure determination method based on neutron powder diffraction data. Diffraction pattern of this compound showed the monoclinic symmetry (space group, $P2_1$). In the structure of Li_5AlS_4 , aluminum atom is coordinated to four sulfur atoms to form a AlS_4 tetrahedron. Lithium atoms occupy crystallographically different five sites. Among them, Li1, Li2 and Li3 are coordinated to four sulfur atoms to form LiS_4 tetrahedra, respectively, while Li4 and Li5 atoms are coordinated to six sulfur atoms to form a LiS_6 octahedra.

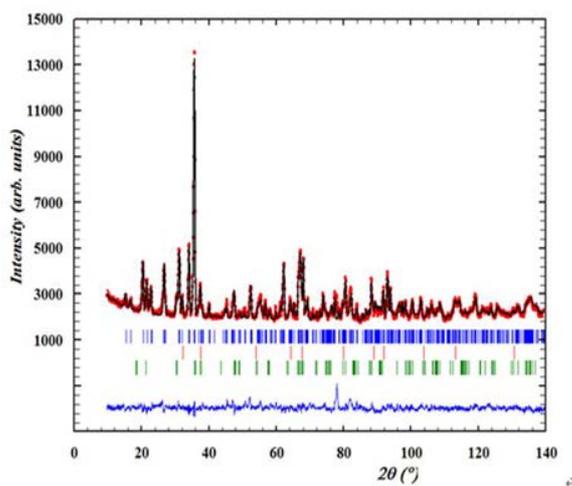


FIG.1 Rietveld Refinement of Li_5AlS_4

$R_p = 3.10\%$, $R_{wp} = 4.34\%$, $R_{exp} = 2.01\%$, $\chi^2 = 4.65$

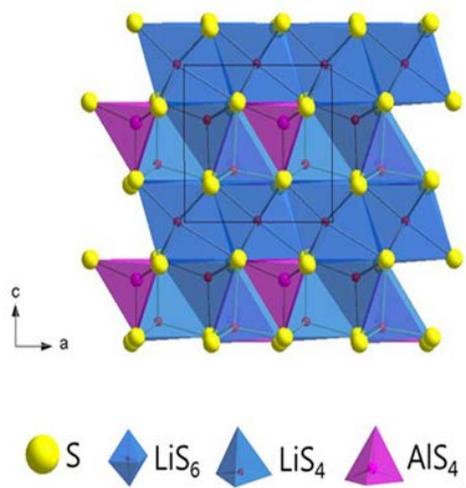


FIG.2 Structure of Li_5AlS_4



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Graphene-Embedded Alumina-PMMA Hybrid Materials

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Recently, bio-mimetic alumina-polymer composite materials attract attention due to their enhanced fracture toughness (K_{IC}). In their structure, plate-type alumina grains are aligned each other and hybridized with polymer to have a “brick-mortar-bridge” structure. In this study, we attempted to improve the strength and toughness of the alumina-polymer composite materials by embedding mechanically strong graphene in the matrix. Graphene-embedded ceramic-polymer composite materials have not been reported so far. Our graphene-embedded alumina-PMMA(poly-meta-acrylic acid) composite shows high fracture toughness due to interference of crack propagation by embedded graphene in alumina grain. The graphene-embedded alumina-PMMA composite materials were prepared by sintering a mixture of graphene and plate-type alumina, and subsequent polymer embedding. After the polymerization reaction, the PMMA penetrates into interlayer space between the alumina layers, which was modified by organo-silane grafting. The fracture toughness and flexural strength value of the composites were measured. As a result, increased fracture toughness ($\sim 5.6 \text{ MPa}\cdot\text{m}^{1/2}$) and strengths ($> 200 \text{ MPa}$) were observed in our synthesized composites.

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발표코드: MAT.P-1105

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermoelectric Property of chemically exfoliated n-type $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$

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Bismuth telluride-related alloys are the best bulk thermoelectric materials, which are ever known so far. Bi_2Te_3 has a hexagonal layered structure comprised of five atom thick stacks of Te-Bi-Te-Bi-Te held by weak van der Waals forces. In this study, we attempted to synthesize n-type Bismuth chalcogenide nanoplatelets by exfoliation method and measure thermoelectric property of the sintered bulk material. Lithium cations were intercalated into interlayer space between the $[\text{Bi}_2(\text{Te},\text{Se})_3]$ layers using the reducing power of solvated electrons in n-hexane. The intercalated lithium was removed by reaction with water, which created stable colloidal suspension of exfoliated nanoplatelets. Thermoelectric property of the $\text{Bi}_2(\text{Te},\text{Se})_3$ nanoplatelets was found to be recovered by minimizing surface oxides by chemical reduction of the exfoliated suspensions. Using spark plasma sintering technique, bulk materials of bismuth chalcogenide, composed of plate-like grains with ~50 nm thickness, were synthesized from the exfoliated and ultrasonicated samples. The resulting compounds showed reduced thermal conductivity due to enhanced phonon scattering at highly dense grain boundaries without deterioration of power factor. The peak ZT value of the present compound (ZT~0.8) is comparable to that of n-type single crystalline $\text{Bi}_2(\text{Te},\text{Se})_3$, which is one of the highest among the reported n-type materials synthesized by soft chemical route.

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발표코드: MAT.P-1106

발표분야: 재료화학

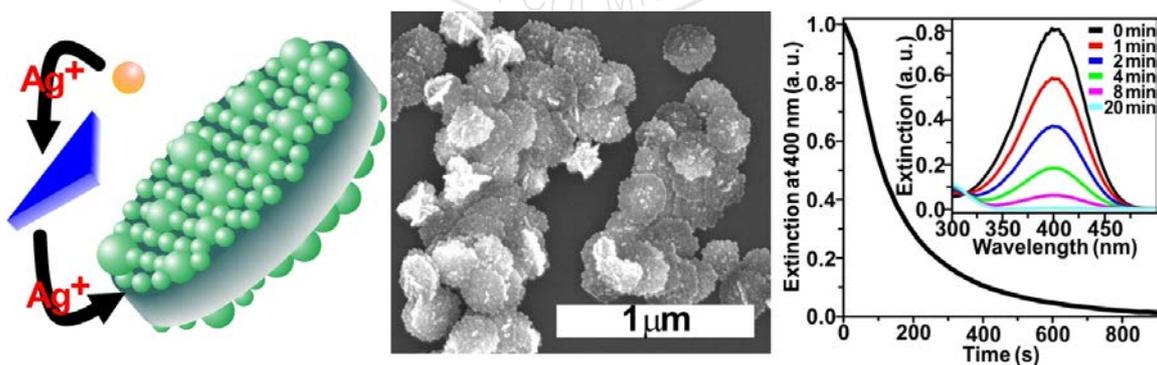
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Large Bumpy Silver Nanostructures with Controlled Sizes and Shapes for Catalytic Applications

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고려대학교 신소재공학부

We have synthesized disc-like large silver nanomaterials ($D = \sim 250$ nm) that have nanostructured bumps on the surface using smaller nanoplate seeds ($D = \sim 100$ nm). The size and shape of the bumpy nanostructures are rationally controlled by changing the concentrations of nanoplate seeds, silver ion, reductant, and citrate ion. Importantly, the synthetic mechanism of these bumpy nanostructures is remarkably similar to that of the conventional seed-mediated growth based on tiny seeds ($D = \sim 5$ nm). We have further investigated the catalytic properties of the bumpy nanostructures for the reduction of 4-nitrophenol, which is associated with a concomitant color change from yellow to colorless



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Transparent and Conducting Graphene/ZnO Hybrid Films Fabricated by Aerosol Chemical Vapor Deposition

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ZnO/graphene hybrid films have been synthesized with aerosol chemical vapor deposition (Aerosol CVD). The ZnO/graphene hybrid films, in which the graphene nanosheets are embedded in the matrix of ZnO, were fabricated from colloidal suspensions of the graphene oxide (GO) with an aqueous zinc precursor. The graphene nanosheets were dispersed into aqueous solution of 1 wt % sodium dodecyl sulfate (SDS), which results in stabilization of the GO in colloidal suspensions. The resulting ZnO/graphene hybrid films have reduced resistivity, compared to bare ZnO film. The hybrid films exhibit optical transmittance of about 80 % in visible regions and sheet resistance of ~20 k Ω /square. Both experimental data shows the present hybrid is promising as a transparent and conducting material in optoelectronic devices.

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장소: 창원CECO

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발표분야: 재료화학

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Enhanced thermoelectric properties of In, Yb double filled CoSb_3 based skutterudites nanocomposites

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With serious concerns regarding the exhaustion of fossil fuel resources and environmental pollution, there has been renewed interest in thermoelectric power generation which can recycle the waste heat as an energy saving technology. The energy conversion efficiency of thermoelectric devices depends partly on the non-dimensional figure of merit (ZT) of thermoelectric materials. Numerous works have been done to improve the ZT values of thermoelectric materials, and thermoelectric nanocomposites processed by dispersion of nanopowders into bulk materials have drawn much attention in recent years. For thermoelectric nanocomposites, improvement of ZT values has been suggested due to decrease in lattice thermal conductivity without adverse effects on electrical resistivity. Among many kinds of materials, CoSb_3 -based skutterudites nanocompounds are the most widely used thermoelectric materials but has a low figure of merit due to the high thermal conductivity. To solve this problem, filling voids with rare earth atoms is an effective way to lowering thermal conductivity which causes scattering of phonons, necessarily enhances thermoelectric properties of skutterudite compounds. In this study, double-filled CoSb_3 based skutterudite nanocomposites were processed by Spark Plasma Sintering (SPS) of mechanically alloyed $\text{In}_x\text{Yb}_y\text{Co}_4\text{Sb}_{12}$ nanopowders. The results showed that a pure skutterudite phase could be obtained by mechanical alloying with appropriate ball-milling time and SPS process. The structure and composition of the samples are characterized by using XRD and EDS. Thermoelectric characteristics of the filled-skutterudite nanocomposites were evaluated at a temperature range from room temperature to 873 K as a function of the atomic fraction of dispersed filler atoms.

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발표코드: MAT.P-1109

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발표종류: 포스터, 발표일시: 수 16:00~19:00

High Efficiency Ambipolar Blue Emitting Materials Based on Amino-Methyl-Chromen Derivatives for OLEDs

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New blue emitting materials, 7-diphenylamino-4-methyl-coumarin (DPA-MC) and aminotri(4-methylcoumarin) (T-MC) including coumarin moiety were synthesized by Ullman reaction. Optical and electronic properties were examined by UV-Vis. Absorption spectrum, PL spectrum, and cyclic voltammetry. UV-Vis. spectra of DPA-MC and T-MC in a film state showed maximum absorption wavelengths of 382 nm and 399 nm, respectively. PL spectra of DPA-MC and T-MC show maximum emission wavelengths of 463 nm and 481 nm respectively. Non-doped OLED devices were fabricated by using the synthesized materials as an emitting material layer. DPA-MC compound showed highly efficient luminescence properties. EL spectrum of DPA-MC exhibited a maximum value of 463 nm and DPA-MC device provided luminescence efficiency of 3.83 cd/A, power efficiency of 2.46 lm/W and CIE coordinates of (0.154, 0.190) at a current density of 10 mA/cm². In particular, Power efficiency increased by more than 1.6 times in DPA-MC (2.46 lm/W), which is higher than commercialized material, DPVBi (1.46 lm/W). High EL performance might come from ambipolar effects of a molecular structure.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nano hybrid materials of cobalt hydroxides

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We synthesized various forms of $\text{Co}(\text{OH})_2$ in aqueous solution and their nanocomposites with carbon materials. The exfoliated $\text{Co}(\text{OH})_2$ nanosheets were self-assembled with graphene oxide through Coulomb interactions. Graphene oxide/ $\text{Co}(\text{OH})_2$ nanohybrid materials were reduced by annealing under Ar_2/H_2 mixed gas atmosphere. The prepared nanohybrid materials of carbon- $\text{Co}(\text{OH})_2$ were characterized by HR-TEM, SEM, XRD, UV-vis absorption spectroscopy, Raman spectroscopy, Zeta-potential, laser scattering particle size analyzer. The electrochemical storage capacity showed significant increases compared to the as-prepared the pristine $\text{Co}(\text{OH})_2$.

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발표코드: MAT.P-1111

발표분야: 재료화학

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Cobalt Boride Nanoparticles Immobilized on Layered Double Hydroxide Nanosheets

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Cobalt boride nanoparticles (Co₂B-NPs) immobilized on layered double hydroxide nanosheets (LDH NS) was successfully synthesized. LDH-NS were incorporated with the black colloids of Co₂B-NPs with average of 20-30 nm size distribution, synthesized by the reduction of Co²⁺ by NaBH₄. This assembly of high density Co₂B-NPs on the exfoliated LDH-NS which could be applied as a hybrid supporter for Co₂B-NPs catalysts was characterized by XRD pattern, SEM and HR-TEM. The catalytic activity were measured for hydrogenation reaction of p-nitrophenol and monitored by using UV-Vis spectrophotometer at room temperature. After the completion of the reaction, the catalysts showed catalytic conversion on the first reaction cycle up to 100%. These LDH-Co₂B nanocomposites are expected to provide 'new platform' for the development of heterogeneous nanocatalysts

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

자기 조립법에 의한 양자점이 함치된 고분자 입자의 합성 및 LED 응용

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본 학술 발표에서는 양자점을 포함하는 고분자 입자를 자기 조립 기술에 의해 합성하고 이를 LED 에 응용하는 연구 결과를 발표하고자 한다. 디스플레이 소자나 생물학적 진단 등에 활용이 높아질 것으로 예상되는 양자점은 그 표면 특성을 제어하기 위하여 세라믹 절연층으로 코팅하거나, 고분자 입자 내부에 함치시키는 연구가 몇몇 연구진들에 의해 진행되어 왔다. 대부분의 방법들이 양자점의 표면에 리간드를 치환한 뒤, 졸-겔 반응이나 중합 반응을 거쳐 양자점이 포함된 복합 입자를 제조하는 루트를 취하고 있다. 이 경우, 리간드 치환 과정에서 양자점의 광학적 활성이 저하될 수 있다는 단점을 내포하고 있다. 본 연구에서는 에멀전 액적을 자기조립틀로 활용하여 액적 내부에서 고분자 물질과 양자점의 자기 조립에 의해 고분자-양자점 복합 입자를 합성하는 내용을 소개하고자 한다. 이러한 물리적인 자기 조립을 거칠 경우 리간드 치환 과정이 불필요하므로 양자점의 발광 특성의 저하가 어느 정도 방지될 수 있다는 장점을 기대할 수 있을 것이다. 본 연구에서 제조된 CdSe 또는 CdSe@ZnS 등의 양자점이 포함된 poly(St-co-MMA) 입자를 합성할 수 있었으며, 이를 blue LED 칩에 PDMS resin 과 함께 도포하여 CRI(color rendering index)가 높은 백색 LED 를 제조할 수 있었다. 본 발표에서는 고분자-양자점 복합 입자의 제조에 대한 결과와 더불어, LED 의 발광 특성 향상에 대한 연구 결과를 소개하고자 한다.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Tailorable Permselective Membranes Made of 2D Cucurbit[6]uril Polymers

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Separation of small molecules by nanoporous membranes is of great interest in industries, especially for pharmaceutical and biological applications. Despite the recent progress in the fabrication of the nanoporous membranes via electroless gold deposition, atomic layer deposition, and conformal initiated chemical vapor deposition, a simple and general method for the fabrication of the nanoporous membranes with tailorable surface properties has yet to be developed. Here, we demonstrate a facile fabrication of the nanoporous permselective membranes using the two-dimensional (2D) polymers by a simple deposition of 2D polymers on the supporting membranes, and their tunable separation properties. The 2D polymers were synthesized via thiol-ene photopolymerization of (allyloxy)₁₂cucurbit[6]uril and dithiol linker in solution. The membrane that has 2D polymers on the surface has its own selectivity. Furthermore, the post-synthetic modification of the membranes via host-guest chemistry allows tuning the separation selectivity of the membranes. The details of this work will be presented.

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발표코드: MAT.P-1114

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Highly Conductive and Transparent Heating Glass by Spray Deposition of Silver Nanowires

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Herein using silver nanowire, we designed conductive and transparent heater for excellent performances in solving problems for frost and fogs by reaching desired temperature in optimized condition for vehicle and other conventional uses. We fabricated a hybrid film on top of glass and PET substrate by simply spraying the AgNWs and immerse the sprayed product in a polymer solution to develop a high quality conducting composite under room temperature for heating windshield for vehicles. Measurement of sheet resistance changes, scanning electron microscopy (SEM), optical microscopy (OM), UV-vis spectroscopy, and heating test with IR monitoring were used to investigate the adhesion properties as well as comparing the performance of AgNW/glass hybrid film with and without the coating of GO as the outer most layer. We successfully demonstrated that our hybrid film on substrates, with low sheet resistance value, was able to heat up all types of substrates within desired time with standard voltage of 12 V. Therefore, this polymer treated and GO protected AgNW transparent heater have potential use in various applications in the future vehicle and smart window industry.

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발표코드: MAT.P-1115

발표분야: 재료화학

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Gap Controlled Reduced Graphene Oxide for High Performance Supercapacitors

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Since appearance of graphene, supercapacitor field have paid attention to that because of its excellent conductivity, surface area, stability and easy to functionalization.^[1] In this work, we developed a facile, cost effective and efficient method for preparing gap controlled reduced graphene oxide (rGO) using three kinds of bis-diazonium salt (BDs) for supercapacitors. Fabricated rGO-BDs1, rGO-BDs2 and rGO-BDs3 was characterized by SEM, TEM, Raman spectroscopy and XPS, further shown electrochemical characteristics for supercapacitor properties. The series of rGO-BDs show different interlayer distances that each material has specific gap size due to their unique structural properties. Surprisingly the rGO-BDs2 exhibits excellent specific capacitance. Because, in here, its gap size corresponds to solvated electrolyte ion size, further this can affect to smooth absorption/desorption of electrolyte on electrode and to increase the specific capacitance.^[2] And the rGO-BDs1 and rGO-BD3 like subnanopores material also show higher capacitance than the rGO having narrow gap. Our results demonstrate that graphene material containing suitable gap size corresponding to electrolyte ion can be applied to Li ion battery, fuel cell, gas storage, and energy conversion/harvesting systems.[1] Y. Yoon et al. Adv. Mater. 2013, 25, 4437-4444[2] J. Chmiola et al. Science 2006, 313, 1760-1763

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장소: 창원CECO

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발표분야: 재료화학

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Electrochromic cell with graphene quantum dot as an electrolyte

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An electrochromic cell has been paid attention to the possible application. Here, we like to report our fabrication of the electrochromic cell with methyl viologen and Prussian blue as a electrochromic materials and GQD as a supporting electrolyte. This is the first trial to use GQD as a electrolyte. The switching property of methyl viologen was recorded from the transmittance changing at λ_{max} (550nm) for 1000 s. The coloration of methyl viologen was very reversible by applied potentials. The value of transmittance change (ΔT) is around 39 %, which is the best result what we have achieved. Moreover, in terms of stability that is one of the best fittable applications for a carbon based materials with GQD, our study is obviously valuable. And the heat stability test was done by chronoamperometry with GQD compared to the KCl cell. After heating the cell, the chronoamperometric response is more stable and reversible than that of KCl cell. Applying GQDs as an electrolyte is expected to be a novel separator between two electrodes and allows to give an easy processing for the device fabrication. We believe that these new results should open up new possibility of carbon based industry.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nonvolatile Molecular Memory of an Azobenzene Monolayer through Solution-processed Reduced Graphene Oxide Contacts

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Solution-processed fabrication of molecular devices without the use of lithographic techniques is currently a major goal in plastics-based molecular electronics. Reduced graphene oxide (rGO), a single-layer sp²-carbon atomic sheet that is electronically compatible with graphene, has attracted attention because of its excellent solution dispersion and its semimetal property of high conductivity, which allows for good electronic contacts with organic molecules. In particular, like noble metals, graphene can act as a building block for molecular assembly using bottom-up fabrication and can provide chemically compatible contacts via the formation of carbon-carbon bonds and stable contacts that avoid contact fluctuations at the interface with organic molecules. In this study, an rGO solution process for the fabrication of a flexible molecular monolayer electronic device was designed that allows for the generation of a physical soft top contact to AB molecules covalently attached to an rGO bottom contact. the solution-processed fabrication of a molecular monolayer-based nonvolatile memory flexible device on a plastic substrate was successfully accomplished. We found that an rGO soft contact top electrode can play an important role in the conformational-change-dependent conductance switching process of an ABC10 SAM. Voltage-controlled trans-cis isomerizations of ABC10 molecules in a SAM were applied to an rGO/ABC10 SAM/rGO device, which showed stable nonvolatile memory operations.

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발표코드: MAT.P-1118

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reusable Phase Transfer Catalyst, Graphene Oxide

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Graphene and its derivatives have attracted great interest for use in composite materials and catalyst. We have successfully demonstrated that GO sheets can be functioned as phase transfer catalyst (PTC) for the Michael addition. As reactants, trans- β -nitrostyrene and 2,4-pentanedione and their derivatives were used, as well as differently sized alkali metal bases. GO was compared with 18-crown-6 ether (CE), the well-known conventional PTC. The GO promoted the formation of C-C bonds in the Michael adducts, giving short reaction time and high yield compared with CE. The used GO PTC could be recovered by simple filtering and washing and could be reused many times, while CE was difficult to recover. Furthermore, the GO PTC was effective with differently sized metal cation bases, while the CE worked effectively only with a specifically sized metal cation. And also, GO has the potential to provide an environment friendly, inexpensive and easy way to produce commercial products on a large scale. Thus, the GO PTC provides a novel method for the synthesis of new C-C bonds, and can be used in an open system. This is the first observation of GO's ability to provide greatly enhanced phase transfer catalysis.

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Push-pull 구조의 유기 단분자 재료의 합성과 organic photovoltaic cells 재료로서 적합성에 관한 연구

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Push-pull 구조의 유기 단분자 재료는 전자의 밀도가 높은 electro-donor group 과 전자의 밀도가 낮은 electro-acceptor group 의 유기 구조를 이중결합(π -bridge)을 이용하여 연결한 유기 화합물이다. 이러한 유기분자는 분자 내에서 전하이동 현상이 일어나 장파장의 빛을 효과적으로 흡수 할 수 있으며 분자구조에 따라서 HOMO 와 LUMO 의 에너지 준위를 쉽게 조절 할 수 있다. 본 연구에서는 1-chloro-1-phenyl-2,2-dicyanoethylene(CPDE)을 전자 수용체 구조로, triphenylamine group 을 전자 공여체 구조로 사용하여 push-pull 구조의 유기 단분자 재료를 합성 하였다. 합성된 유기 재료는 분자내 전하이동 현상에 의해 band-gap energy 를 낮출 수 있어 organic photovoltaic cells(OPVs)의 재료로 사용 하고자 한다. 합성한 유기재료의 구조는 NMR, FT-IR 이용하여 확인 하였으며 UV-Vis, DSC, TGA, PL, CV 를 이용하여 열적특성 분석 및 OPVs 재료로서 적합성에 대하여 평가 하였다.

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발표코드: MAT.P-1120

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal behavior of surface plasmon resonance in dynamic suprastructure multilayer

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Delicate thermodynamic control at confined space has been of importance in recent nano/micro-plasmonic sensing to be more accurate and to use lower quantity of specimens than conventional devices. In our study, experimental and computational study on thermal behavior of surface plasmon resonance (SPR) was carried out using various sizes of Au nanoparticles (NPs; 4, 18, and 57 nm) and thermo-reversible polymer, poly(N-isopropylacrylamide) (PNIPAm) on SPR chip. It was interesting that SPR angle shift on temperature was dependent on NP sizes, where the smaller size the better sensitive. It is probable that both plasmonic interaction and polymer dynamicity were collaboratively affected and presumably the latter dominated in the thermal monitoring of SPR signals. The simulations clearly indicated that the interaction between the Au NPs and polymers was strengthened by increasing temperature and NP sizes, resulting in decreasing sensitivity. These results are supportive to develop further accurate devices using plasmonics and polymer dynamics, such as plasmonic sensing devices, thermo-actuators, hybrid organic solar cell, and flexible display.

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장소: 창원CECO

발표코드: **ELEC.P-1121**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Oxidation of Glucose at Nanoporous Gold Surfaces Prepared by Anodization in Carboxylic Acid Solutions

노성진 정화경 이금섭 김민주 김종원*

충북대학교 화학과

세 가지 종류의 카복실산(포름산, 아세트산, 프로피온산) 용액 하에서 양극산화 반응을 통한 나노다공성 금 (Nanoporous gold, NPG) 구조의 형성과 NPG 전극 표면 상의 전기화학적 글루코오스 산화반응을 관찰하였다. 세 가지 카복실산 용액 조건 중에서 포름산 용액 조건 하에서 양극산화를 통해 형성된 NPG 전극이 글루코오스 산화 활성이 가장 우수하였다. 포름산 용액 조건의 양극 산화 과정에서 가장 우수한 글루코오스 산화 활성을 얻기 위한 최적 조건은 인가 전위 5.0 V 와 반응시간 4 시간이었다. 카복실산 용액 하에서 형성된 NPG 상에서 전기화학적 글루코오스 산화 활성을 염소 이온의 부재 및 존재 하 조건에서 관찰하였다. 또한, 포름산 용액 하에서 최적 조건으로 형성된 NPG 전극상에서 글루코오스의 전류법 검출 결과를 통해 정량적인 글루코오스 분석에 활용할 수 있는 가능성을 제시하였다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1122**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochromic properties of Nickel oxide thin film by sol-gel method

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부경대학교 화학과

Nickel oxide(NiO) is a attractive electrochromic material which shows the color change between pale yellow(reduction) and dark brown(oxidation). NiO films are usually prepared by RF magnetron sputtering and pulsed laser deposition. These methods are not cost effective for large-scale production. Electrochromic properties of Ni oxide thin films have been investigated in basic electrolytes(KOH and NaOH) due to low coloration efficiency(CE) in LiClO₄/PC electrolyte. In this study, Nickel oxide electrochromic films were prepared by the wet-coating method on flexible PEN/ITO and glass/ITO substrate using silica-sol with nanocrystalline NiO particles. The electrochromic properties of the NiO film were characterized using the FE-SEM, UV-Vis spectroscopy and cyclic voltammetry. The electrochromic device was assembled by the combination of the prepared NiO and WO₃ electrodes with a liquid Li⁺ electrolyte and polymer gel electrolyte. The NiO/WO₃ EC device showed high performance in its contrast ratio and durability.

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장소: 창원CECO

발표코드: **ELEC.P-1123**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

리튬이차전지 성능 향상을 위한 dicarboxyl 보론 및 인 계 리튬염 의 제조와 적용

오상덕* 이재훈¹ 정현민^{1,*}

금오공과대학교 응용화학¹ 금오공과대학교 응용화학과

최근 리튬이차전지에서 전해액을 통한 전지의 수명, 고율방전 특성, 안전성, 저온방전 특성 등을 크게 향상시키고자 노력이 진행되고 있다. 본 연구는 전해액 성분개발을 통해 리튬이온배터리의 성능향상을 연구 목적으로 했으며 기존의 oxalato borate 계 리튬염 등의 성능향상 첨가제 개념의 리튬염 보다 더 나은 성능의 신규 리튬염 확보를 주요목적으로 연구하였다. 산화/환원안정성 계산데이터를 통해 기존 oxalato borate 계 대비 동등이상의 적용가능성을 보이는 dicarboxylate 보론과 인 계 리튬염을 합성 하였고, anode half cell test, LNMO cathode half cell test, high temperature cell swelling test, low temperature discharge power test 를 진행하였다. 그 결과 anode half cell test 에서 첨가제의 SEI 막 형성 특성을 관찰 할 수 있었고, high temperature cell swelling test 에서 기존 대비 5% swelling 억제 효과, low temperature discharge power 특성에 대한 10~20 % 출력향상이 나타나는 결과를 관찰할 수 있었다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1124**

발표분야: 전기화학

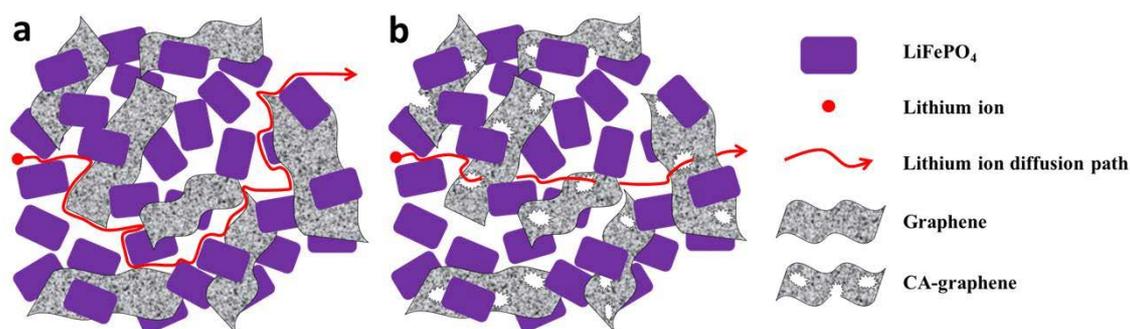
발표종류: 포스터, 발표일시: 수 16:00~19:00

다공성 활성화 그래핀으로 감싸인 LiFePO_4 복합체의 합성과 고출력 리튬이온 이차전지에의 응용

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리튬이온 2 차전지의 양극재료인 LFP (LiFePO_4)는 열적 안전성, 장기수명, 싼 가격 등의 장점을 갖지만 전기전도도가 낮다는 단점 때문에 초기 시장진입이 더디게 진행되고 있다. 전기전도도가 높은 탄소계열 물질, 특히 그래핀을 LFP 에 혼합하면 이 단점을 보완할 수 있다. 하지만 그래핀은 이차원의 평면 물질로써, 리튬이온이 그래핀을 통과하여 이동할 수 없어 이동거리가 길어지기 때문에 충전-방전 시 리튬이온의 확산속도가 느려진다. 본 논문에서는 KOH 활성화 방법을 이용하여 무수한 기공을 가진 다공성 활성화 그래핀을 합성하고, LFP 와의 복합체를 만들어 리튬이온 이차전지의 양극물질로 적용하였다. 다공성 활성화 그래핀/LFP 복합체가 뛰어난 출력특성과 수명안정성을 보이는 것을 일반 그래핀/LFP 복합체와의 비교를 통하여 확인하였다. 이것은 다공성 그래핀이 리튬이온의 확산경로를 제공함으로써 전극의 전기전도도와 이온전도도를 동시에 향상시켰기 때문이다.



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1125**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Surface Enhanced Raman Scattering Active Au Core Pt and Pd shell Substrates for In-situ Examination of Electrochemical Reactions

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충북대학교 화학과

간단한 전기화학적 석출을 통해 만든 dendritic Au rod (DAR) 구조를 중심부 기관으로 이용하여 표면 증강 라만 산란(Surface Enhanced Raman Scattering, SERS)에 큰 활성을 가지는 백금과 팔라듐 층을 만들었다. 일산화탄소를 이용한 SERS 와 전기화학적 특성 규명을 통해 모든 결과가 Pt/Pd 껍데기 층에서 측정된다는 것을 알 수 있었다. DAR@Pt/Pd (중심부@껍데기) 기관의 SERS 증강 인자는 각각 4.5×10^4 , 3.5×10^4 이며 이러한 활성은 뾰족한 모서리를 가지는 독특한 DAR 구조와 중심부 기관으로 쓰인 DAR 의 전자기적 증강의 장거리 효과 때문이다. DAR@Pt/Pd 의 균일한 형태로 인해 SERS 활성의 재현성이 좋았으며 전압 인가 시에도 안정한 전기화학적 SERS 거동을 보였다. DAR@Pt/Pd 기관을 이용해 표면에서 개미산의 전기화학적 산화반응과 SERS 를 동시에 관찰하여 DAR@Pt 와 DAR@Pd 표면에서의 개미산 산화반응에 대한 전기화학적 촉매활성을 비교하였다. 개미산의 산화를 관찰하는 동안 1000 cm^{-1} 이하의 스펙트럼 영역에서 전극 표면의 산화/환원과 개미산의 탈수반응으로부터 생성된 일산화탄소의 거동에 중점을 두고 SERS 를 관찰하였다. DAR@Pt/Pd 는 매우 높은 SERS 활성과 안정성을 가진 백금, 팔라듐 기관으로서 다른 중요한 전극 반응들의 분광학적 연구에 활용될 수 있을 것으로 기대된다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1126**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical sensor for hydroquinone based on electrochemically reduced GO-terthiophene-CNT

한형순 유정민 정해상 전승원*

전남대학교 화학과

GO-TT-CNT hybrid material was prepared in situ polymerization of graphene oxide (GO), multi-wall carbon nanotube (CNT), and terthiophene (TT). The GO-TT-CNT hybrid material was characterized by Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and field emission scanning electron microscope (FE-SEM). The electrochemical detection of HQ (hydroquinone) was verified by cyclic voltammetry (CV), differential pulse voltammetry (DPV), and amperometric response. Electrochemically reduced GO-TT- CNT (ER(GO-TT-CNT)) was obtained by electrochemical reduction of GO-TT-CNT in PBS solution of pH 5. The ER(GO-TT-CNT) was employed to detect HQ. The effects of ER(GO-TT-CNT), pH (4.04 ~ 9.01) of PBS solution were investigated for the detection of HQ. The detection limits of HQ was $3.5 \times 10^{-2} \mu\text{M}$. Catechol (CC), resorcinol (RS), H₂O₂, ascorbic acid (AA) as an interference materials give negligible effect on the HQ responses, demonstrating the high selectivity of the proposed biosensor.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1127**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic activity of oxygen reduction by cobaltporphyrin functionalized with graphene oxide in alkaline solution

유정민 정대철 전승원*

전남대학교 화학과

The Cobalt[5, 15-(p-aminophenyl)-10, 20-(pentafluorophenyl)porphyrin] (CoAPFP) functionalized with graphene oxide (GO) by N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC hydrochloride) was used amide coupling reagent. Electrochemical investigation revealed that the ERGO-CoAPFP was exhibited much better catalysis and higher improved for oxygen reduction reaction (ORR) than GO-CoAPFP. ERGO-CoAPFP is a simple and facile method to improve the electrocatalytic activity. The ERGO-CoAPFP catalysts were tested in ORR using electrochemical techniques such as cyclic voltammetry (CV) and rotating ring disk electrode (RRDE) hydrodynamic voltammetry to quantitatively obtain the ORR kinetic constants and the reaction mechanisms on a glassy carbon electrode (GCE) in 0.1 M KOH solution. The electrocatalytic oxygen reduction reaction of RRDE modified with ERGO-Co-APFP established a pathway of four electron transfer reductions to H₂O

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1128**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical determination of Orange II by electrochemically reduced graphene oxide grafted with 5-amino-1,3,4-thiadiazole-2-thiol-Pt nanoparticles

윤미라 전승원*

전남대학교 화학과

Graphene nanosheets can be produced from easily available starting materials. We synthesized GO-ATDT with graphene oxide and 5-amino-1,3,4-thiadiazole-2-thiol (ATDT). The subsequent platinum nanoparticles were decorated on GO-ATDT surface. Lastly, the glassy carbon electrode surface was coated with GO-ATDT-Pt and was reduced by electrochemical process. The ERGO-ATDT-Pt was characterized by UV-vis, IR, Raman spectroscopy, transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS). Electrocatalytic activities were verified by cyclic voltammetry (CV), chronoamperometry (CA) and differential pulse voltammetry (DPV). In pH 4.0 HAc-NaAc buffer, a reversible oxidation/reduction peak was observed for Orange II. This sensor possesses the advantages of high sensitivity, good selectivity, low detection limit and stability.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1129**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

I- Anion selective electrodes based on urea derivative as an ionophore

이경미 전승원*

전남대학교 화학과

The PVC membrane electrodes based on urea derivate as an ionophore were prepared and studied for the iodide-ion selective electrode. This membrane exhibits a linear stable response over a wide concentration range (1.0×10^{-5} ~ 1.0×10^{-2}) with a slope of -57.5mv/decade and a detection limit of $\log[I] = -5.23$. The selectivity series of the membrane gives the follow as $I^- > SCN^- > Sal^- > ClO_4^- > NO_3^- > Br^- > NO_2^- > Cl^- > F^-$. The proposed electrode showed good selectivity and response for iodide anion over a wide variety of other anions in pH 6.0 tris buffer solutions. The crystal structure of ionophore as studied using X-ray diffraction.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1130**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

PEDOT functionalized graphene oxide with MnO₂ nanoparticles for enhanced electrocatalytic oxygen reduction

최주은 전승원*

전남대학교 화학과

Poly(3,4-ethylenedioxythiophene) [PEDOT] functionalized GO with MnO₂ nanoparticles on the glassy carbon electrode MnO₂/PEDOT/rGO was prepared by electrochemical and chemical methods. The electrochemical behavior of MnO₂/PEDOT/rGO and its electrocatalytic O₂ reduction were investigated via cyclic voltammetry (CV) in 0.1 M KOH aqueous solutions. The hydrodynamic voltammetry (RDE) results confirmed that H₂O was the major product of O₂ reduction via four-electron transfer. The MnO₂/PEDOT/rGO showed the significant electrocatalytic performance on the reduction of O₂. The MnO₂/PEDOT/rGO was characterized by scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDS).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1131**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Glucose-Oxidase Label-Based Redox Cycling for an Incubation Period-Free Electrochemical Immunosensor

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Indian Oil Corporation (IOCL) R & D Centre ¹부산대학교 화학과

Catalytic reactions of enzyme labels in enzyme-linked immunosorbent assays require a long incubation period to obtain high signal amplification. We present herein a simple immunosensing scheme in which the incubation period is minimized without a large increase in the detection limit. This scheme is based on electrochemical-enzymatic (EN) redox cycling using glucose oxidase (GOx) as an enzyme label, $\text{Ru}(\text{NH}_3)_6^{3+}$ as a redox mediator, and glucose as an enzyme substrate. Fast electron mediation of $\text{Ru}(\text{NH}_3)_6^{3+}$ between the electrode and the GOx label attached to the electrode allows high signal amplification. The acquisition of chronocoulometric charges at a potential in the mass transfer-controlled region excludes the influence of the kinetics of $\text{Ru}(\text{NH}_3)_6^{2+}$ electrooxidation and also facilitates high signal-to-background ratios. The reaction between reduced GOx and $\text{Ru}(\text{NH}_3)_6^{3+}$ is rapid even in air-saturated Tris buffer, where the faster competitive reaction between reduced GOx and dissolved oxygen also occurs. The direct electrooxidation of glucose at the electrode and the direct electron transfer between glucose and $\text{Ru}(\text{NH}_3)_6^{3+}$ that undesirably increase background levels occur relatively slowly. The detection limit for the EN redox cycling-based detection of cancer antigen 125 (CA-125) in human serum is slightly higher than 0.1 U/mL for the incubation period of 0 min, and the detection limits for the incubation periods of 5 and 10 min are slightly lower than 0.1 U/mL, indicating that the detection limits are almost similar irrespective of the incubation period and that the immunosensor is highly sensitive.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1132**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dependence of the capacitance between an electrode and an electrolyte solution on the thickness of aluminum oxide layers deposited using atomic layer deposition

정진교 장병용¹ 양해식*

부산대학교 화학과¹ 부경대학교 화학과

Self-assembled monolayers cannot be used to readily prepare insulating layers that are a few nm thick and are pinhole-free onto electrodes. Here, atomic layer deposition (ALD) is used to prepare aluminum oxide (Al_2O_3) insulating layers, whose thickness is controllable and which are pinhole-free toward electroactive species such as $\text{Ru}(\text{NH}_3)_6^{3+}$ and ferrocenemethanol, on indium tin oxide electrodes. The controllability of the uniform thickness of the Al_2O_3 layers enables us to investigate the dependence of the total capacitance between an electrode and an electrolyte solution on the thickness of the ALD layer over a wide range of thicknesses. When the thickness is greater than ca. 2 nm, the total capacitance is dominated by only the ALD layer capacitance. Consequently, the reciprocal of the total capacitance is linearly proportional to the ALD layer thickness. From this finding, a schematic diagram for the potential profile across the ALD layer and in the electrolyte solution is proposed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1133**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

ZnO Nanorod Electrodes Modified with Redox-Active Gold Nanoparticles for the Electrochemical Detection of Alkaline Phosphatase

고은솔 Prabhu 이동일*

연세대학교 화학과

Thiolate-protected gold nanoparticles containing less than a few hundred atoms have attracted much research interest recently because of their unusual physical and chemical properties. In particular, Au₂₅ nanoparticles have been extensively studied due to their exceptional stability with unique electrochemical and optical properties. In this poster, we demonstrate that thiolate-protected Au₂₅ nanoparticles can be utilized as a redox mediator for the amperometric sensing of 4-aminophenol. Glutathione stabilized Au₂₅ nanoparticles were uniformly anchored on hydrothermally grown highly oriented ZnO nanorods/ ITO electrode surface. Au₂₅ nanoparticles immobilized on ZnO exhibit well-resolved redox peaks and the peak currents were found to be controlled by Au₂₅ loading. The oxidation current of Au₂₅ was found to linearly increase with the addition of 4-aminophenol, indicating its electrocatalytic activity towards 4-aminophenol. On this basis, the composite electrode was used to detect alkaline phosphatase (ALP), a well-known label enzyme that dephosphorylates 4-aminophenylphosphate to produce 4-aminophenol which was subsequently oxidized by Au₂₅/ZnO/ITO electrode. The stable and reproducible immobilization of Au₂₅ nanoparticles on ZnO nanorods resulted in a highly sensitive detection of ALP which finds potential applications for the construction of biosensors and immunosensors.

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발표코드: **ELEC.P-1134**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Atomic Layer Deposition (E-ALD) of CdS on CIS/Au(111)

정찬용 이치우^{1,*}

고려대학교 소재화학과 ¹고려대학교 신소재화학과

CIS 박막은 광 흡수계수가 크고 밴드갭이 크기 않기 때문에 태양광 전지에 사용하기 좋은 흡수 재료 중 하나이다. CdS 와의 접합을 통하여 태양전지를 구성할 수 있는데 현재의 태양전지는 가격이 비싸서 에너지 문제 해결에 어려움이 있다. 이에 전기화학 방법으로 금 전극 표면에 CIS 를 입히고 그 위에 다시 CdS 를 전착하여 얇은 박막을 만드는 연구를 진행 중에 있다. 본 실험은 단결정 금 전극 표면에 구리, 인듐, 셀레늄(CIS)을 입히고 그 위에 CdS 를 전착한 얇은 필름의 제작을 위하여 Electrochemical Atomic Layer Deposition(E-ALD) 방법을 사용하였다. 이 실험으로 전기화학적 전착에 의한 n-형 반도체 CdS 와 p-형 반도체 CIS 에 따라 p-n 접합을 제작하는 것이 가능하다는 것을 보여준다. CdS on CIS/Au(111) 박막의 전착된 화합물의 형상은 금속 현미경과 Scanning Electron Microscope (SEM)을 통하여 확인 하였고, 구조와 성분 분석은 X-ray Diffraction (XRD)과 Energy Dispersive X-ray Spectroscopy (EDS)를 사용하였다. 또한 전착 되는 과정의 전압 및 전류의 변화는 Sequence 프로그램을 통하여 시간에 따라 측정하였다.

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발표코드: **ELEC.P-1135**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Improvement of Electrochemical Properties of IrO₂ Nanowires on Au Microwire by Reduction

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Developing nano-scaled material has often enhanced electrochemical performance for detection of biomolecules. Recently, we have successfully synthesized IrO₂ nanowires (NWs) on a Au microwire by vapor transport method. At the present time, we have reduced IrO₂ to Ir on the surface of IrO₂ NWs under hydrogen atmosphere. Morphology has been changed dramatically upon reduction of IrO₂ NWs, which was characterized with scanning electron microscopy (SEM). After reduction, the electrochemical performance of IrO₂ NWs exhibited significant enhancement showing higher capacitance and catalytic activity for oxygen reduction and H₂O₂ redox reactions than before. Especially for glucose detection, surface reduction of IrO₂ enabled glucose sensing through direct glucose oxidation reaction without aid of enzyme, which was impossible for non-reduced IrO₂ NWs. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (NRF-2011-0015619).

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발표코드: **ELEC.P-1136**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Measurement of Nitric Oxide Using Single Crystalline RuO₂ Nanorods Grown on a Carbon Fiber Microelectrode for Nitric Oxide Sensing

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Single crystalline ruthenium oxide nanorods were successfully grown on a single carbon fiber (CF, diameter = 5~10 μm) by simple thermal annealing (RuO₂ nanorods-CF). The morphology and structure of RuO₂ nanorods-CF were characterized by FE-SEM, XRD and Raman spectroscopy. Nitric oxide is well known for its crucial physiological functions as a vasodilator, neurotransmitter, mediator of anti-tumor activities, etc. Therefore, the as-prepared RuO₂ nanorods-CF is tested for its feasibility as an amperometric NO microsensor. The sensor is composed of a RuO₂ nanorods-CF (or bare CF) working electrode and a Ag/AgCl counter/reference electrode. Electrochemical activities of these materials for electrochemical oxidation of nitric oxide are characterized by linear sweep voltammetry (LSV), constant potential amperometric experiments (i-t). In addition, the sensor is applied for real-time in-vivo NO measurements at the cortical surface of a living rat brain. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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발표코드: **ELEC.P-1137**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Application of Electrochemical Dual Microsensor for Simultaneous Measurements of CO and NO Distribution in Mouse Kidney

나지선 하예진 이영미*

이화여자대학교 화학나노과학과

Endogenously produced carbon monoxide (CO) and nitric oxide (NO) gases have similar biological functions such as vasodilation and neurotransmission. For years, studies have suggested that two gases do not work independently, but rather coregulate each other. Nevertheless, researchers still can't reveal their interactions clearly due to the lack of proper analysis techniques. In this presentation, we present the development of an electrochemical dual CO/NO sensor and its biological application. The sensor is made up of a dual platinum working electrode (WE) and a Ag/AgCl counter/reference electrode. The dual WE possessing two platinum disks (WE1 and WE2, 76 and 25 μm in diameter, respectively) which are etched to form a micropore-shaped electrode and then electrodeposited with porous platinum layer. The larger WE1 is additionally modified with electrochemical deposition of tin. Modifications of two sensing disks different in their sizes as well as in their disk surface treatments give apparently different selectivity of CO at WE1 and NO at WE2. For the sensor application, we employ the CO/NO dual microsensor on mouse kidney in order to examine the location-dependent CO and NO distribution levels. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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발표코드: **ELEC.P-1138**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Application of a Dual Microsensor for Simultaneous Nitric Oxide and Potassium Ion

김미선 이영미*

이화여자대학교 화학나노과학과

Nitric oxide is known to be closely to potassium ion (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. A technique, which could analyze NO and K^+ simultaneously, would be able to provide more information to understand biological processes mediated by NO/cGMP/ K^+ pathway more clearly. We demonstrate the development of a dual microsensor for simultaneous measurements of NO and K^+ ion. A sensor possesses two microdisks: one disk is used for amperometric NO measurement and the other is used for potentiometric K^+ measurement. Sensor performances, such as sensitivity and, selectivity, are characterized and the results show the possibility for the biological applications. As-prepared sensor is applied for the NO/ K^+ measurements at biological organ tissues, rat kidney. The levels of NO and K^+ are clearly location dependent over the kidney surface and it is considerably matched with results studied by various method previously. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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장소: 창원CECO

발표코드: **ELEC.P-1139**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic Characteristics of $\text{Ru}_{1-x}\text{V}_x\text{O}_2$ nanowires on Au microwire

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Single crystalline Ru/V mixed metal oxide nanowires ($\text{Ru}_{1-x}\text{V}_x\text{O}_2$ NWs) on commercial gold microwire ($d = 25 \mu\text{m}$) were successfully synthesized by a simple vapor phase transport process. The morphology and crystalline structure of $\text{Ru}_{1-x}\text{V}_x\text{O}_2$ NWs on Au microwire ($\text{Ru}_{1-x}\text{V}_x\text{O}_2$) were characterized by scanning electron microscopy (SEM), high resolution transmission electron microscopy (HR-TEM), X-ray diffraction pattern (XRD), Raman spectroscopy and AFM. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) experiments were performed to show favorable electron-transfer kinetics of $[\text{Fe}(\text{CN})_6]^{3-/4-}$ and $\text{Ru}(\text{NH}_3)_6^{3+/2+}$ compared to bare Au microwire. The $\text{Ru}_{1-x}\text{V}_x\text{O}_2$ -Au microelectrode revealed catalytic activity for amperometric H_2O_2 reduction and oxygen reduction at physiological pH (7.40), where the activity increased as the amount of vanadium increased. Moreover, it showed high H_2O_2 selectivity against ascorbic acid (AA), acetamidophenol (AP), uric acid (UA) and dopamine (DA). $\text{Ru}_{1-x}\text{V}_x\text{O}_2$ NWs exhibited potential applications in biofuel cells and bio sensors.

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발표코드: **ELEC.P-1140**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Amperometric Ascorbic Acid Sensor Based on Zwitterionic Carbon Nanotubes Modified with and without Gold Nanoparticles

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Recently, we reported synthesis of zwitterionic carbon nanotube (f-CNT) and Au nanoparticle (AuNP) modified f-CNT, AuNP-f-CNT, and their application to oxygen reduction. The f-CNT denotes zwitterionic poly(vinylimidazoliumpropylsulfonate)-functionalized multi-walled CNT. In this presentation, we extend the applicability of AuNP-f-CNT to nonenzymatic sensing for ascorbic acid (AA) at physiological pH. For selective detection of AA, working potential (E_{app}) was determined by analyzing linear sweep voltammograms obtained in the solutions containing AA and possible interferents, i.e., glucose, uric acid, dopamine, acetamidophenol, and NADH. Amperometric i-t curves on the AuNP-f-CNT modified electrode at E_{app} (0.05 V) represented highly sensitive and selective detection of AA. The AuNP-f-CNT modified electrode showed sensitivity of $550 \mu\text{A mM}^{-1}\text{cm}^{-2}$ for the linear dynamic range of zero to 12 mM AA with the response time of 0.8 s and detection limit of 0.8 μM .

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장소: 창원CECO

발표코드: **ELEC.P-1141**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characteristic and continuous manufacturing of Gas diffusion layer`s(GDL) using Carbon fibers

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한국에너지기술연구원 에너지융합소재연구단 ¹한국에너지기술연구원 에너지소재연구센터

고분자전해질연료전지(PEMFC)의 전극소재인 가스확산층(GDL)은 수소 및 공기를 촉매층으로 균일하게 공급하고, 반응생성물인 물의 배출, 전자전도, 촉매지지층으로서의 역할 등 여러 가지 중요한 기능을 갖는다. 따라서 GDL의 특성향상 및 설계 최적화를 위한 연구가 활발히 수행되어져 왔으며, 연료전지의 보급 확대에 따라 이의 생산기술도 시장점유를 위한 중요한 소재기술로 부각되고 있는 상황이다. 본 연구에서는 탄소섬유를 기반으로 한 탄소섬유웹의 제조, 물리적특성 및 전기전도를 향상시키기 위한 수지 및 전도성분말의 함침, 탄화 과정을 거쳐 제조되는 가스확산기재(GDM) 연속생산연구를 진행하였다. 탄소섬유의 이방성 배열이 우수하고, 두께가 균일한 탄소섬유웹을 제조하기 위하여 습식초지방법을 사용하여 폭 50cm 인 탄소섬유웹을 연속생산하였으며, 유기섬유의 종류 및 첨가량 변화에 따른 특성을 분석 비교하였다. 또한 탄소섬유 웹에 전도성분말을 수용성수지와 혼합하여 연속 함침하기 위한 최적조건을 선정하기 위하여 함침 및 탄화 후 연료전지 전극소재로서 요구되는 특성들을 비교 분석하였다.

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발표코드: **ELEC.P-1142**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pt를 다중 흡착 시킨 Au 전극의 표면 분석 및 유기분자 산화 특성 연구

김세철 이충균^{1,*} 신동완¹

충남대학교 분석과학기술대학원 ¹충남대학교 화학과

금 전극 표면의 변형을 통한 유기 분자의 산화 특성 연구의 일환으로, 백금 층의 두께와 형태에 따른 여러가지 특성을 분석, 연구하였다. 전극 표면의 변형 방법으로 비가역적 흡착방법을 중첩하여 사용함으로써 백금층의 높이와 덮힘 면적이 다른 두 종류의 전극을 비교 분석하였다. 본 연구 결과에서 백금의 흡착 층의 두께에 따라서 CO의 산화 전압의 위치가 변화하였고, 에탄올 산화가 크게 증가하는 것을 관찰하였다.

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장소: 창원CECO

발표코드: **ELEC.P-1143**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Plasmon Enhanced Photoelectrochemical Properties of Surface-Textured Mesoporous Titania Inverse Opal Structure

김광현 THIYAGARAJAN PRADHEEP 안효진¹ 김선이 장지현*

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We report an inverse opal structure, a type of photonic crystals, helps to improve a photoconversion efficiency of photoanode via photon trapping effect caused by the large dimension of nanostructures. Surface-texturing of inverse opal structure ensures much larger surface area of large scale nanostructures while providing photon trapping effect. Additionally, gold nanoparticles deposited on the surface have a great influence on a plasmon-enhanced photon trapping effect. Photon trapping by structural factor and surface Plasmon enhancement by gold nanoparticles of the surface-textured mesoporous titania inverse opal structures create synergetic effects to enhance the photoelectrochemical properties of the devices under the visible light illumination, which occupies the great portion of the solar spectrum.

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장소: 창원CECO

발표코드: **ELEC.P-1144**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A portable phenol selective sensor composed of tyrosinase, gold nanoparticles and screen printed carbon chips

Karim Md. Nurul 이혜진*

경북대학교 화학과

In this poster, a portable amperometric phenol biosensor fabricated on screen printed carbon electrodes where gold nanoparticles (AuNPs) were electrochemically deposited followed by the covalent attachment of tyrosinase on AuNP's. The sensing methodology is based on measuring the current changes due to the electrocatalytic reactions of phenol in the presence of tyrosinase on AuNP deposited biosensor. The phenol sensing signal was characterized using both cyclic voltammetry and square wave voltammetry (SWV). A detection limit of 47 ppb alongside a linear range of 47 ppb to 15 ppm for phenol was achieved in conjunction with SWV. The developed sensor was finally employed to the measurement of phenol concentration in environmental water samples.

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장소: 창원CECO

발표코드: **ELEC.P-1145**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Voltammetric Studies of Copper Ion Transfer Reactions Facilitated by Picolinamide-PV at Liquid/liquid Interfaces

이상혁 이혜진*

경북대학교 화학과

In this poster, the voltammetric characterization of transfer reactions of Cu(II) and Cu(I) cations by picolinamide-PV across a polarized water/1,2 dichloroethane (DCE) interface was presented. The direct transfer process of two different copper ionic species across the interface was first studied using cyclic voltammetry. Both ions limits the potential window such that each ion transfer reaction was not clearly distinguished within the potential window set by ionic electrolyte components present in both water and DCE phases. A potential ligand, picolinamide-PV which can selectively complex with copper ions was then incorporated into the DCE phase which can facilitate the transfer of copper ions by selective complexation across the interface. The transfer characteristics of Cu (II) and Cu(I) ions assisted by picolinamide-PV was thoroughly investigated using cyclic voltammetry and their possible sensing application is demonstrated.

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발표코드: **ELEC.P-1146**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Gold Nano-Particles on Nickel Oxide for Electrochemical Supercapacitor Applications

김선이 THIYAGARAJAN PRADHEEP 장지현*

울산과학기술대학교(UNIST) 친환경 에너지 공학부

Electrochemical supercapacitor using porous metal oxide has received great attention as an alternative energy device because of high specific capacitance, low cost, and easy control on the surface morphology. However metal oxide suffered from poor conductivity and low cycle stability. In this study, we present an easy and cost-effective method to improve the conductivity of metal oxide via simple deposition of gold nanoparticle on 3D nickel oxide (NiO). 3D-structured NiO with flower shape has been synthesized via sol-gel methods and the prepared sample was characterized using SEM, XRD, BET, and cyclic voltammetry. By coupling of gold nanoparticles with 3D-nickel oxide pseudocapacitor materials, the specific capacitance was remarkably improved due to the improved conductivity. Furthermore, the capacitance retention and kinetic property are enhanced.

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장소: 창원CECO

발표코드: **ELEC.P-1147**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electro-catalytic applications of marine sponge

이은정 심윤보* 김동민

부산대학교 화학과

A glucose sensor was constructed on a screen printed carbon electrode(SPCE) employing marine sponge as an electron transfer mediator, and the nicotinamide adenine dinucleotide dependent glucose dehydrogenase(NAD-GDH) as a catalytic subunit. Scanning electron microscopy(SEM-EDX) confirmed the presence of the fiber and the content of Iron in the sponge. To construct the sensor, the conducting polymer, 2,2':5',2''-terthiophene-3'(p-benzoic acid)(TTBA) was electropolymerized onto a gold nanoparticles(AuNPs)/screen printed carbon electrode(SPCE). The electrode was modified with fiber through the amide bond formation between the conducting polymer and the fiber. The sensor was characterized using cyclic voltammetry(CV) and electrochemical impedance spectroscopy(EIS). The optimization of the sensing parameters was investigated according to the PH, temperature, concentration, and sonication time.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1148**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Covalent Functionalization Based Heteroatom Doped Graphene Nanosheet as a Metal-Free Electrocatalyst for Oxygen Reduction Reaction

박민주

울산과학기술대학교(UNIST) 화학공학과

Oxygen reduction reaction (ORR) is an important reaction in energy conversion systems such as fuel cells and metal-air batteries. Carbon nanomaterials doped with heteroatoms are highly attractive materials for use as electrocatalysts by virtue of their excellent electrocatalytic activity, high conductivity, and large surface area. This study reports the synthesis of highly efficient electrocatalysts based on heteroatom-doped graphene nanosheets prepared through covalent functionalization using various small organic molecules and a subsequent thermal treatment. A series of nitrogen-doped reduced graphene oxide (NRGO_n) nanosheets exhibited varying degrees and configurations of nitrogen atoms within the graphitic framework depending on the type of precursors used. On the basis of the rotating disk electrode (RDE) and rotating ring-disk electrode (RRDE) experiments, NRGO₃, with a high degree of pyridinic-N content, displayed the desired one-step, quasi-four-electron transfer pathway during ORR, similar to commercial Pt/C. We also demonstrated the potential of covalent functionalization of sulfur and boron-doped graphene nanosheets.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1149**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical and spectrochemical properties of newly synthesized terthiophene phenyl acrylic acid

Eswarreddy 심윤보* 김동민

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A novel terthiophene phenyl acrylic acid (TTPAA) was synthesized and characterized by FT- IR, ¹H & ¹³C NMR, mass spectroscopy, and elemental analysis. The synthetic route involves three steps including Grignard reaction, Suzuki coupling, and followed by Knoevenagel condensation reaction to get the title compound (TTPAA). Spectroelectrochemical properties compared with poly(2,21:5,211-terthiophene-31-p-benzoic acid) (pTTBA). The monomer was electrochemically polymerized on platinum electrode, then poly-TTPAA film was characterized by voltammetry using different scan rates, impedance spectrometry, and in situ UV- Visible spectroscopy. Thickness and surface morphology of polymerized electrode was characterized by using AFM image.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1150**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical detection of cancer cells using interaction between antimetabolite compounds and the cell surface receptors

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A sensor probe for the electrochemical detection of cancer cells was constructed using antimetabolites. In order to sensitively detect and differentiate between the cancer and non-cancerous cells the overexpression of the receptors on the surface of cancer cells is exploited in the present study. The antimetabolite compound was immobilized on the gold nanoparticles composited with a, {5-([2,2':5',2''-terthiophen]-3'-yl)pyrimidin-2-amine} (polyAPTT), amine functionalized conducting polymer. The formation of each layer is confirmed by XPS, Cyclic voltammetric and Impedometric experiments. The sensor probe is successfully used for the detection of cancer cells using electrochemical techniques.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1151**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bimetallic Au-M (M = Ni, Co, Mn, Fe) alloy dendrites as excellent catalysts for oxygen reduction and glucose oxidation

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We report a facile single step electrochemical method to synthesize Au-M (M = Ni, Co, Fe) alloy dendrites. Prepared alloy dendrites have a large surface area, good electrical conductivity and chemical inertness, they are characterized by SEM, EDX, and Cyclic voltammetry techniques. The atomic ratio of AuNi alloy was tuned by using different deposition potential and examined for oxidation of glucose and oxygen reduction reaction (ORR) in alkaline media and applied for fuel cell application. AuNi alloy dendrite was found to be efficient catalyst that are comparable that of commercial Pt.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1152**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

몰리브덴 브론즈의 생성에 관한 전기화학적 연구

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전기변색(electrochromism)이란 용어는 1961년 Platt에 의해 처음으로 사용되었으며, 전극 물질에 전기화학적으로 산화 또는 환원 반응을 일으킬 때 가역적으로 색 변화가 일어나는 현상을 말한다. 유기 또는 무기 전기변색 물질로 이루어진 소자는 기존의 음극선관, 액정 디스플레이, 발광 다이오드에 비교하여 응답속도가 느리지만 적은 비용으로 넓은 면적의 소자로 제작될 수 있고, 소비전력이 낮기 때문에 스마트 창, 스마트 거울, 전자 종이 등에 응용될 수 있다. 그 중에서도 Molybdenum 과 Molybdenum oxide 는 다양한 색깔 구현이 가능하여 전기 변색 물질로 널리 사용되는 것 중 하나이다. 산화 몰리브덴의 전기변색 성질은 양이온과 전자의 동시 공급을 통하여 Molybdenum bronze 로 합성된 형태인 $AxMoyOz$ 로 정의된다. 본 실험은 K_2SO_4 용액에서 3 step 으로 1)LSV 2)CA 3)LSV 로 실험을 진행하였으며 3)단계에서 end potential 을 변화시킴으로 각기 다른 컬러가 만들어졌다. 만들어진 샘플은 EQCM, XRD, EDS 그리고 SIMS 통해 분석을 하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1153**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of potassium permanganate pretreatment of pitch fiber on the electrochemical performance of pitch-based activated carbon fibers

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Pitch-based activated carbon fibers (ACFs) were obtained in this work from a combination of pretreatment with different amounts of potassium permanganate (KMnO₄) and chemical activation with potassium hydroxide. The influence of the KMnO₄ treatment on the textural properties of the pitch-based ACFs was investigated by means of N₂/77 K adsorption isotherms. The investigation also involved the use of the Brunauer-Emmett-Teller equation and the Dubinin-Radushkevich method. The electrochemical performance of the ACFs was confirmed by cyclic voltammograms (CV). Moreover, the specific surface area of the pitch-based ACFs increases in proportion to the amount of KMnO₄ pretreatment and reaches its highest value of 2114 m²/g with 0.5 g of KMnO₄ because the surface oxygen groups of the pitch fibers act as an active site during chemical activation.

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장소: 창원CECO

발표코드: **ELEC.P-1154**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Fluorination on Electrochemical Performance of coal tar Pitch-based Activated Carbons for EDLC

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In this work, we investigated the electrochemical performance of porous coal tar pitch-based activated carbons (C-ACs) by Fluorination. The influence of fluorine treatment time on electrochemical performance of the C-ACs was investigated. The textural properties and morphologies of the C-ACs were analyzed by reference to $N_2/77\text{ K}$ adsorption isotherms and field emission scanning electron microscope (FE-SEM), respectively. The electrochemical performance of the C-ACs was confirmed by cyclic voltammograms (CV). This was suggested that the fluorine functional groups on the C-ACs led to the combination effect of both electric double-layer capacitor and pseudocapacitance in the present system

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1155**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Core/Satellite Nanoassembled Catalyst for the Oxygen Reduction Reaction

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Noble-metal nanostructures are widely used in a variety of applications ranging from electrocatalysis to electronics, electrochemical synthesis, and electrochemical analysis owing to their inertness and catalytic properties. Among the noble metals, Au is regarded as a poor catalyst for a sluggish oxygen reduction reaction (ORR) due to the weak chemisorptions properties caused by the filled d-band. To improve the activity of Au, we have successfully synthesized a series of well-defined core-satellite nanostructures with different porosities, i.e., the core-to-satellite gap distances controlled on a molecular scale. The dependence of the ORR on the gap distance between the core and the satellites was systematically investigated by varying the length of the alkanedithiol linkers. The structures and electrocatalytic activities of the Au core-satellite catalysts are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), cyclic voltammetry (CV), and rotating disk electrode (RDE) voltammetry.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ELEC.P-1156

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Observation of connection between formic acid oxidation current , catalyst poison and rotating disk electrode (RDE) rotation rate

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Rotating disk electrode(RDE)는 전극을 회전시켜서 전극표면과 용액 사이의 diffusion layer 를 감소시키고 mass transfer 를 원활하게 함으로서 전극에서의 반응이 잘 이루어지도록 하는 역할을 한다. 그러나 Formic acid 에서는 RDE 의 회전 속도가 증가할수록 산화 전류량과 촉매독 양이 모두 감소하는 것을 관찰하였다. 이에 우리는 RDE 의 회전 속도가 증가할수록 Formic acid 분자가 백금 전극의 반응점에 흡착하여 산화되기 전에 빠르게 지나가게 되어 흡착량이 감소되고 결과적으로 산화 전류의 감소와, 촉매독이 감소한다는 가설을 가지고 실험을 계획하였으며, 전극 표면의 roughness 도 이에 영향을 주는 것을 발견하고 이를 포함한 실험도 추가하였다. 본 연구에서는 개미산이 산화하는 여러 전압에서 RDE 의 회전속도를 다르게 하였고, 대시간전류법을 이용하여 일정한 시간이 지난 후 개미산 산화와 촉매독이 생성되는 것을 방지하기 위해서 Iodine 을 이용하여 의 개미산 산화 전류와 촉매독을 측정하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1157**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel conductive polymer-graphene oxide composite for oxygen electroreduction as a nonmetallic catalyst

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Graphene oxide (GO) and PolyAPT were deposited onto a glassy carbon electrode (GCE) through electrochemical polymerization of APT. Both cyclic voltammetry (CV) and the rotating disk electrode (RDE) techniques were employed to investigate the kinetics and mechanism of the oxygen reduction reaction (ORR) by the GO-PAPT modified electrode. In comparison to a GO/GCE or a PAPT/GCE, the GO-PAPT-modified electrode shows a significant electrocatalytic enhancement of the ORR as reflected in a current increase (50 μ A). Koutecky-Levich plots suggest a four-electron process for oxygen reduction in 0.1 M NaOH solution. The electrocatalytic stability of the GO-PAPT layer and its excellent tolerance toward the poisoning by methanol and ethanol is demonstrated, highlighting this electrode as a promising metal-free electrode material for oxygen reduction in alkaline fuel cells.

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장소: 창원CECO

발표코드: **ELEC.P-1158**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characteristics of PAA-PVP-Fe-EA polymer and its application to bioelectrocatalytic system

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단국대학교 화학과

A series of novel, electro-active poly(acrylicacid-4-vinylpyridine) (PAA-PVP) polymer of pentacyanoamminferrate $[\text{Fe}(\text{CN})_5\text{NH}_3]$ were prepared and then characterized using UV-vis spectroscopy and electrochemical techniques. Also, quaternized iron hydrogel polymer with ethylamine was prepared as a potential redox mediator in an bioelectrocatalytic system. The redox polymer presented here are described in shorthand as $[\text{Fe}(\text{CN})_5(\text{poly}(\text{acrylicacid-4-vinylpyridine})\text{-ethylamine})]$ (PAA-PVP-Fe-EA) which were immobilized on the ITO Electrodes without or with gold nanoparticles (AuNP). The electrical signals were measured by voltammetry technique. The AuNPs immobilized onto ITO Electrodes provided about a three times higher electrochemical response compared to that of a normal ITO electrode. Also, catalytical current was amplified by GOx which is electrically mediated by new iron redox film, converting the film into an electro catalysts for the electron reduction of oxidation of glucose. The resulting catalytical current was linearly related with the concentration of glucose.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1159**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of new polymer compounds for the development of a biofuel cell

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단국대학교 나노바이오의과학과 ¹단국대학교 화학과

Miniaturized biofuel cells in the future can be used as alternative energy supply sources for nano-microelectronic devices and biosensors. Also, biofuel cells have a tremendous opportunity to provide much higher energy densities and smaller footprints than batteries for powering implantable medical devices, leading to less intrusive implantable devices with longer lifetimes. The main advantage of biofuel cells is that they are able to convert chemical energy of biological environment into electrical current. This paper introduces a new cathode redox polymer based on mediated oxygen reduction to water by bilirubin oxidase (BOD). The immobilized electrocatalyst enabling the reduction is the electrostatic adduct of bilirubin oxidase from *Myrothecium verrucaria*, and the redox polymer of poly (acrylic acid-4-vinylpyridine-acrylamide) (PAA-PVP-PAA) complexed with $[\text{Os}(\text{dichloro-bipyridine})_2]^{2+/3+}$, cross-linked on the screen printed carbon electrodes (SPCEs). We have investigated the enzymatic electrode formulations that have the high potential to achieve higher current densities and longer stability on the electrodes.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1160**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Electrochemical Properties of Lithium Pre-doped Carbons for Li-ion Capacitors

이지한 조은아 박수진*

인하대학교 화학과

In this work, the electrochemical properties of lithium pre-doped carbons were studied in lithium-ion capacitors (LICs). The Li pre-doping carbons were prepared with various Li contained solutions using natural graphites and graphite oxides for negative electrode. The characteristics of Li pre-doping carbons were confirmed by XRD, XPS, and AAS. The electrochemical properties were determined by galvanostatic charge-discharge cycling and impedance spectroscopy measurements. From the results, it was found that the highest cycling performance of the Li pre-doped graphite oxides was attributed to the pre-doped lithium component. Consequently, the oxygen functional groups and a wide interlayer spacing of GO lead to increasing the contents of Li pre-doping.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1161**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic oxidation reactions of dopamine and uric acid under various pH ranges at carbon nanotube electrodes

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전북대학교 화학과

Dopamine(DA) and uric acid(UA), which play important roles in biological system, are electrochemically active. Oxidatively treated carbon nanotubes were coated on the glassy carbon surfaces and the prepared electrodes were employed for electrochemical reaction of DA and UA. Under various pH ranges (pH 3 ~ pH 11), cyclic voltammetry was used for measuring electrocatalytic oxidation reaction of DA and UA. The oxidation peak potential of DA and UA shifted positively with the decrease of pH. DA and UA showed the maximum oxidative current at pH 5. Higher currents at carbon nanotube electrodes were measured than at the bare glassy carbon electrode. It was shown that the carbon nanotube electrode improved the electrocatalytic activity for the oxidation reaction of DA and UA.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1162**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Porous Gold-on-palladium Nanoparticles with High Catalytic Activities

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The high cost of catalysts caused by the exclusive use of platinum and platinum-based catalysts in the fuel cell electrodes is one of the major barriers to limit the commercial application. Recently, Pd-based nanoparticles (NP) catalysts, as a promising alternative to Pt, have attracted increasing attention especially in the development of efficient fuel cell electrocatalyst. In this presentation, we describe the facile preparation of well-dispersed porous Pd and Au-on-Pd NPs of controllable sizes. The surface of porous Pd NPs was covered with a layer of Au via a galvanic replacement reaction in an aqueous medium. Porous Au-on-Pd NPs possess a much higher surface-to-volume ratio than AuPd nanospheres. The catalytic activity toward the ORR of the prepared catalysts in an alkaline solution was investigated as a function of the Au/Pd composition ratios. The structures and electrocatalytic activities of the porous Au-on-Pd catalysts are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), cyclic voltammetry (CV), and rotating disk electrode (RDE) voltammetry.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1163**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Electrocatalytic Activity of Highly Porous Hollow AuPd Mesospheres for Oxygen Reduction in Alkaline Solution

손정우 심준호*

대구대학교 화학·응용화학과

A variety of approaches to preparing bimetallic (or trimetallic) nanostructures comprised of noble metals such as Au, Pt, Ag, and Pd have been evaluated for their impact on the oxygen reduction reaction (ORR), including electrochemical reduction, simultaneous chemical reduction of mixed metal ions, and successive reduction of metal ions on the surface of sacrificial nanoparticles, known as galvanic replacement reaction (GRR). Among them, GRR, as an effective and simple tool, has been widely employed to synthesize bimetallic nanostructures with porous, hollow, and core/shell particles. In this presentation, highly porous hollow AuPd nanostructures have been synthesized via a GRR of hollow cobalt mesospheres in metal ion precursor solutions (HAuCl₄ and K₂PdCl₄, respectively). A series of characterizing techniques, including scanning and transmission electron microscopy (SEM and TEM, respectively), energy-dispersive X-ray (EDS) spectrometry, and X-ray diffraction (XRD), were applied to systematically explore the changes in the morphology, composition, and crystal structure. The electrocatalytic activities of these nanomaterials for the ORR are investigated by rotating disk electrode (RDE) and cyclic voltammetry (CV).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1164**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot Synthesis and Electrocatalytic Activity of Porous Gold Nanoparticles

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Recently, the direction of research in the quest for better materials has shifted to the preparation of porous metals in the nanoscale range owing to their remarkable catalytic properties, which are superior to those of non-porous metals. Among the many different nanomaterials, porous Au nanoparticles (pAuNPs) are very attractive for various applications, mainly because of their unique optical, catalytic, and electrocatalytic properties. In this presentation, we describe a simple one-pot approach for the synthesis of pAuNPs without any extra surfactant, seed, control, and so on and their nonenzymatic electrocatalytic activity toward the electrochemical oxidation of glucose and NADH. The shape and structure of the pAuNPs catalysts were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and UV-vis absorption spectroscopy to examine the morphology and to analyze the optical properties of the synthesized products. To investigate the glucose and NADH detection, the pAuNPs were loaded on a glassy carbon (GC) electrode with Nafion as the capping agent for the nano-catalysts. The prepared GC/pAuNPs/Nafion electrode exhibited an improved performance at low overpotential in glucose and NADH detection.

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발표코드: **ELEC.P-1165**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Capacitive Behaviour of Reduced Graphene Oxide in a Ionic Liquid Containing Double- Cationic Charge

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동국대학교 화학과

A ionic liquid with di-cationic group was synthesized and used to evaluate the supercapacitive behaviour of a reduced graphene oxide(rGO) in comparison with LiClO₄. The morphological properties of GO and rGO were characterised by XRD, TEM, Raman spectroscopy, and rGO was found to have a typical structural nature after reduction. The electrochemical performance of the GO and rGO was studied by cyclic voltammetry, impedance spectroscopy and galvanostatic charge/discharge in different aqueous electrolytes, 0.1 M C₆(TMA)₂(BF₄)₂ and 0.1 M LiClO₄. Superior capacitive properties were observed from rGO in both electrolytes.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The study of electrochemical performance about all-solid lithium ion batteries made by polyaniline films with nano-cube structure as cathode and solid polymer electrolyte

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There is currently a great interest in the development of thin, flexible, lightweight, and environmentally friendly batteries. It is applied to many applications and designs previously impossible, such as high-performance sportswear, wearable displays, new classes of portable power, and embedded health monitoring devices. To get these electronics, it should avoid using the liquid electrolyte and the electrode has to get advantages such as mechanical flexibility. Therefore, the cell has to be made form of all-solid for flexible batteries. As cathode materials, conducting polymers have many advantages such as their inherent fast redox switching, high conductivity, mechanical flexibility, low weight and possibility to be integrated into existing production processes. We achieved the polyaniline-paste including minimum solvent, which has high density about 50 mg/mL. It shows similar physical properties with paints or pigments. The synthesis of polyaniline was confirmed by FT-IR. The surface morphologies of doped polyaniline-paste were confirmed by SEM. As results, overall particle has approximately 40~50 nm of uniform size and has cubic-like shape. We had tested to operate the lithium ion battery used an electrode of polyaniline-paste as cathode with the liquid electrolyte. Further, we had tested electrochemical performances of polyaniline-paste using polymer-electrolyte instead of liquid electrolyte. The cell made out of polyaniline and solid electrolyte, achieved $\sim 87 \mu\text{Ah}/\text{cm}^2$ (64.0 mAh/g) at second cycle and $\sim 67 \mu\text{Ah}/\text{cm}^2$ (50.1 mAh/g) at 100th cycle as all-solid lithium ion battery.

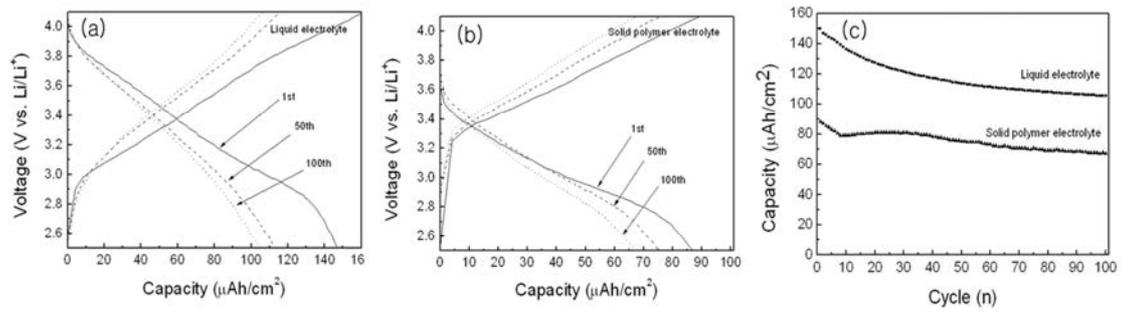


Figure 1. (a) Charge-discharge curves of polyaniline-paste electrode (70µm) using the liquid electrolyte, and (b) charge-discharge curves using solid polymer electrolyte and (c) cycle performance.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Electrochemical Performance of FeF₃/Reduced Graphene Oxide Nanocomposites as a Cathode Material for Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) have high energy density, high operating voltage, environmental friendliness, and long cycle lifetime. They are applied to the energy storage systems such as the mobile phones, laptop computers, and electric-vehicles (EVs). However, modern energy storage devices still require the development of LIBs with the enhanced reversible specific capacities. Although the significant improvements of the specific capacities of LIBs have been achieved in the past decade, the increase of the capacity has mainly been limited by the electrode materials, especially the cathode materials. Therefore, it needs to develop the cathode materials with the higher reversible specific capacities. FeF₃ is of great interest as a potential alternative cathode material for the commonly used cathode materials such as LiCoO₂, LiFePO₄ etc because of its low cost, abundance, environmental friendliness and high theoretical capacity of about 237 mAhg⁻¹ in the voltage range of 2.0-4.5 V. However, FeF₃ has drawbacks of poor capacity retention and rate performance due to its low intrinsic electrical conductivity and slow diffusion of lithium ions. In this study, FeF₃/reduced graphene oxide nanocomposites were synthesized through utilizing reduced graphene oxide as a conducting agent. From this, the improvements of discharge capacity, cycling stability, and rate performance of FeF₃ were achieved in the voltage range 2.0-4.5 V at room temperature compared to those of bulk FeF₃.

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발표코드: **ELEC.P-1168**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

pH sensors based on conductive polymers coated on metal alloy dendrite

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Some conductive polymers functionalized with carboxylic acid, benzoic acid, pyrimidine groups were synthesized and polymerized electrochemically on a metal alloy dendrite / screen print carbon electrode (SPCE), which were examined for pH sensors. The SEM image shows that the metal alloy dendrite grew homogeneously in a hierarchical structure. The fabricated pH sensors were characterized with SEM, EDX, impedance spectroscopy, and cyclic voltammetry. Analytical parameters affecting the pH sensor performance were optimized in terms of applied potential, temperature, humidity, and polymerization condition. The linear calibration plots for pH analyses were obtained between pH1 ~ pH13.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Synthesis and Electrochemical Performance of Carbon-Coated V_2O_5 Nanocrystals by Using Citric Acid as a Carbon Source

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Vanadium pentoxide (V_2O_5) with a layered structure has been considered as an attractive cathode material for Li-ion batteries (LIBs) because of its low cost, abundance, and relatively high theoretical capacity (about 294 mAhg^{-1} with 2 Li insertion/extraction per unit formula) compared with more commonly used cathode materials such as LiCoO_2 (140 mAhg^{-1}) and LiFePO_4 (170 mAhg^{-1}). However, the practical application of V_2O_5 is limited by its poor structural stability, low electrical conductivity and slow electrochemical kinetics, which lead to poor long-term cycling stability and rate performance. In this study, carbon-coated V_2O_5 nanoparticles have been synthesized through a facile thermal-decomposition of vanadium precursor $(\text{NH}_4)(\text{VO})\text{C}_6\text{H}_5\text{O}_7$ in which citric acid ($\text{C}_6\text{H}_8\text{O}_7$) was used as both a carbon source and reducing agent. The highly crystalline V_2O_5 nanoparticles are coated by a carbon layer with a thickness of approximately 3-6 nm. The carbon-coated V_2O_5 nanoparticles showed the enhanced electrochemical performances, compared to those of commercial micron-sized V_2O_5 and V_2O_5 nanoparticle synthesized with oxalic acid ($\text{C}_2\text{H}_2\text{O}_4$), which is commonly used as a reducing agent. For example, it exhibited a high initial discharge capacity $\sim 293 \text{ mAh g}^{-1}$ (2 Li per V_2O_5) between 2.1-4.0 V vs. Li/Li^+ at 0.1 C rate and good capacity retention of $\sim 90 \%$ after 30 cycles. At high current densities, the excellent rate capability and cycling stability were achieved.

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발표코드: **ELEC.P-1170**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

FeF₃/carbon foam (CF) nanocomposites for improving electrochemical performances as a cathode material for lithium-ion batteries

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Lithium-ion batteries (LIBs) have high operating voltage, high energy density, low self-discharge ratio, and long cycle lifetime. However, further researches to develop LIBs with enhanced reversible lithium-storage capacities are still necessary for their widespread applications in electric vehicles and energy storage systems. The specific capacities of LIBs are mainly limited by their electrode materials, especially the cathode side. Therefore, development of cathode materials with a higher theoretical capacity is needed. FeF₃ is one of the promising cathode materials because of its low cost, safety and environmental friendliness compared to commercialized LiCoO₂. In addition, FeF₃ has a higher theoretical capacity of about 237 mAh g⁻¹ at 2.0-4.5 V than that of LiCoO₂ (a reversible capacity of 140 mAh g⁻¹). However, FeF₃ has drawbacks of poor electrical conductivity and sluggish lithium-ion diffusion, which lead to inferior cycle retention and rate capability. In this study, FeF₃ nanoparticles were impregnated into the mesopores of carbon foam (CF) and crystallized inside the pores through the calcination under argon where CF was utilized as both a template and a carbon source. The synthesized FeF₃/CF nanocomposites were thoroughly characterized by BET, XRD, SEM, and TEM. The nanocomposites exhibited the improved electrochemical performances, e.g., discharge capacity, cycling stability and rate capability, in the voltage range of 2.0-4.5 V at room temperature, compared to bulk FeF₃.

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발표코드: **ELEC.P-1171**

발표분야: 전기화학

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Metal oxide Integrated Cobalt Phthalocyanine Nano Hybrid for an Efficient Cathode Catalyst in Microbial Fuel Cells

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The increasing cost of precious metals, especially platinum, as oxygen reduction catalysts impede their widespread use in microbial fuel cells for practical application. It is therefore of importance to develop alternative catalysts based on nonprecious metals. Electrochemical results revealed that cobalt oxide incorporation increased the ORR activity of cobalt phthalocyanine adsorbed on carbon particles. When applied to MFCs, the maximum power density of 780 mW m⁻² was achieved with the C-CoOx-CoPccathode, which was about 50 % higher than that with carbon supported CoPc. The voltage output of the MFC dropped only 19 % from its initial voltage after 100 days' operation, suggesting that the synthesized catalyst showed enough long-term stability. The voltage drop was partially resulted from the covering of biofilm on the catalyst layer, 89~92 % of which was reinstated upon scrapping off the biofilm. This work shows that C-CoOx-CoPc could be a potential alternative to Pt in MFCs for sustainable energy generation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemically reduced graphene oxide and horseradish peroxidase deposited pencil graphite electrode for the detection of hydrogen peroxide

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A new disposable biosensor based on the electrochemically pretreated pencil graphite electrode (PGE) for the determination of hydrogen peroxide (H_2O_2) has been developed. The disposable biosensors were constructed by using direct electrochemical immobilization of horseradish peroxidase (HRP) with in situ electrochemical reduction of graphene oxide (ErGO-HRP-PGE) on commercial graphite pencil leads. Before performing the electrochemical in situ immobilization, the PGE was electrochemically pretreated in 0.1M phosphoric acid solution by potential cycling between -0.3 V and +2.0 V. It was found that the electrochemical treatment could improve the redox characteristics of PGE and the with pretreatment showed improved sensitivity to H_2O_2 compared with the results obtained from non-pretreated GPE. The detailed characteristics of the ErGo-HRP-PGE were evaluated and the experimental parameters are optimized by using cyclic voltammetry and chronoamperometry. The optimized results obtained will be presented in the poster.

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발표코드: ELEC.P-1173

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphite oxide/SnO₂ Nanocomposites with High Cycle Stability for Lithium Ion Batteries

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Li ion battery (LIB) 가 전기자동차 (EV)의 전원으로 활발히 적용되기 위해서는 기존의 소형 전자기기에 사용되는 LIBs 의 성능을 뛰어넘는 고출력, 고에너지용량 및 안정성 향상이 요구되며, 이를 위해서는 새로운 음극 및 양극 소재 개발이 필수적이다. 이와 같은 관점에서 SnO₂ 는 유망한 음극소재이나 Li 과 alloy 형성 과정 중 부피 팽창으로 전기화학적 안정성을 담보할 수 없다. Graphene oxide (GO)의 넓은 표면적은 효과적으로 전극 전체에 network 를 제공하여 전자 전달을 도와주고, 높은 mechanical flexibility 를 가져 SnLi_x 와 Li₂O matrix 형성에 의해 유발된 부피 변화를 수용하는 것을 돕는다. 결과적으로 nanocomposite 은 고에너지와 출력, 가역성을 가지는 우수한 음극 재료임이 널리 알려져 있다. 하지만, GO layer 간의 약한 π - π 인력은 300%에 이르는 SnO₂ 의 부피 변화를 완벽하게 보완하기에는 충분하지 않다. 따라서, 본 연구에서는 long range ordering 이 존재하는 graphite oxide(GTO)가 SnO₂ 의 부피 변화를 좀더 효과적으로 buffering 하는지를 확인하기 위하여, GTO/SnO₂ (rSGTO) nanocomposites 을 합성하였다. rSGTO nanocomposite 은 GTO 를 DMSO/H₂O 혼합용매에 분산시킨 후 Sn⁴⁺를 첨가한 용액을 10h reflux 후 얻어진 침전물을 에탄올로 washing 하고 dry 과정을 마친 후 400 °C Ar 분위기 하에서 2 시간동안 열처리를 하여 제조되었다. rSGTO (GTO : SnO₂ of 45 : 55)는 50 cycle 충-방전 후에 761 mAh·g⁻¹ (77 % retention, 97 % Coulombic efficiency)에 이르는 매우 높은 가역적 용량을 갖는 것으로 확인되었고, GO/SnO₂ (rSGO) nanocomposite 는 상대적으로 낮은 용량 (ca. 567 mAh·g⁻¹)과 빠른 용량감소(73 % retention, 99 % Coulombic efficiency)를 갖는 것을 확인하였다. 이는 SnO₂ 나노입자가 GTO 구조 내부에서 SnO₂ 의 리튬치환반응에 대한 mechanical strain 을 최소화되고 그로 인해 최적의 이론적 비에 가까운 높은 Li 저장 성능을 얻을 수 있음을 의미한다.

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TiO₂ 나노입자 크기에 따른 염료감응형 태양전지 효율 변화 연구

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염료감응형 태양전지(Dye-Sensitized Solar Cells, DSSCs) 광전변환효율 향상을 위한 방법으로는 광전류(Jsc)-광전압(Voc) 특성을 향상시켜야 하는데 이 두 가지 기능을 모두 향상 시킬수 있는 핵심이 TiO₂ 광전극이다. 본 연구에서는 크기가 다른 TiO₂ 나노입자를 이용하여 광산란층을 광전극 위에 적층하거나, 서로 다른 크기의 입자를 혼합하여 비교적 큰 TiO₂ 입자에서 산란되는 광을 이용하여 Jsc 값이 증가로 인한 광전변환효율 향상을 목표로 실험하였다. 20 nm TiO₂ 나노입자를 이용하여 제조한 투명 전극용 TiO₂ paste 와 태양광선 산란 효과를 위해 250 nm, 500 nm TiO₂ 나노입자를 이용한 산란층 TiO₂ paste, 그리고 20 nm 와 250 nm, 500 nm TiO₂ 나노입자를 혼합한 혼합 TiO₂ paste 를 이용하여 여러 가지 방법으로 TiO₂ 전극을 형성하고 최적의 다층구조 TiO₂ 전극막을 설계하고 평가하였다. 이 실험에서는 20 nm TiO₂ paste, 혼합 TiO₂ paste, 산란층 TiO₂ paste 을 여러가지 방법으로 적층하여 scattering 효과로 인한 다중산란층의 단위셀을 만들고 SEM 을 이용하여 다중산란층 구조의 다중층 구조를 확인할 수 있었다. Solar simulator 측정을 통해서 셀 효율은 9.09%로 단일산란층보다 0.33% 향상 된 것을 확인하였다.

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Prussian Blue and its analogues for Na-ion batteries

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Prussian Blue(PB)는 face-centered cubic lattice 구조로 (C≡N)- 음이온들이 cube 의 각 코너에 octahedral 을 형성하여 low-spin Fe(III)는 C 원자와 결합하고, high-spin Fe(II)는 N 원자와 결합하여 교대로 배열되어 있다. PB 는 전기 촉매 특성을 가지고 있으며 표면에 전기화학적 또는 화학적 증착 후에 전기활성 층들을 형성할 수 있으며 재충전 가능한 배터리의 전원으로 사용할 수 있다. PB 와 유사한 framework 를 가지는 NaFe₃[Fe₂(CN)₆], KFe₃[Fe₂(CN)₆], Fe₃[Fe₂(CN)₆]의 화합물을 ice-bath 상태에서 공침법으로 합성하였다. 이후 framework 형성의 구조를 XRD, SEM 및 다양한 분석방법으로 확인하였으며, 이들 소재를 SIB 의 양극으로 사용하기 위해 capacity 및 cyclability 를 확인하였다.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-step electrochemical reduction of graphene oxide and in situ immobilization of cytochrome c

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부산대학교 바이오피지오 센서 연구소 ¹부산대학교 바이오피지오 센서 연구소 ²부산대학교 바이오피지오 연구소

A simple in situ immobilization method of cytochrome c by using an electrochemical reduction of graphene oxide (ErGO-cyt c) on glassy carbon electrode (GCE) will be introduced. The prepared ErGO-cyt c electrodes showed enhanced electro-catalytic activity to an enzymatically generated superoxide radical and the electro-catalytic enhancement was studied by cyclic voltammetry and chronoamperometry. The immobilized cyt c is retains direct electrochemistry and bio catalytic activity toward the reduction of superoxide. The performance of the electrode was characterized by comparison with the absence of cyt c, electrochemically reduced graphene oxide. The results indicated that the ErGO embedded Cyt c provided significant improvement in an electro-catalytic activity and sensitivity compared with the results obtained from bare or only ErGO modified GCE. Experimental parameters are optimized and will be presented in the poster.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1177**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the relationship between the outer Helmholtz plane potential and the supporting electrolyte concentration

남광모 장병용*

부경대학교 화학과

Electrochemical reactions are activated by the potential difference between the electrode and the solution. Normally, the potential difference is defined by the potential at the outer Helmholtz plane (OHP) because the supporting electrolyte of high concentration deforms the electric field to eliminate the potential drop outside of the OHP. Sometimes, the measurement of electrochemical information under such conditions can make distorted results. Here, we studied the effect of the supporting electrolyte concentration on the electrochemical information. We measured the electron transfer rates of Fe(CN)₆³⁻ reduction at different concentrations of the supporting electrolytes using the Fourier transform electrochemical impedance spectroscopy method. From the results, we calculated k_0 values and fitted them to the Frumkin effect equation in order to evaluate the potential of the OHP. Finally, we correlated the OHP potential to the concentration of the supporting electrolyte.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1178**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical control of the transport of ions

PIAOHUSHAN 손용근*

성균관대학교 화학과

Membrane separation method was frequently applied in recent years. Because, it can be used in large quantity scales and automatic separation was possible. But, the mechanism of the separation for many ions were not reported. So, we performed several transport experiment of organic and inorganic ions of identical charge but have different character to understand the mechanism of the ionic transport in detail. Conducting polymer modified membrane was prepared in two steps. First, gold was sputtered on the PC(polycarbonate) membrane. Second, a polypyrrole layer was electrochemically deposited on the Au surface in aqueous solution until the pores were covered perfectly. Then ion transport was performed under various potential conditions. The transport tendency of ions through the membrane was depending on the nature of them. 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 Knowledge Economy(No. 2010501010002B)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ELEC.P-1179**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of tunneling effect of 16-MHDA layers on gold substrate by using Self-Assembled mono- or multi-layer(s) method

Wang Wenxiu 손용근*

성균관대학교 화학과

Organic thin film transistors (OTFT) are highly attractive for a mount of application, but one of the main problems with traditional OTFT is the high operating voltage is usually large, because of the poor capacitive coupling through the dielectric layers. Through decreasing the thickness of the insulating layer to reduce the supply voltage is one of the possible ways to make nanometer-scale FET. Fortunately using of self-assembled monolayer or multi-layers might solve this problem. In this paper the insulator which we studied is 16-mercaptohexadecanoic (16-MHDA) self-assembled multi-layers on gold wafer. These molecules are deemed to be insulating and also the tunneling current will decrease exponential with the increasing of molecule length. Many works have shown the electronic transport through molecules of alkanethiol (C8, C10, C12, C16 etc.) however in these studies only molecular monolayer was studied, it was too thin to avoid the tunneling current. Here we have used 16-MHDA self-assembled mono- and multi-layers on gold surface to discover the dielectric characters and the critical thickness of the 16-MHDA layers. 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 Knowledge Economy (No.2010501010002B)

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **EDEC.P-1180**

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

2012 여수 EXPO 전시장의 STEAM 교육요소와 중등과학 교육과정과의 연계성 연구

하동수* 김민아

순천대학교 화학교육과

본 연구에서는 중등 과학영역을 중심으로 2009년 개정 교육과정을 비교한 후, 과학영역에 해당하는 2012 여수세계박람회장내 전시물의 STEAM 교육요소를 조사·분석하였고, 이를 국가 교육과정에 근거한 성취기준 및 평가기준 개발 연구에 기초하여 연구자가 직접 개발한 평가기준을 토대로 연계성을 비교·평가 하였다. 교육과정과 전시물의 조사·분석·비교·평가를 통해 실제 여수세계박람회의 전시물과 교육과정이 어느 정도 연계되고 있는지를 분석하였다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: EDEC.P-1181

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

과학적 상호작용 수업에서 모델진화에 영향을 주는 상호작용 분석

- 중학교 물질분야(결합)

김혜영 박현주^{1,*}

조선대학교 화학교육과 ¹조선대학교 과학교육학부

이 연구는 과학적 상호작용 수업에서 학생이 형성하는 결합 모델 진화에 영향을 주는 상호작용의 특성을 조사한 것이다. GEM 순환전략을 이론 및 실험적 근거로 이용하여 소집단토론이 학생의 과학적 모델 변화에 어떤 영향을 주는지에 대하여 분석하였다. 연구는 수도권 소재의 중학교 2학년 1개 반을 대상으로 진행되었으며, 연구를 위한 수업설계는 물질분야의 결합 수업을 담당한 교사와 상호협력적이며 유기적인 관계를 통하여 이루어졌다. 자료 수집은 수업 참여 및 관찰, 비디오 녹화, 음성 녹음, 교사와 학생 면담, 학생활동지 등을 통하여 진행하였다. 자료의 분석은 정신모형이 모둠모형으로 화합하는데 있어 나타나는 표현의 특징과 사고모형이 표현모형으로 표출되는데 있어 교사-학생의 상호작용을 통해 비계설정의 영향의 두 가지 측면에서 이루어졌다. 연구 결과는 다음과 같다. 첫째, 정신모형이 모둠모형으로 화합하는데 있어 모둠원의 의견을 모아 공동구성하는 모둠이 4개 모둠, 개인의 의견을 모둠모형으로 나타내는 모둠이 2개 모둠으로 표현의 변화 없음이 가장 많았고, 표현의 확장 및 다양해진 모둠과 표현의 축소 및 제한적인 모둠은 각각 1개 모둠으로 나타났다. 둘째, 사고모형이 표현모형으로 표출하는데 있어 어려움을 겪는 학생들에게 도움을 주는 교사의 비계설정을 분석한 결과 모둠의 특성별로 각기 다른 비계설정이 이루어진다는 결론이 나왔다. 즉 학생들이 부분적 개념을 가지고 있는 경우 열린 질문, 동의, 격려를 통해 사고를 확장하게 하고, 표현의 시도를 하지 못하는 모둠은 정보, 힌트를 통해 사고모형을 표현모형에 연결시킬 수 있게 하고, 오개념의 방향으로 상호작용하는 모둠에게는 교사의 주도적 열린 질문으로 목표모형에 도달할 수 있도록 비계설정을 하는 것으로 조사되었다. 이 연구는 학습목표를 도달하기 위해 과학적

상호작용을 이용한 모델링 수업 중에 나타난 상호작용의 유형과 모둠원의 구성에 따라 상세화하였다는데 그 의미를 찾을 수 있겠다. 참고문헌 John Clement,(2008). Six Levels of Organization for Curriculum Design and Teaching.John J. Clement(2008). Student/Teacher Co-construction of visualizable Models in Large Group DiscussionBarbara C. Buckley(2000). Investigating the role of Representations and Expressed



일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: EDEC.P-1182

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

현직 교사에게 묻습니다. 사범대학에서 무엇을 배워야 할까요?

한재영* 김경은¹

충북대학교 사범대학 화학교육과 ¹남성중학교 과학

한국의 중학교 및 고등학교 교사들은 많은 경우가 사범대학에서 공부를 하고 교직으로 진출해 있다. 그리고 사범대학의 입학생들은 교사가 되기를 꿈꾸며 다양한 대학 과목을 수강하여 자신의 능력을 계발해 나간다. 즉 사범대학은 중등 교육과 연계된 여러 가지 경험을 예비 교사에게 제공하여야 한다. 그런데 현재 사범대학에서 제공하는 교육은 교육 현장의 요구나 필요성과 어느 정도 연계되어 있을까? 이 연구에서는 신임 화학 교사들을 대상으로 사범대학에서 무엇을 배워야 하는지 질의?응답한 내용을 통해 이 문제를 다루어 본다. 교사의 다양한 역할 중 수업을 가장 중심적인 것으로 놓고, ‘수업을 잘 하기 위해 사범대학에서 배워야 할 것은?’이라는 질문에 대해 2013년 화학 1급 정교사 자격연수에 참가한 교사 44명이 자유롭게 작성한 글을 분석하였다. 현직 교사들의 생각은 교과내용, 교수법, 교재연구, 수업 실연, 실험 능력, 흥미 유발, 학생 상담 및 이해, 교육관, 기타 등으로 분류할 수 있었다. 교사들은 전공 과학 내용에 대한 이해가 수업에 기본적인 바탕이 된다고 응답하였다. 교수법에 대해서는 다양한 교수학습법이나 수업 모형을 실습을 통해 익히는 것이 필요하고 멀티미디어 활용법도 알아야 한다고 답하였다. 그리고 교재연구를 통해 중등 교육과정과 교과서를 분석해볼 필요가 있다고 생각하고 있었다. 수업 지도안을 작성하여 수업 실연을 많이 해 보고 수업에 대한 평가와 반성이 필요하다고 응답하였다. 또한 대학 전공 실험보다 중고등학교에서 수행되는 실험을 수행해 보는 것이 필요하며, 학생의 흥미를 유발하기 방법이나 자료를 준비해 두는 것이 좋다고 답하였다. 한편, 학생 상담을 통해 학생을 이해하고 관계를 개선하는 것이 과학 수업에도 도움을 주며, 교사 자신의 교육관을 수립할 필요가 있다고 생각하고 있었다. 이러한 현직 화학 교사의 생각을 사범대학 화학교육과 교육과정 개선에 반영하여 예비 교사의 수업 능력 발달을 지원할

필요가 있다.(이 논문은 2013 년도 정부(교육부)의 재원으로 한국연구재단의 지원을 받아 수행된 기초연구사업임(2010-0010983)).



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장소: 창원CECO

발표코드: EDEC.P-1183

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

제7차, 2007 개정 및 2009 개정 교육과정 중?고등학교 교과서 중의 물질의 분리 관련 부분의 내용분석

이재환 류재정^{1,*}

경북대학교 일반대학원 과학교육학과 ¹경북대학교 화학교육과

제 7 차, 2007 개정 및 2009 개정 교육과정에 속하는 국내에서 출간된 중?고등학교 과학 및 화학 교과서에서 물질의 분리 부분에 대한 전반적인 내용구성, 서론 부분, 실험 부분, 정의 또는 원리, 활용, 역사 및 종류, STS 관련 및 기타 내용으로 구분하여 비교 분석하였다. 특히 선행연구[1,2]를 토대로 크로마토그래피 부분의 내용을 중점적으로 살펴 보았다. 연구 결과, 각 교육과정별로 크로마토그래피에 대한 전반적인 내용과 내용 수준에 있어서는 큰 차이가 없었고, 대부분 크로마토그래피 관련 내용이 다양하지 못하였다. 특히 교육과정이 개정될수록 크로마토그래피 관련 내용의 비중과 분량이 감소하였고, 2009 개정 교육과정 고등학교 교과서에서는 크로마토그래피 관련 내용이 삭제되었다. STS 가 강조되는 현대 사회에서 크로마토그래피 관련 내용은 충분한 교육적 가치가 있으므로, 다음 교육과정에서는 대폭 개선되어 크로마토그래피에 대한 교재 내용이 보다 많이 알찬 내용으로 소개되길 기대한다. 1. Analysis of Chromatographic Part in Middle School and High School Chemistry Textbooks; J. J. Ryoo; Chemical Education, 25 (1998) 196-206. 2. Content Analysis of Chromatographic Part in Middle School Science and High School Chemistry Textbooks of the 7th Education Curriculum, Jae Jeong Ryoo, Jeong Hwan Kim, Seoung Hey Paik, Journal of the Korean Chemical Society, 52 (2008) 423-433.

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장소: 창원CECO

발표코드: EDEC.P-1184

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

실험비계(experimental scaffolding)를 통한 과학개념구성 수업모형

개발연구 -액체의 증기압에 적용한 수업사례-

우현승 정대홍*

서울대학교 화학교육과

연구에 의하면 고등학교 학생들의 평균 인지수준은 구체적 조작수준 비율이 형식적 조작수준보다 높아서 추상적 사고가 필요한 형식적 개념을 습득하기에 어려움이 따른다. 따라서, 화학 2에 집중되어 있는 형식적 개념과 물질의 특성, 이를테면 증기압, 삼투압, 엔탈피, 화학평형 등은 학생들의 이해도와 수업참여도를 고려하여 적절한 수업방법이 필요하지만 학교에서는 현실적인 문제로 강의식 수업에 치중하고 있는 실정이다. 이에 따라 본 연구에서는 추상적 사고가 필요한 형식적 개념을 새롭게 구성하는 경우, 특히 학생의 인지수준과 학습하고자 하는 개념간의 인지수준 차이가 클 때 적용할 수 있는 수업모형을 연구, 개발하였다. 이 수업모형은 학습자 스스로 지식을 구성하면서도 인지적 부담을 최소화하여 최종적으로 개념수준을 상승시키는 것을 목표로 하였고, 전통적인 강의식 개념학습의 형태를 탈피하기 위해 개념지식과 과학적 탐구력을 함께 습득할 수 있도록 설계하였다. 그 핵심전략으로 수업의 3 단계 구성과 각 단계별 비계를 지속적으로 제공하는데, 단계별 비계는 과학적 탐구를 유발하는 실험비계를 제시하는 것이다. 발표에서는 수업모형의 알고리즘과 각 단계의 구성특징, 특히 단계별 실험비계의 특성에 대해서 구체적으로 기술할 것이다. 또한 본 수업모형을 액체의 증기압 수업에 적용한 사례를 제시하는데, 주목할 점은 직접 개발하고 특허등록을 마친 증기압 측정기구를 실험비계로 사용한 것이다. 따라서 자체개발한 증기압 기구의 원리와 조작방법, 실제 증기압 측정 방법도 함께 제시할 것이다.

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장소: 창원CECO

발표코드: EDEC.P-1185

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

이온화 에너지, 전자 친화도, 전기 음성도의 정의에 대한 예비교사 의 이해

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본 연구에서는 7 차 교육과정과 2009 개정 화학 교과서와 대학 일반화학교재, 무기화학교재를 대상으로 이온화 에너지, 전자친화도, 전기음성도의 정의를 진술하는 방식에 대해 분석하고, 예비교사를 대상으로 설문을 통해 이온화 에너지, 전자친화도, 전기음성도의 개념에 대한 이해를 알아보았다. 교재분석 결과, 이온화 에너지는 기체상태의 중성원자로부터 정의되어 있는데 일부 교재에서는 중성원자 뿐 아니라 이온으로도 이온화 에너지를 정의하고 있었다. 또한 전자친화도는 대부분의 교재에서 공통적으로 기체상태의 중성원자로 정의하고 있지만 일부교재에서는 전자친화도를 비금속 원소로부터 정의하고 있었으며, 정의를 마무리하는 진술에 있어서 방출하는 에너지, 에너지변화 두 가지 유형으로 정의하고 있었다. 전기음성도는 대부분의 교재에서 결합과 관련지어 정의하고 있는데 일부교재에서만 결합에 대한 언급이 없었고, 정의되는 입자는 교재마다 일정한 기준이 없었고, 정의가 마무리되는 진술부분에서도 교재마다 차이가 있었다. 또한 이온화 에너지, 전자친화도, 전기음성도가 제시 되는 단원이 동일했던 교재가 있고 각각 다른 단원에서 따로 제시된 교재도 있었는데, 개념들이 같은 단원에서 함께 제시되어 그들을 비교 설명한 교재로 학습하는 것이 학습자들이 개념을 이해하는데 있어 좀 더 명확할 것으로 보인다. 설문조사 결과, 이온화 에너지의 정의에 대해서 예비교사들은 에너지차원에서 이온화 에너지가 흡수에너지임을 대부분 알고 있었으나, 이온화 에너지가 정의되는 입자차원에서는 이해가 낮았다. 전자친화도의 정의에 대해서는, 에너지측면에서 전자친화도가 방출에너지임을 알고 있는 예비교사의 비율이 낮은 편이었다. 설문 응답으로는 전자친화도를 전기음성도와 혼동한 응답과 에너지출입의 이해 부족에서 오는 응답 등 여러

오류 응답들이 있었다. 전자친화도의 정의에 대한 이해도 전반적으로 낮았으며, 전자친화도와 혼동한 오답이 많았다. 이는 전자친화도와 전기음성도를 구분하는데 어려움이 있다는 것을 의미한다.



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장소: 창원CECO

발표코드: **EDEC.P-1186**

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

액체 혼합물의 끓음과 증발에 대한 고등학생, 예비교사, 현직교사 의 입자모형적 이해 조사

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액체의 증발과 끓음에 대한 많은 연구가 이루어져 왔으나, 에탄올 수용액과 같은 액체 혼합물에 대한 연구는 부족하다. 액체 혼합물이 끓을 때에는 혼합물 중 끓는점이 낮은 액체의 끓는점에서 먼저 끓고, 다시 끓는점이 높은 액체의 끓는점에서 끓는다는 대체적 개념이 많이 있다. 이러한 인식의 근원과 해결점을 찾기 위한 방안으로서 고등학생, 예비교사, 현직교사를 대상으로 에탄올 수용액의 끓는 현상과 증발 현상에 대하여 입자모형을 그려보게 하였다. 그 결과 증발 상황에서는 증기상에서 물과 에탄올 입자는 모두 있으나, 끓음 상황에서는 에탄올의 입자만 그리는 경우가 많았다. 연구대상의 여러 다양한 입자모형과 분석을 통해 액체 혼합물의 끓음의 교수학습에 대한 시사점을 살펴보았다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **EDEC.P-1187**

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

초등학교 과학 영재 교육 프로그램의 개발과 적용

하동수* 이강별 최원호

순천대학교 화학교육과

본 연구에서는 렌줄리의 삼부심화학습모형에 근거하여 초등학교 과학 영재 교육 프로그램을 개발하여 적용하였다. 프로그램을 적용하면서 실시한 수업 관찰과 설문 조사 결과를 바탕으로 몇 가지 시사점을 알 수 있었다. 첫째, 학생들은 학교에서 경험하지 못한 실험 활동에 흥미와 호기심을 가지나 참여 학생의 학교급을 고려하여 학생 수준과 경험에 맞는 활동을 선정할 필요가 있다. 둘째, 학생들의 다양한 흥미를 충족하기 위해 공통 과제와 함께 선택 과제를 고려할 필요가 있다. 셋째, 변인 통제와 같은 탐구 활동을 어려워하기 때문에 추론 및 통합탐구능력 향상을 위한 노력이 필요하다. 넷째, 반복적인 탐구 활동도 과학에서 매우 중요하다고 인식시킬 필요가 있다. 다섯째, 사고할 수 있는 시간을 위하여 수업 활동 시간을 충분히 확보할 필요가 있다. 여섯째, 현대 과학이 협동을 통해 진행된다는 측면에서 개별 활동보다는 협동을 통한 활동을 수행하는 경험을 늘릴 필요가 있다.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1188

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of calcination temperature and organic buffers on the catalytic nitrate reduction by Pd-Cu/TiO₂ catalyst

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We have investigated the effect of calcination temperature and organic buffers on catalytic nitrate reduction (50 NO₃--N mg/L) by Pd-Cu bimetallic catalyst supported by TiO₂ (Pd-Cu/TiO₂). Pd-Cu/TiO₂ calcinated at 450 and 550 °C showed 77 and 31% of nitrate removal efficiency in 1 h which was much lower than that at 350 °C showing 100% removal due to the sintering of metal particles at high temperature. Transmission electron microscopy analysis supported the sintering of metal particles by showing the bigger particle size of Pd and Cu calcinated at 450 and 550 °C than that at 350 °C. Complete nitrate reduction was observed at pH 6 (MES) and 7 (MOPS), while 58-74% of nitrate was degraded by TiO₂/Cu/Pd at pH 8-10 (TRIS, TAPS, and CHES) in 1 h. Especially, its removal efficiency at pH 8 prepared with TRIS buffer dramatically dropped (58%) due mainly to the significant leaching of Cu (35%), resulting in loss of catalytic sites for nitrate reduction. The by-product selectivity (nitrite, ammonia, and nitrogen gas) seemed to be controlled by the suspension pH rather than that by metal leaching in this study.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1189

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reductive dechlorination of octachlorodibenzo-p-dioxin by nanosized zero-valent Metals: Modeling of rate kinetics and congener profile

이충섭 장윤석*

포항공과대학교 환경공학부

Polychlorinated dibenzo-p-dioxins (PCDDs), a group of recalcitrant toxic compounds, are ubiquitous in nature. Amongst them, octachlorodibenzo-p-dioxin (OCDD) is not only prevalent in soil and sediment due to its high lipophilicity and hydrophobicity, but also detected in ground water and surface water. The present study examined the degradation of OCDD in aqueous solutions using four different zerovalent metal nanoparticles; zero-valent aluminum (nZVAL), zero-valent zinc (nZVZ), zero-valent iron (nZVI) and zero-valent nickel (nZVN). Only nZVZ was found to efficiently degrade OCDD into lower chlorinated congeners [OCDD \rightarrow 1,2,3,4,6,7,9-HxCDD (63%) \rightarrow 1,2,3,6,8,9-HpCDD (21%) \rightarrow 1,2,4,7,8-PeCDD (46%) \rightarrow 1,2,4,7-TeCDD (19%)] under ambient conditions. Simulations were also performed to predict the OCDD dechlorination pathway using a linear free energy relationship (LFER) model. Additionally, toxic equivalent quantity (TEQ) and homologue patterns were calculated by LFER modeling. The experimentally observed congener profiles were in excellent agreement with the model-predicted results, especially considering the complexity of the OCDD dechlorination pathway (256 theoretically possible reactions). This study proposes nZVZ as a suitable candidate for OCDD dechlorination and constitutes the first report on OCDD degradation using zero-valent metal nanoparticles under ambient conditions.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1190**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of Dechlorane plus exposure to micro-biota in the soil mimic condition

이충섭 장윤석*

포항공과대학교 환경공학부

Dechlorane plus (DP-C₁₈H₁₂Cl₁₂), a high chlorinated flame retardant, is listed as a high production volume (HPV) chemical. The technical DP product consists of two isomers: syn and anti in a ratio 1:3 and it is used in electrical hard plastic connectors in televisions and computer monitors, wire coatings, and furniture. In our study, we evaluated the effects of DP on bioactivities in the soil mimic condition. By using various bacteria including Escherichia coli (E.coli); dibenzofuran (DF) degrading-bacteria Agrobacterium sp. PH-08; phosphorus solubilizing bacteria Gluconacetobacter liquefaciens sp. G1, which play specific roles in ecosystem, we could predict the potential interaction among two isomers and biota. The different behavior between syn- and anti-isomer was presented in cell viability, ROS level and bioactivities. DP at low concentration could be toxic to bacteria but the toxicity level was decreased in suspended medium, such as soil extracted solution as well as specific growth medium. It was caused due to the high hydrophobicity of DP. This characteristic could limit the interaction between DP and microorganism, which could in turn be a limitation in terms of DP biodegradation.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1191**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic Degradation Behaviors of TiO₂/graphene composites

이동수 박수진*

인하대학교 화학과

In this work, the TiO₂ (P25, Degussa AG, Germany) and graphene composites were prepared from a thermal reaction of graphene oxide. The surface morphology of TiO₂/graphene composites was examined by scanning electron microscopy (SEM). The structural properties of TiO₂/graphene Composites were examined by X-ray diffraction (XRD). The surface properties of the TiO₂/graphene were characterized by X-ray photoelectron spectroscopy (XPS). The textural properties of TiO₂/graphene composites were investigated by N₂/77K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. From the results, it is confirmed that the adsorption of methylene blue and absorption of visible light are improved by carbon doping on the TiO₂ surface.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1192**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of TiO₂/Activated Carbon composites for Adsorption Behaviors of Organic Dye

이동수 이민상 박수진*

인하대학교 화학과

In this work, TiO₂/Activated Carbon composites were synthesis by a sol-gel method with prepared using titanium isopropoxide (Ti(OCH(CH₃)₂)₄, Sigam aldrich) as a Ti source. The surface morphology of TiO₂/Activated Carbon composites was examined by scanning electron microscopy (SEM). The structural properties of TiO₂/Activated Carbon composites were examined by X-ray diffraction (XRD). The textural properties of TiO₂/Activated Carbon composites were investigated by N₂/77K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. The photocatalytic activities of TiO₂/Activated Carbon composites were tested using methylene blue (MB) solution under UV and visible light irradiation. From the result, it was apparent that photocatalytic activities of TiO₂/Activated Carbon composites are higher than non-treated TiO₂ due to a wider adsorption wavelength of TiO₂/Activated Carbon composites.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1193

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Monitoring of surface reaction kinetics on vivianite and green rust with Cr(VI) in aqueous phase

박미소 신영호 이우진*

한국과학기술원(KAIST) 건설 및 환경공학과

A number of soils and surface/ground-waters in industrial regions have been widely contaminated by chromium due to its improper disposal and leakage from ore processing, electroplating, leather tanning etc. Hexa- and tri-valent chromium (Cr(VI) and Cr(III)) are the most common oxidation states of Cr in environments and Cr(VI) is more mobile and toxic than Cr(III). Vivianite ($\text{FeII}_3(\text{PO}_4)_2 \cdot 8(\text{H}_2\text{O})$) and green rust ($[\text{FeII}_4\text{FeIII}_2(\text{OH})_{12}] [4\text{H}_2\text{O} \cdot \text{CO}_3]$) are mixed-valent iron compounds that can mainly consist of ferrous iron (Fe(II)). It has been well known that Fe(II) has high reduction potentials for organic and inorganic compounds, therefore, we studied Cr(VI) reduction into Cr(III) by vivianite and green rust in aqueous phase for understanding the surface reaction and kinetics. In this study, batch kinetic tests were performed in anaerobic conditions under different pH (5-9) and reactant concentration. Aqueous Cr(VI) concentrations were quantified using diphenylcarbazide method with UV-vis at 540nm. Also, Cr(VI) reduction kinetics on vivianite and greenrust surfaces were estimated by EPA 3060A methods. Furthermore, X-ray spectroscopic and microscopic analysis, i.e., XPS, XRD, and SEM/TEM etc., conducted to identify the reduction mechanism of aqueous Cr(VI) on vivianite and green rust surfaces.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1194**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Hydrodechlorination of Chlorophenols by Pd-Y Zeolite and Pd-MCM-41 Mesoporous Material

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Chlorinated phenols are used in many industrial areas such as pesticides, herbicides, disinfectants, and wood preservatives. However the toxic chlorophenols have become current environmental concerns. In this study, mesoporous material MCM-41 and Y zeolite support palladium catalysts were prepared and the catalytic HDC of chlorophenols (especially 2,4-dichlorophenol, 2,6-dichlorophenol, and 2,4,6-trichlorophenol) was investigated. MCM-41 and Y zeolite were used as porous-based support materials for palladium particles. These Pd-MCM-41 and Pd-Y were utilized in adsorption and hydrodechlorination of chlorophenols (especially 2,4-dichlorophenol, 2,6-dichlorophenol, and 2,4,6-trichlorophenol). 2,4-Dichlorophenol was completely decomposed within 2 hr when the reaction was catalyzed by Pd-MCM-41 with Na₂SO₄. On the other hand, 3,4-Dichlorophenol was completely decomposed within 2 hr when the reaction was catalyzed by Pd-Y with Na₂SO₄ or K₂CO₃.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1195**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Role of Simultaneous Nb Doping and Fullerol Complexation for Visible Active Titania

임종훈 최원용*

포항공과대학교 환경공학부

Titania has been widely studied in many fields because of high photo oxidation power, excellent stability, non-toxicity, and low material cost. Although it has various advantages, its application for visible active photocatalysis is limited due to a large bandgap (~3.2 eV) and fast recombination of photo-generated charge pairs. Therefore, many researchers have modified titania to increase visible light activation with various methods such as dye sensitization, composition with other visible active photocatalyst and doping. In this study, we propose simultaneous Nb doping and fullerol complexation to solve the main drawbacks of titania. Nb-doped TiO₂ (Nb-TiO₂) was firstly synthesized by a simple sol-gel method, and then surface modification with adsorbed fullerol. As prepared samples were characterized by XRD, TEM (EELS mapping), XPS, DRS and Mott-Schottky plot. Their photocatalytic activity were tested for the reduction of chromate, oxidation of iodide and degradation of 4-chlorophenol. The photoactivity was also evaluated with photoelectrochemical measurements. From all data, we could confirm the role of Nb doping and fullerol complexation. Fullerol adsorption enhanced the visible light absorption through a surface complex charge transfer mechanism. Nb doping retarded recombination of photo-generated charge pairs by formation trapping site (Ti vacancy) and increased the charge transfer by a charge compensation mechanism (substitution of Nb⁵⁺ in a Ti⁴⁺ position). As a result, the photocatalytic activity of C60/Nb-TiO₂ was higher than other samples under visible light ($\lambda > 420$ nm).

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1196**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Uncertainty evaluation of dioxins analysis in fish

신은수 장윤석*

포항공과대학교 환경공학부

The uncertainty of measurement is defined as 'parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand' by ISO GUM. All measurements have the uncertainty, and it is derived from various components. In order to take more closer to the true value, we should know the uncertainty to prevent decline the confidence of measurement. In this study, we considered many components of uncertainty, and made the 'cause and effect' fish bone model. Various components exist, for example, accuracy of balance, deviation of syringe volume, expanded uncertainty of standard solution's concentration, and peak assignment. First, we classified the components to type A and type B uncertainty. Standard uncertainty of each component is calculated each formula, and then it is combined. Expanded uncertainty is obtained by multiplying the combined standard uncertainty by a coverage factor. We calculated the expanded uncertainty in the analysis of PCDD/Fs and DL-PCBs in *Scomber japonicus*. The result is expressed as 1.3644 ± 0.094 pg-TEQ/g wet weight with a level of confidence of approximately 95% and coverage factor 2. Acknowledgement : This research was supported by a grant (12162MFDS015) from Ministry of Food and Drug Safety in 2012.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1197

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of safety management of dioxins and PCBs in food

신은수 장윤석*

포항공과대학교 환경공학부

Fish samples (37 food, total 480 samples) collected in nine major cities have been analysed for a range of dioxins (29 congeners; PCDD/Fs 17 congeners and dioxin-like PCBs 12 congeners) using the isotope dilution method, HRGC/HRMS. The detected dioxin levels were pleuronectes platessa 0.3675, trichiurus lepturus 0.8506, scomber japonicus 1.1159, cetacea 0.9797, paralichthys olivaceus 0.5979, cololabis saira 0.2263, gadus macrocephalus 0.0789, pleuronichthys cornutus 0.8689, arctoscopus japonicus 1.4749, freezed calamus bajonado 0.4140, Theragra chalcogramma 0.0336, engraulis japonica 0.6978, theragra chalcogramma 0.0410, misgurnus anguillicaudatus 0.2206, silurus asotus 0.2587, miichthys miiuy 0.0735, pampus argenteus 0.3603, ostracion solorensis 0.0851, seabastes inermis 0.2646, carassius carassius 0.3756, scomberomorus niphonius 0.9286, selachimorpha 0.0628, cynoglossus joyneri 0.0412, oncorhynchusmasou 0.2606, mugil cephalus 0.2902, lophiomussetigerus 0.1520, astroconger myriaster 0.5851, oncorhynchusketa 0.2512, pleurogrammus azonus 0.6773, cyprinuscarpio 0.2689, anguilla japonica 0.4023, konosirus punctatus 1.5930, larimichthys polyactis 0.3028, stephanolepisirrhifer 0.0538, thunnusthynnus 0.2136, clupea pallasii 1.1986, okamejei kenojei 0.082 pg WHO05-TEQ/g weight, respectively. The contribution of dioxins levels were 34% in scomber japonicus, 29% in ngraulis japonica, 7% in trichiurus lepturus, 4% in larimichthys polyactis, 4% in thunnusthynnus, 4% in paralichthys olivaceus. In the study, PCDFs, penta-PCBs and hexa-PCBs in congeners of dioxins in fishes were mainly detected when converted into TEQ(toxicity equivalents). Acknowledgement : This research was supported by a grant (12162MFDS015) from Ministry of Food and Drug Safety in 2012.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1198**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Concentration Profiles of Polychlorinated Biphenyls and Organochlorine Pesticides in Serum from Korean General Population

신은수 장윤석*

포항공과대학교 환경공학부

Polychlorinated biphenyls(PCBs) and Organochlorine pesticides(OCPs) are groups of persistent organic pollutants(POPs). It have been reported that exposure to high dose of PCBs and OCPs cause diverse adverse health effect. Recent studies suggests that long term exposure of low dose of POPs can be related to chronic disease like metabolic syndrome, diabetes, and arthritis. To evaluate risk of chronic effect of pops, this study assess POPs concentration in Korean general population without environment-related disease. Totally 370 serums sampled from healthy adults consist of 159 from Ansan/Ansung, 90 from Uljin, and 121 from Daegu, respectively. All subjects were selected for the healthy control for the case-control study to assess relationship between POPs concentration and environment-related disease. The serum samples were then extracted on C18 SPE cartridges followed by clean-up with silica and florisil cartridge. GC-HRMS measurements were performed on a JMS-800D (JEOL, Japan) interfaced with a 6890N gas chromatography. Demographic information, lifestyle factors, and dietary intake were determined for all participants by trained interviewers using a standardized questionnaire. The most abundant OCP compound was p,p'-DDE, followed by b-HCH, p,p'-DDT, trans-nonachlor, and HCB among 22 OCPs measured. Among the PCB congeners analyzed, PCB153 was detected in the highest concentrations, followed by PCB118, PCB180, PCB138, and PCB187. Although the result shows similar concentration patterns with previous monitoring studies, regional differences in numerical value were found. Therefore further studies are necessary to evaluate effect of other life styles factors on concentration differences, and to establish concentration range in Korean healthy population.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1199

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of mobile phase modifiers about ionization efficiency of biomass burning marker Levoglucosan

신은수 장윤석*

포항공과대학교 환경공학부

Levoglucosan (1,6-anhydro- β -D-glucopyranose) is one of the biomass burning markers generated from biomass burning, such as woods consisting of cellulose and hemicellulose, and it is very useful as a biomass burning marker compared to other monosaccharide anhydrides (MAs), including mannosan and galactosan because of its abundance in the atmosphere. Levoglucosan is very hydrophilic and polar compounds. Thus, several studies have been attempted for the identification of levoglucosan using Gas chromatograph-Mass spectrometry (GC-MS) after derivatization process and Liquid chromatograph/Electrospray ionization Tandem Mass Spectrometry (HPLC/ESI-MS/MS). In this study, the latter was applied for the levoglucosan analysis due to the several advantages in time and labor-saving. Mobile phase modifiers for enhancement of ionization efficiency of analytes have been widely used as "post column infusion" system. Representative weak base, such as ammonium hydroxide (NH₄OH), was basically applied for this study and also, trimethylamine(TMA) and triethylamine (TEA) were attempted for enhancement of deprotonation of levoglucosan. The purpose of this study was to find the proper and efficient mobile phase modifier facilitating ionization of levoglucosan in negative-ion electrospray ionization mass spectrometry.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1200**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Role of Interlayer Graphene Layer on the Free-Standing TiO₂ Nanotube Based Dye-Sensitized Solar Cells

서인철 강순형*

전남대학교 화학교육과

Since the first discovery of high efficient dye-sensitized solar cells (DSSCs) at 1991, the enormous attention has been focused on the development of DSSCs to improve the conversion efficiency up to 15 %. In particular, one-dimensional (1-D) TiO₂ materials such as nanorods, nanotube, nanowhisker, and nanotubes as a photoanode have quite received lots of interest because of the fast electron transport rate rather than zero-dimensional TiO₂ nanoparticle. However, the development of 1-D TiO₂ nanotube (TONT) directly aligned on the transparent conducting oxide (TCO) substrate has been in the bottleneck. Recently, the free-standing anodic TONT was achieved by simple chemical dissolution process, followed by transferring to the TCO substrate. In here, the graphene as an interlayer to bond the detached TONT to TCO substrate was firstly introduced to improve the electron transport rate. Related several analyses (FE-SEM, XRD, UV-VIS spectrophotometer) would be performed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1201

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Double Layered Nanoarchitecture Based on Anodic TiO₂ Nanotubes for Dye-Sensitized Solar Cells

안보은 강순형*

전남대학교 화학교육과

Bo Eun Ahn and Soon Hyung Kang*Department of Chemistry Education, Chonnam National University, Gwangju 500-757, KoreaE-mail address: skang@jnu.ac.krDye-sensitized solar cells (DSSCs) have been widely attracted due to low manufacturing cost, environmental friendliness, and high efficiency. However, there are still several drawbacks to attain the conversion efficiency above 15 % for the commercialization. In particular, in the photoanode comprised of TiO₂ nanoparticles, the trap-limited diffusion process leads to the high charge recombination with a reduction of electron collection efficiency, even though it shows large surface area ensuring a high dye loading for light harvesting. One-dimensional TiO₂ nanotube (TONT) with three different thicknesses (10, 18, 28 μm) prepared by electrochemical one-step anodization in 0.25 wt% NH₄F of ethylene glycol was suggested to overcome this problem. Herein, the overcoating of TiO₂ nanoparticle was introduced to support the surface area because nanotubular structure has low surface area resulted from large inner diameter (approx. 100 nm) of nanotube. This bilayered TiO₂ nanotube/nanoparticle film was characterized by XRD, FE-SEM, and J-V analysis.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1202**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of WO₃ Nanorods onto Carbon Cloth by Hydrothermal Method and Its Application for Photoelectrochemical Devices

김윤옥 강순형*

전남대학교 화학교육과

Metal oxides such as TiO₂, WO₃, ZnO, SnO₂ etc. have widely investigated because of low cost, environmental friendliness, and the application to various energy related devices. In particular, WO₃ having the energetic band gap of 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 photoresonance in the strong acidic condition. Accordingly, we prepared the WO₃ nanorods(NRs) on the carbon cloth substrates by hydrothermal method. The morphological and crystalline properties of as-synthesized WO₃ NRs were confirmed by a field emission scanning electron microscope and a X-ray diffraction. In particular, A length of approximately 1 μm and a diameter of about 250 nm were obtained with the hexagonal structure. Based on these analyses, WO₃ NRs based photoelectrochemical devices would be developed and their photoelectrochemical behavior would be assessed.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1203**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ruthenium Bipyridyl-sensitized Photocatalytic Reduction of CO₂ : the Role of Ruthenium bipyridyl-Nafion Cluster

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Successful photosynthetic conversion of CO₂ to CO was achieved using Ru(bpy)₃²⁺-sensitized Re(bpy)(CO)₃Cl/Nafion system (bpy = 2,2'-bipyridine) under visible light irradiation. The molecular Re(I) catalyst was able to photo-reduce CO₂ moderately using triethanolamine (TEOA) as an electron donor (in DMF solvent) in the presence of Ru(bpy)₃²⁺ sensitizer (quantum yield of 0.09). However, the addition of nafion to the Re(I)/Ru(bpy)₃²⁺/DMF/TEOA system enhanced the photo-conversion rate (quantum yield of 0.13). Control experiments using monochromatic light irradiation revealed that photo-excitation of Ru(bpy)₃²⁺ initiated the CO₂ reduction process on the Re(I) center. The selective quenching of Ru(bpy)₃²⁺ photoluminescence by Re(I) complex further confirmed that electron transfer from Ru-to-bpy charge transfer excited state is responsible for CO₂ reduction. In the presence of Nafion, about 10% of Ru(bpy)₃²⁺ is immobilized in the polymer structure and provides heterogeneity to the system exhibiting enhanced CO₂ reduction efficiency compared to the homogenous Re(I) catalytic system. The lifetime of excited Ru(bpy)₃²⁺ is expanded with the existence of Ru(bpy)₃²⁺-Nafion cluster, which encourage the collision of Re(I) catalyst and sensitizer as well.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1204

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Variation of hydrogen gas and distribution of products in the reductive dechlorination of tetrachloroethylene by Ni-Pd/hematite catalysts

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한국과학기술원(KAIST) 건설 및 환경공학과

This study was conducted to investigate the variation of hydrogen gas and distribution of products in the reductive degradation of tetrachloroethylene (PCE) by bimetallic catalysts. Bimetallic catalyst was applied to effectively degrade PCE, one of the recalcitrant toxic contaminants. We used Ni as a second metal and Pd as a noble metal to synthesize bimetallic catalysts with hematite as a support material. Reductive dechlorination of PCE by bimetallic catalysts was observed in closed batch reactors containing certain contents of noble metal and second metal with hematite in pH 7 MOPS buffer solution (30 mM) under 4% H₂/96% N₂ condition. Both metals in the catalyst were reduced by using sodium borohydride. PCE removal in Pd(3%)/hematite catalyst was highest (100%) in 6 hr, while the removal efficiencies were in the order of Ni(10%)-Pd(3%)/hematite > Pd(1%)/Hematite > Ni(10%)/hematite > Ni(5%)/hematite. The concentration of hydrogen gas in the reaction system decreased when only Pd was used to synthesize bimetallic catalyst. As the concentration of Pd increased, decrease in the concentration of hydrogen gas increased as well. From the by-products study, chlorinated products such as TCE, 1,1-DCE, cis-1,2-DCE, trans-1,2-DCE, and VC were not observed in this reaction system. Instead, the formation of other products from PCE by Ni-Pd/hematite were in the order of acetylene ethane ≥ ethylene. Acetylene was transformed to 19% in 6 hr, compared to the initial concentration of PCE. The results obtained in this study can be used to provide basic knowledge to understand reductive dechlorination of chlorinated organics by bimetallic catalyst and to establish optimal composition of the bimetallic catalyst to treat the contaminant in soil and groundwater.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1205

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Continuous nitrate reduction by bimetallic Pd-Cu/nZVI catalyst

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The continuous nitrate reduction was investigated by bimetallic Pd-Cu/nZVI catalyst to develop a durable and stable treatment system for continuous catalytic nitrate reduction with high removal efficiency. Pd-Cu/nZVI catalyst was synthesized with impregnation method by addition of Cu (2.0 wt.%) and Pd (0.5 wt.%) precursor solutions. The final solution was filtered in an anaerobic chamber and vacuum dried for 24 h. The purged nitrate solution (30 mg/L as NO₃-N) was continuously added to a reactor with a constant hydraulic retention time (2 h) and the catalytic denitrification was initiated by the injection of the prepared catalyst (0.2 g). A remarkable nitrate removal (above 90%) was maintained for 9 h with Pd-Cu/nZVI, while a significant decrease in the removal efficiency (85 to 0%) was observed with nZVI only. Additionally, Pd-Cu/nZVI catalyst showed the high removal efficiency (over 70%) until 20 h.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1206

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bifunctional TiCl₄ Treatment in CdSe Quantum Dots Sensitized TiO₂ Microrods for Photoelectrochemical Water Splitting

강순형

전남대학교 화학교육과

Since Fujishima and Honda first adapted titanium dioxide (TiO₂) semiconductor as a photoanode for a solar light-driven water splitting cell, considerable attention has been focused on enhancing the photoelectrochemical (PEC) conversion efficiency [1]. Generally, TiO₂ has been regarded as one of the most promising materials due to its excellent photocatalytic activity, low cost, and chemical stability [2]. However, the energy band-gap of TiO₂ is too large to allow for efficient visible-light absorption. Thus, advancing the visible light harvesting ability of TiO₂ has been considered a key issue. One of challenging works, the sensitization of TiO₂ with quantum dots (QDs) was performed with the TiCl₄ treatment showing the bifunctional effects. At first, TiO₂ microrods (TOMRs) were synthesized using a facile hydrothermal method and subsequently surface-treated with TiCl₄ solution at different concentrations. CdSe QDs were assembled on the TiO₂ films as a sensitizer to improve the light harvesting efficiency in visible light, because the TiO₂ absorbs only UV light. As the concentration of TiCl₄ solution to 200 mM was increased, the surface coverage of anatase TiO₂ nanoparticles and the loading of CdSe QDs also increased. Furthermore, the anatase TiO₂ between the rutile TOMR and the CdSe QD facilitates the charge separation, which suppresses the charge recombination. Due to these beneficial effects, the photoelectrochemical performance was significantly enhanced with the increased TiCl₄ concentration. References[1] Fujishima A, Honda K. Nature 1972; 238: 37-39.[2] Kang S H, Lim J -W, Kim H S, Kim J -Y, Sung Y -E. Chem. Mater 2009; 21: 2777-2788.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1207**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

CO Oxidation performances of Au/Ag-CeO₂ catalysts

나율이 박요한 손영구*

영남대학교 화학과

Au and Ag-coped CeO₂ were prepared by a facial hydrothermal method. Their fundamental properties were first examined by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis absorption (UV-Vis) and BET surface area measurements. Catalytic activities of the materials were further tested by temperature programmed hydrogen reduction and CO oxidation reaction mass spectrometry. We found that the CO oxidation activity was significantly determined by the relative amounts of the two codoped metals.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1208**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

CO and Ethanol oxidations of CeO₂ particles, cubes and wires

박요한 손영구*

영남대학교 화학과

CeO₂ particles, cubes and wires were prepared by coprecipitation and hydrothermal methods, and examined by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis absorption (UV-Vis), X-ray photoelectron spectroscopy (XPS), FT-IR and BET surface area measurements. CO oxidation activity was tested by temperature programmed mass spectrometry. Ethanol oxidation was also examined by UV-Vis absorption spectroscopy.

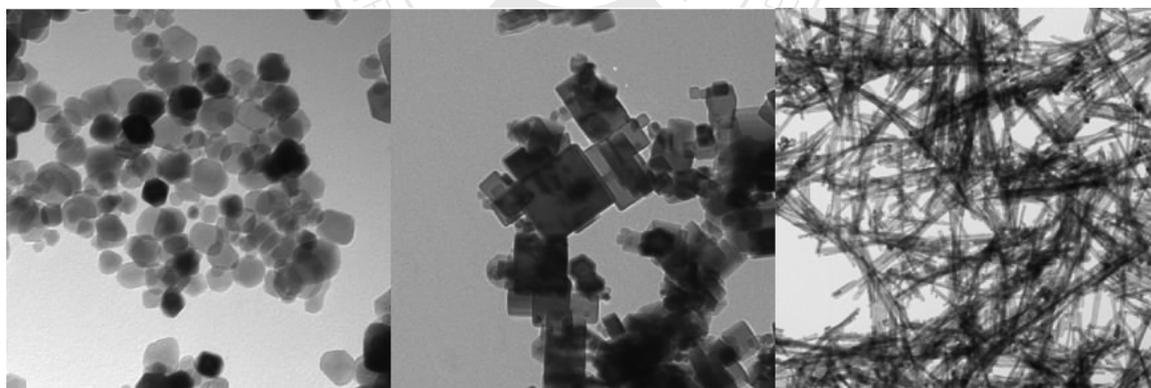


Figure. TEM images of particles, cubes and wires

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: **ENVR.P-1209**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inverse Opal SnO₂ based sensitized solar cells

윤건 강순형*

전남대학교 화학교육과

Nowadays, the exploration of new photo electrode architectures to improve the light-harvesting and charge-collection properties of sensitized solar cells and related devices has been regarded as a challenging work. Here, we demonstrate the synthesis of the inverse opal SnO₂ film for sensitized solar cells by gravimetric sedimentation method, subsequently followed by the spin-coating or drop casting method. Using 430 nm poly styrene (PS) beads, we synthesized the 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. Based on these results, SnO₂ inverse opal film was applied to sensitized solar cell to identify their unique properties and evaluated exploring the photocurrent-voltage measurement.

일시: 2013년 10월 16~18일(수~금) 3일간

장소: 창원CECO

발표코드: ENVR.P-1210

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Reductive Degradation of Tetrachloroethylene (PCE) by Nickel-Palladium Nanoparticles *via* Pulsed Laser Ablation in Liquid

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경상대학교 화학과

Tetrachloroethylene (also known as perchloroethylene, PCE) is a common groundwater contaminant, due to its common use as a dry-cleaning solvent. Current treatment methods are limited in their ability to remove PCE from contaminated sites in an efficient and cost effective manner. Nickel and nickel oxide 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 (1064 nm, 10 Hz, 7 ns) is used to produce the nickel and nickel oxide nanoparticles in deionized water and methanol. The morphological properties and phase identification of the nickel and nickel oxide nanoparticles were characterized by field emission scanning electronic microscope (FE-SEM) and X-ray diffraction (XRD). Synthesized palladium/nickel (Pd/Fe) bimetallic nanoparticles were applied to the degradation of PCE under various experimental conditions. Rapid catalytic degradation of PCE suggests that the nickel nanoparticles prepared in this work can be used for remediation of polychlorinated compounds in polluted environments.

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발표코드: **ENVR.P-1211**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced dechlorination of m-dichlorobenzene using Fe/Pd/C nanoparticles

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Chlorinated organic compounds (COCs) are widespread environmental contaminants found both in ground water and soil. Disposal of chlorinated organic wastes in such a way as to minimize the environmental hazards has become an urgent issue nowadays. Synthesis and use of reactive Fe particles have shown significant environmental implications for the remediation of groundwater and sediment contaminated with COCs. Among COCs, m-Dichlorobenzene cannot be easily and effectively decomposed with currently available biological and chemical treatment methods. The good of this work is a development of an effective dechlorination of COCs using Fe/C nanoparticles produced via a pulsed laser ablation in liquid (PLAL). The present work presents a relatively simple method to fabricate Fe nanoparticles for the dechlorination of m-dichlorobenze. Fe nanoparticles were produced by laser ablating onto an Fe plate immersed in deionized water with a reducing agent, ascorbic acid. Rapid dechlorination of m-dichlorobenze suggests that Fe/Pd/C bimetallic nanoparticles can be used for remediation of m-dichlorobenzene in polluted environments.

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발표코드: **ENVR.P-1212**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

A facile method for preparation of metal and non-metal co-doped TiO₂ nanoparticles by TiCl₄ solution sol-gel process

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계명대학교 화학과

Titanium dioxide (TiO₂), which was doped with different metal ions and Nitrogen co-doped TiO₂ nanoparticles were prepared by standard sol-gel methods. Nitrogen doped TiO₂ nanoparticles were successfully prepared by the addition of ammonia water. Metal doped TiO₂ nanoparticles were prepared by using metal sources (i.e., SnCl₂, NiCl₂, and ZnCl₂). The resulting materials were characterized by X-ray diffraction (XRD), Transmission electron microscopy (TEM), X-ray photoelectron spectroscopy(XPS) and BET surface area measurement. XRD results showed that metal and non-metal co-doped TiO₂ nanoparticles into anatase phase and Zn, N co-doped TiO₂ nanoparticles BET surface area was 133 m²/g.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of metal/nonmetal-doped TiO₂ Photoelectrode for Dye-Sensitized Solar Cells Application

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Metal/nonmetal-doped TiO₂ nanoparticles were synthesized through the hydrolysis of TiCl₄. For comparison, pure TiO₂ nanoparticles were synthesized using the same technique. The synthesized Metal/nonmetal-doped TiO₂ were characterized by X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy, UV-vis diffuse reflectance spectroscopy, and N₂ sorption techniques. To prepare the metal/nonmetal-doped TiO₂ electrode, transparent films were fabricated using metal/nonmetal-doped TiO₂ paste onto glass substrate coated with transparent conductive oxide (FTO) by the doctor-blade method. For comparison, the pure TiO₂ electrode was fabricated using pure TiO₂ paste, respectively. Consequently, we obtained the energy conversion efficiency of the DSSCs based on the metal/nonmetal-doped TiO₂ electrode is higher than that of the DSSCs based on pure TiO₂ electrode. The DSSCs based on the metal/nonmetal-doped TiO₂ electrode improved V_{oc}, J_{sc}, and η, as compared to the pure TiO₂ electrode.

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발표코드: **ENVR.P-1214**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of hydrophilic/hydrophobic functional groups with silica mesoporous by controlled concentration of silica and surfactant

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Hydrophilic/hydrophobic functional groups with silica mesoporous was prepared by sol-gel method. This method is using tri-block copolymer surfactant and CTACl as a template. Preparation of silica mesoporous was by adjusting the molar ratio of the silica and surfactant. The preparation of hydrophilic/hydrophobic functionalized silica mesoporous was characterized by Brunauer-Emmett-Teller (BET) method, Transmission electron microscopy (TEM) and FT-IR.

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발표코드: **ENVR.P-1215**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of High Efficiency Dssc with Reduced TiO₂ Nanoparticles

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We report a simple one-step chemical method to fabricate partially reduced TiO₂ (TiO_{2-x}) nanoparticles for the photoanode of dye sensitized solar cell (DSSC). The reduced TiO₂ which has oxygen vacancy or Ti³⁺ on the surface was synthesized by treating 0.1M NaBH₄. Oxygen vacancy enhances the electrical conductivity which increases charge transportation and reduces the band gap from UV region to visible light region. The shifted conduction band of TiO₂ increases the open-circuit voltage (V_{oc}), the difference between the energy potential of conduction band of TiO₂ and redox potential of iodide/tri-iodide. The DSSC fabricated with reduced TiO₂ NPs showed not only increased current density (J_{sc}) but also enhanced open-circuit voltage (V_{oc}), leading to great enhancement in the cell efficiency.

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발표코드: ENVR.P-1216

발표분야: 환경에너지

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Enhanced Release of Bioavailable Iron in Ice

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Iron is a crucial but limiting micronutrient for the growth and metabolism of marine organisms. The main source of bioavailable iron is through the chemical and physical reactions of iron containing Aeolian dust particles in the atmosphere. Dust aerosols has been reported to be one of the most efficient ice nuclei and for such reason there is a great possibility that atmospheric iron could be trapped in tropospheric ice. In this work, we investigated the unique chemical and physical reactions of iron oxide in ice related to its production of bioavailable iron. In the dark condition, the release of bioavailable iron was significantly enhanced in the ice phase in the presence of various organic ligands. In comparison, dissolution of iron from iron oxide in the aqueous phase was negligible even in low pH environment. This unique phenomenon in the ice phase can be explained by the 'freeze concentration effect'. When solutions are frozen, ice crystal forms and solutes, dissolved gases, and protons are concentrated in the quasi liquid region present between crystals. Due to such characteristic condition, many chemical reactions can be different in the ice phase compared to the aqueous counterpart. Therefore, the enhanced release of dissolved iron in the ice phase might suggest a crucial pathway of providing bioavailable iron to the ocean. References 1. Kim, K.; Choi, W.; Hoffmann, M. R.; Yoon, H.-I.; Park, B.-K. Environ. Sci. Technol. 2010, 44, 4142-4148. 2. Jeong, D.; Kim, K.; Choi, W. Atmos. Chem. Phys. 2012, 12, 11125-11133. 3. Kim, K.; Yoon, H.-I.; Choi, W. Environ. Sci. Technol. 2012, 46, 13160-13166. 4. Kim, K.; Choi, W. Environ. Sci. Technol. 2011, 45, 2202-2208.

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발표코드: **ENVR.P-1217**

발표분야: 환경에너지

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Preliminary Testing of MIRAN SapphIRe Portable Ambient Air Analyzers against a Chemical Simulant, Methyl Salicylate

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When we encounter a contaminated or potentially contaminated area with chemical warfare (CW) agents, we must survey the area for the presence of toxic or explosive vapors to respond immediate danger. However, the vapor detectors commonly used are not designed to detect and identify CW agents on the spot. Indeed, little data are available concerning the ability of these commonly used, commercially available detection devices to detect CW agents. Here we try to test the capabilities of Miniature Infra-Red Gas Analyzer (MIRAN) SapphIRe Portable Ambient Air Analyzer to detect chemical warfare agent vapors when it is released. In this test, we used a chemical simulant, methyl salicylate (MeS) instead of live CW agents. Results of MeS to the MIRAN were consistent and reliable when above the minimum detectable levels in the laboratory environment although the MIRAN detectors are not sensitive enough to provide sufficient warning for the safety of first responders.

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발표코드: **ENVR.P-1218**

발표분야: 환경에너지

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Characteristics of recovered ITO and glass substrate from discarded TFT-LCD

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성균관대학교 화학과

Indium tin oxide (ITO) has been widely used in transparent conductive electrode for display. Furthermore, glass substrate is considered as an important material because it takes about 8% of total price of TFT-LCD panel. In this study, our interests were focused on the recovery of ITO and glass substrate from discarded display. Recovery of ITO was done by electrochemical methods mainly chronopotentiometry. After removing of ITO, upper layer of the TFT-LCD did not show any electrical conduction. The color filter and black matrix were removed from TFT-LCD by using acid remover. Optical transmittance of recovered glass substrate was about 90% at 380nm to 770nm. Analysis of the ITO was done by using X-ray photoelectron spectroscopy (XPS), Energy dispersive x-ray spectroscopy (EDX) and Inductive coupled plasma (ICP) and Scanning microscope (SEM). 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 Knowledge Economy (No.2010501010002B)

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Synthesizing colloidal stable zero-valent iron nanoparticles with polymers for rapid nitrate reduction

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This study examines the effect of 2 common polymers on the size, zeta potential, colloidal stability and their reactivity to nitrate reduction of zero valent iron (nZVI). The polymers are poly(1-vinylpyrrolidone-co-vinyl acetate)(PVPVA) and polyethylene glycol(PEG) known as biodegradable and non-toxic materials. Pre-grafting method, synthesizing nZVI by sodium borohydride reduction of iron and polymer mixture solution, is applied and investigated. PVPVA and PEG coated nZVIs are dispersed and stable than bare nZVI and PVPVA is more stable than PEG because of difference in molecular weight and length of structure. Both synthesized nZVIs have ability to reduce nitrate into ammonium with 86.89 % maximum nitrate removal efficiency. However surplus coating materials on the surface inhibit the contact of nitrate since limited surface of nZVIs. These results could be implacable for in-situ nitrate remediation by injecting polymer-stabilized nZVI coated by PVPVA and PEG.