일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PLEN-1**

발표분야: 기조강연

발표종류: 특별강연, 발표일시: 목 13:30, 좌장: 박승범

Materials for Bio-Integrated Electronics

John A. Rogers

Department of Materials Science and Engineering, University of Illinois

Biology is curved, soft and elastic; silicon wafers are not. Semiconductor technologies that can bridge this gap in form and mechanics will create new opportunities in devices that adopt biologically inspired designs or require intimate integration with the human body. This talk describes the development of ideas for electronics that offer the performance of state-of-the-art, wafer-based systems but with the mechanical properties of a rubber band. We explain the underlying materials science and mechanics of these approaches, and illustrate their use in bio-integrated, 'tissue-like' electronics with unique capabilities in cardiac electrophysiology, brain-machine interfaces, and continuous health/wellness monitors. Demonstrations in humans and live animal models illustrate the functionality offered by these technologies, and suggest several clinically relevant applications.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 이인수

Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry

남원우

이화여대 화학과

Dioxygen is essential in life processes, and enzymes activate dioxygen to carry out a variety of biological reactions. One primary goal in biomimetic research is to elucidate structures of reactive intermediates and mechanistic details of dioxygen activation and oxygenation reactions occurring at the active sites of enzymes, by utilizing synthetic metal-oxygen complexes. A growing class of metal-oxygen complexes, such as metal?superoxo, ?peroxo, ?hydroperoxo, and ?oxo species, have been isolated, characterized spectroscopically, and investigated in various oxygenation reactions. During the past decade, we have been studying the chemical and physical properties of various reactive intermediates in oxygenation reactions, such as high-valent iron(IV)- and manganes(V)-oxo complexes of heme and non-heme ligands in oxo-transfer and C-H activation reactions, non-heme metal-peroxo complexes in nucleophilic reactions, and non-heme metal-superoxo complexes in electrophilic reactions. The effects of supporting and axial ligands on structural and spectroscopic properties and reactivities of metal-oxygen adducts have been extensively investigated as well. In this presentation, I will present our recent results on the reactivities of various metal-oxygen intermediates in electrophilic and nucleophilic oxidation reactions. The synthesis and structural and spectroscopic characterization of mononuclear nonheme metal-dioxygen intermediates will be discussed as well.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-1**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 황도훈

Charge transport in high mobility-solution processed semiconductors

정대성

동아대 화학공학과

Recently there have been many solution processable semiconductors with high charge carrier mobility, including acene-based oligomers, thiophene-based polymers and inorganic nanocrystals. Under the specific optimization in molecular design and/or device processing condition, these semiconductors are now routinely showing charge carrier mobility exceeding 1 cm2/Vs, which is comparable to a-Si. In the case of molecular acene derivatives, which have been developed and studied for more than five years, there are many reports on the systematic analysis of their charge transport behavior. On the other hand, there are only limited number of reports on charge transport studies of high mobility polymers and nanocrystals due to their relatively brief history. At this time, therefore, it would be interesting to do systematic studies on charge transport mechanisms of these brand-new semiconductors. Here I present two solution processable semiconductors ?polymer and nanocrystal- with exceptionally high charge carrier mobility. The origin of their high mobility is discussed combined with various two/three terminal electronic experiments as a function of incident light and temperature.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-2**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 황도훈

Molecular Engineering of Organic Dyes for Dye-Sensitized Solar Cells

권태혁 Torben Daeneke[1] Udo Bach[1] Leone Spiccia[1] Andrew B Holmes[2]

울산과학기술대 친환경에너지 공학부 [1]Monash University [2]Melbourne University

Recently, organic DSCs have received considerable attention as they offer design flexibility, high molar extinction coefficients of dyes, and the potentially low cost of fabrication compared with those based on ruthenium dye sensitizers. However, DSCs require new dye molecule design and device architecture concepts to achieve new record energy conversion efficiencies and then to realize commercial products. To achieve this aim, molecular design strategy is quite important. Also, the traditional iodine/triiodide electrolyte system has a number of significant problems such as health hazards, volatile solvents, corrosive properties and very complex redox chemistry that need to be removed if the technology is to be commercialised. To solve these problems, unique donor-acceptor organic dyes were developed with a new electrolyte system and showed very promising results in organic DSC devices.[1,2] In particular, one of those developed dyes (TH-D3), in organic DSC devices exhibits over 7.5% photo conversion efficiency (PCE)[1] with a ferrocene/ferrocenium electrolyte (Fc) system while devices with the traditional iodine/triiodide electrolyte achieved 6.1% PCE.[1]Reference(1) Daeneke, T.; Kwon, T.-H.; Holmes, A. B.; Duffy, N. W.; Bach, U.; Spiccia, L. Nat. Chem. 2011, 3, 211.(2) Kwon, T.-H.; Armel, V.; Nattestad, A.; MacFarlanem, D. R.; Bach, U.; Lind, S. J.; Gordon, K. C.; Tang, W.; Jones, D. J.; Holmes, A. B. J. Org. Chem. 2011, 76, 4088.

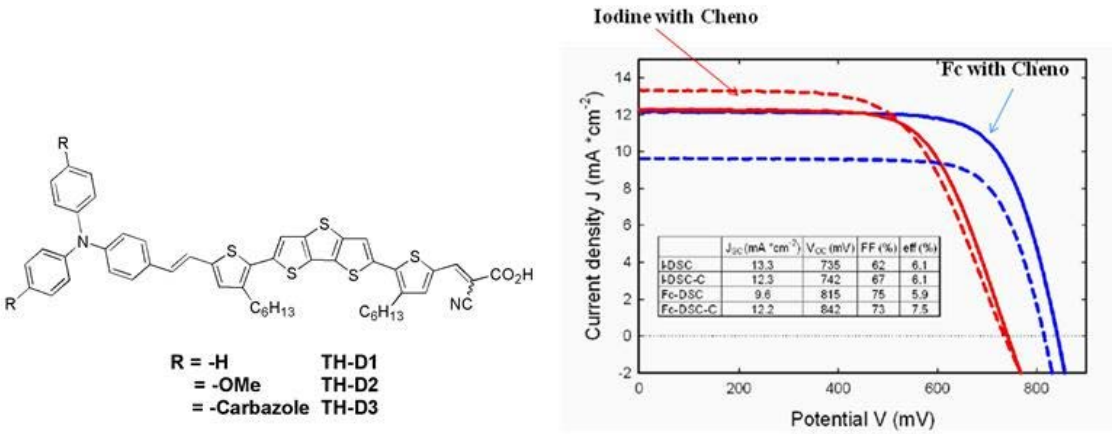

Figure 1. Structure of developed organic dyes and I-V curves (TH-D3 with Fc vs Iodine).

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THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-3**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 황도훈

Conjugated Oligomers and Polymers for Molecular and Organic Electronics

이윤구

대구경북과학기술원 에너지시스템공학전공

Conjugated organic molecules have been used as key materials for a variety of optoelectronic devices such as organic light-emitting diodes(OLEDs), organic thin film transistors(OTFTs), and organic photovoltaic devices(OPVs). Recently, organic photovoltaic devices have attracted much attention owing to their potential cost-effectiveness of light-weight and flexible solar cells. So far, a power conversion efficiency of ~5% has been obtained in OPVs using P3HT and PCBM. To achieve high power conversion efficiency in OPVs, it is necessary to develop new electron-donor polymers which possess several characteristics such as harvesting photons in a wide range of spectrum, efficient exciton dissociation, high hole mobility, suitable HOMO and LUMO energy levels, and good miscibility with the electron-acceptor materials. In this talk, I will present results in studies of conjugated p-n junction oligomers for nano-scale solar cells and low bandgap polymers for bulk-heterojunction solar cells.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-4**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 진영읍

Polymer transistors for sensor applications

정병준

서울시립대 신소재공학과

Semiconducting polymers have been intensively developed for flexible and/or printable electronics such as organic light emitting diodes (OLED), organic photovoltaic devices (OPV) and organic thin films transistors (OTFT). The polymers for OTFTs have been designed and synthesized for catching up the mobility of a-Si TFTs toward display applications. The electronic properties of the synthetic π-conjugated polymers can be tuned via chemical synthesis. It allows organic thin film devices having proper degrees of sensitivity, selectivity and stability for the target chemicals. Therefore, the low-cost sensor application will be one of the promising areas for semiconducting polymers. In this presentation, the sensing responses to various analytes in polymer transistors will be described and the sensing mechanism will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-5**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 진영읍

Organometallic Catalysis for Controlled Olefin Polymerization and Oligomerization

손경선

충남대 화학과

Organometallic catalysis for polyolefin synthesis via coordination polymerization will be discussed in the 1st part. To develop a novel titanocene catalyst for efficient ethylene-styrene (ES) copolymerization at high temperature, which is compatible with most commercial processes, titancenes containing a pendant amine donor were prepared and their catalytic activities were investigated for the copolymerization of ethylene and styrene at 120 °C. In the 2nd part of the talk, selective oligomerization of ethylene to 1-hexene or 1-octene will be presented, focusing on the intermediacy of metallacycles that could provide an opportunity to generate new classes of functionalized ethylene oligomers by chain transfer to a transmetalation reagent.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY1-6**

발표분야: New Trends in Polymer Chemistry: Young Polymer Chemist Symposium

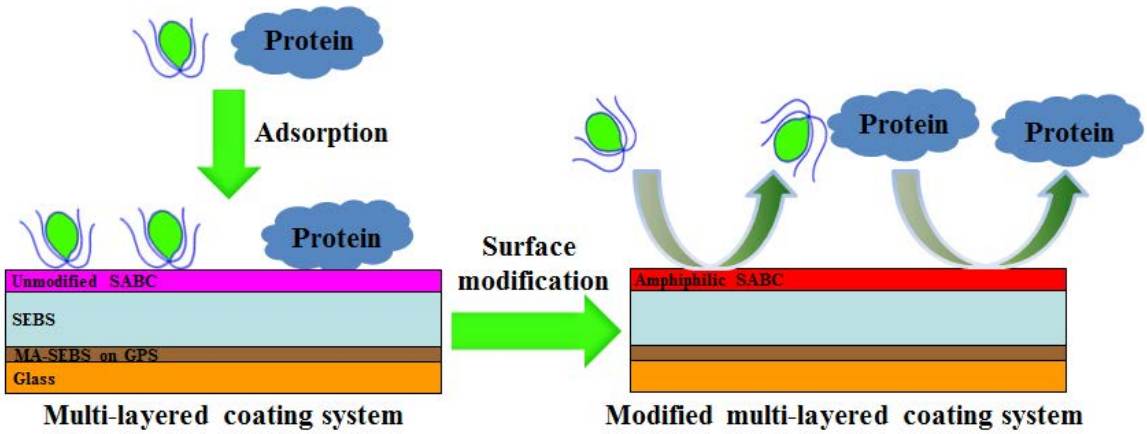
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 진영읍

Amphiphilic surface active block copolymers for antifouling and fouling-release applications

조영진

KIST 생체재료연구단

Antifouling surfaces are critical for the good performance of functional materials in various applications including marine industry, medical implants, biosensors, food packing, protective clothes, and water filtration. The surfaces derived from surface active block copolymers (SABC) having a combination of hydrophobic aliphatic (linear hydrocarbon or propylene oxide derived groups) and hydrophilic PEG side chains have been developed. The surfaces demonstrate superior performance against protein adsorption as well as resistance to biofouling, providing an alternative to coatings containing fluorinated side chains as the hydrophobe, thus reducing potential environmental impact. The surfaces were examined using dynamic water contact angle, captive air-bubble contact angle, atomic force microscopy, X-ray photoelectron spectroscopy and near edge X-ray absorption fine structure analysis. The PS8K-b-P(E/B)25K-b-PI10K triblock copolymer precursor (K3) initially dominated the dry surface. In contrast to previous studies with mixed fluorinated/PEG surfaces, these new materials displayed significant surface changes after exposure to water that enabled fouling resistant behavior. PEG groups buried several nanometers below the surface in the dry state were able to occupy the coating surface after placement in water. The resulting surface exhibits a very low contact angle and good antifouling properties that are very different from K3. The surfaces are strongly resistant to protein adsorption using bovine serum albumin (BSA) as a standard protein challenge. Biofouling assays with sporelings of the green alga Ulva and cells of the diatom Navicula showed adhesion was significantly reduced relative to a PDMS standard as well as to the triblock copolymer precursor of the SABCs.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY2-1**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 박지웅

Toward Generalized Protocols for the Design and Fabrication of Hybrid Plasmonic and Carbonaceous Nanostructures: From Energy, Environment to Optical Biosensing

김동하

이화여대 화학나노과학과

In the Polymer Nanohybrid Materials at Ewha Womans University, a comprehensive approach for the design and synthesis of multifunctional hybrid nanomaterials has been systematically performed to seek their potential applications as key elements in green nanotechnology. Representative areas of interest include energy conversion and storage devices, environmental remediation, biosensing, light-emission, and memory devices. Of the numerous methodologies to achieve these goals, we actively utilize self-assembly processes to construct well-defined hybrid nanoscopic objects suitable for target-oriented applications. Recently, we also pay special attention to surface plasmons as a versatile platform based on which enhanced or tailored properties can be obtained by integrating plasmonic nanostructures into the elements of photovoltaic devices, photocatalysts, optical biosensors, and light-emitting materials. In this talk, I'll introduce recent research activities that have been performed in my research lab with a special focus on the synthesis and applications of active nanomaterials for highly selective/sensitive optical biosensing, visible light active photocatalysis and dye-sensitized solar cells.References1. Y. Wang, et al., Nano Lett. 2009, 9(6), 2384-2389.2. Y. H. Jang, et al., Chem-Eur. J. 2011, 17(7), 2068-2076 (Inside cover article).3. S. T. Kochuveedu, et al., Green Chem. 2011, 13(12), 3397-3405.4. Y. J. Jang, et al., Chem. Commun. 2012, 48(4), 507-509 (Back cover article).5. Y. H. Jang, et al., Nano Lett. 2012, 12(1), 479-485.6. W. J. Lee, et al., ACS Nano 2012, 6(1), 935-943.7. S. T. Kochuveedu, et al., J. Phys. Chem. C 2012, 116(3), 2500-2506.8. D. Li, et al., Small 2012, 8(9), 1442-1448.9. Ji-Eun Lee, et al., Anal. Chem. 2012, 84(15), 6494-6500.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY2-2**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이형일

Tunable Nanotubes and Nanoparticles for Advanced Technology

김철희

인하대 고분자공학과

We report unique methodologies for the construction of supramolecular fluorescent nanotubes and mechanized nanoparticles of which the surface is covered with cyclodextrins (CDs). Their sensory, delivery, and imaging characteristics will be discussed. Recently, we have developed dendron-cyclodextrin nanotubes of which the properties can be precisely tuned, so that they can serve as an efficient sensory platform for proteins, carbohydrates, and metal ions. In addition, CD-based hybrid nanoparticles have been developed for tuning the delivery and imaging properties.

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장소: 부산BEXCO

발표코드: **POLY2-3**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이형일

Synthesis, self-assembly, and bioapplications of cyclic block copolypeptides

임용범 한상헌 김보람

연세대 신소재공학과

Macromolecules that have cyclic structures (macrocycles) are interesting molecules not just because they do not have chain ends but because their topological features can significantly affect their chemical, physical, and biological properties. Macrocycles can more effectively maintain rigid and conformationally constrained structures than their linear counterparts. Meanwhile, self-assembled peptide nanostructures (SPNs) hold great potential as promising biomaterials that can mimic functions of natural proteins or biological nanostructures. By contrast with proteins that consist of very large polypeptide chains with hundreds or more amino acids, SPNs are composed of peptides, relatively small biomacromolecules with less than 50 amino acids in size. When appropriately designed, either as pure peptide molecules or as peptides conjugated to other types of molecules, peptides can be made to self-assemble thereby creating SPNs. Self-assembling peptide nanostructures can mimic or displace the diverse biological functions of natural proteins or organelles with enhanced properties or with functions unprecedented in nature. The precise control of two- and three-dimensional structures is crucial for constructing advanced functional materials of SPNs. Here, I present our recent studies on self-assembling cyclic block copolypeptides.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY2-4**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 이형일

Self-Assembly of Dendritic-Linear Amphiphilic Diblock Copolymers with Fixed Molecular Weight and Block Ratio

김경택

울산과학기술대 나노생명화학공학부

Self-assembly of block copolymers in solution has been a facile way to create a variety of nanostructures. So far, the common strategy to create self-assembled structures of a block copolymer with a preferred morphology has been to control the molecular weight of both the hydrophilic and hydrophoic blocks so that the ratio between two blocks lies in the region where the close packing of the block copolymer prefers a desired geometry. Although this strategy, drawn from the analogy to the packing factor theory of amphiphiles, has proven to be effective, the flexible conformation of linear block copolymers partly limits a through assessment and exploration of the structure-property relationship with respect to self-assembly.We describe a new design concept to synthesize amphiphilic block copolymers to rationally control the topology and morphology of the self-assembled structure. Our design involves a hydrophilic block constructed on a dendritic scaffold for which the number of the peripheral hydrophilic chains can be precisely controlled while the overall molecular weight of the hydrophilic segment is unchanged by matching the molecular weight of individual peripheral chains. This enables us to induce a change in the molecular packing geometry at the interface of the hydrophobic core of the micelle without significantly altering the weight ration between two blocks. As a result, we specifically induce a topological change in micelles and bilayer structures, of which the morphology is dictated by the weight ratio between two polymer blocks. We will show the examples of topological transitions of micelles and vesicles to form new nanostructured materials, which is caused by differences in the steric effect on the corona of the micelles and bilayers.

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장소: 부산BEXCO

발표코드: **POLY2-5**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 김경택

Self-Assembly of Well-Defined Poly(arylene ether sulfone)s Synthesized by Chain Growth Condensation Polymerization

김상율

KAIST 화학과

Well-defined poly(arylene ether sulfone)s containing pyrene and amide moieties were synthesized by chain-growth condensation polymerization. Self-assembly behavior of theses polymers depended strongly on the structural motifs and the polymeric architecture. Interestingly, fan-shaped polymers showed two different gelation-induced fluorescence switching modes. The gel formed from the THF solution exhibited excimer emission due to dimerization of the pyrene groups inside the fibrous structure. In contrast, emission due to the pyrene excimer was quenched after gelation in MC as a result of stacking among the pyrene groups, facilitated by strong intermolecular hydrogen bonds among the amide groups.

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장소: 부산BEXCO

발표코드: **POLY2-6**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 김경택

Synthesis of Bipolar Block Copolymers by Living Anionic Polymerization for Electric and Photonic Materials

이재석

광주과학기술원 신소재공학과, PIMS

The functional polymers with controlled molecular weights and molecular weight distributions were synthesized by establishing the conditions (temperature, reaction time, additive, and initiator) of living anionic polymerization of vinyl monomers with hetero atoms (N, O, and S). Under these conditions, living anionic polymerization was carried out to synthesize the well-defined bipolar block copolymers that electron donors/electron acceptors are integrated. Precisely controlled nanostructures of the block copolymers by thermal annealing were used for polymeric electronic devices such as non-volatile polymer memory and polymer light-emitting diodes. In particular, the relationship between the structure of the block copolymers and the device performance will be mainly demonstrated in this presentation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY2-7**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 김경택

Synthesis of Well-defined Methacrylate Block Copolymers and its Blending with PVDF-TrFe for Actuator Application

백경열

KIST 물질구조제어연구단

A series of ABA triblock copolymers of methyl methacralyte (MMA) and dodecyl metharylate (DMA) [poly(MMA-b-DMA-b-MMA)] were synthesized by sequential atom transfer radical polymerization (ATRP) to examine actuation properties as a novel electroactive material. Obtained well-defined triblock copolymers with various molecular weights of the block segments (PDI ≤ 1.2) showed different morphologies from BCC to lamellar structures, which strongly affect the actuation behaviors. Theses relatively polar methacrylate elastomers showed the higher k values and the superior actuation properties in comparison to corresponding SEBS elastomers. In addition, since these PMMA based triblock copolymers can be compatible with PVDF derivates, those block copolymers were then blended with PVDF-TrFe as a softer additive. Well defined morphologies from cylinder to lamella structures were obtained, of which actuation performance increased with increase of the block copolymer.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY2-8**

발표분야: Precise Macromolecular Synthesis for Advanced Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 김경택

Thermoresponsive Fluorinated Polyacrylamides with Low Cytotoxicity

이형일

울산대 화학과

We report the unique thermoresponsive properties of fluorinated polyacrylamides, poly[N-(2,2-difluoroethyl)acrylamide] (P2F). The thermosensitivity of fluorinated polyacrylamides can be easily controlled by changing the number of fluorine atoms in N-ethyl groups. Moreover, we demonstrate that fluorinated polyacrylamides are less cytotoxic than poly(N-isopropylacrylamide) (PNIPAM).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-1**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 강영종

Controlled adsorption of nanoparticles in honeycomb-patterned thermoresponsive poly(N-isopropylamide) hydrogel surface

허도성

인제대 화학과

Here we show a honeycomb-patterned poly(N-isopropylacrylamide) (PNIPAAm) hydrogel film surface that acts as a smart surface in the adsorptivity of nanoparticles by the environmental temperature change, which is fabricated via a facile method using photopolymerization of the pre-gel solution in a honeycomb-patterned polystyrene template film. Adsorptivity of nanoparticles in the thermosensitive PNIPAAm hydrogel surface is controlled by the dynamic change of surface morphology depending on temperature. For the adsorptivity of nanoparticles in the patterned hydrogel surface, silver nanoparticles are immobilized in the hydrogel, and the adsorptivity is obtained by measuring the released concentration of the silver nanoparticles using ultraviolet-visible (UV-vis) spectroscopy in the aqueous solution. The same experimental procedure is conducted for the unpatterned or flat hydrogel film. Delivery of Ag nanoparticles from the PNIPAAm hydrogel surface is higher in the swelled state below the lower critical solution temperature (LCST) than in the shrunken state, in contrast to the bulk hydrogel. Temperature-sensitivity is significantly higher in the honeycomb-patterned hydrogel than in the unpatterned or flat hydrogel. This study suggests a convenient experimental method for studying the phase-transition behavior of stimuli-responsive hydrogel in the solid?water interface.

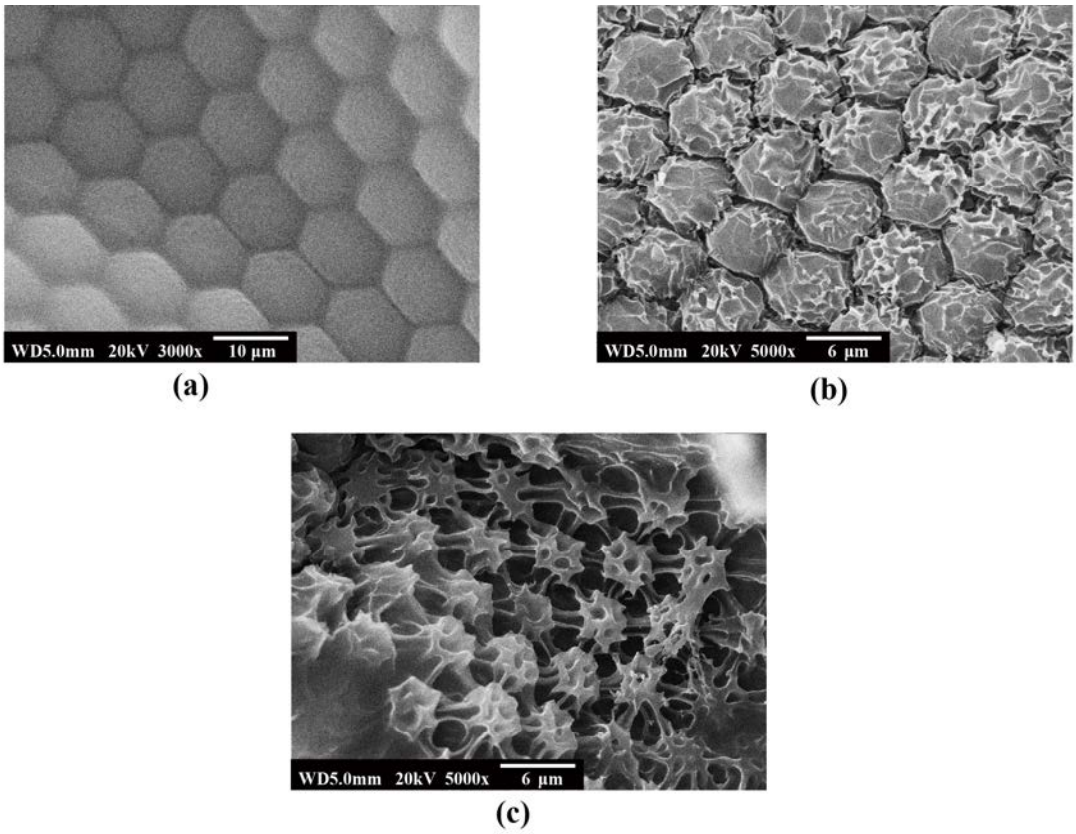

Figure 5. Changes in the surface topography of a PNIPAAm hydrogel filmin response to the temperature change between (a) 27 °C, (b) 32 °C, and (c) 37 °C, as observed by SEM.

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장소: 부산BEXCO

발표코드: **POLY3-2**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 강영종

Electroactive nanostructure polymers for the next generation actuators

구종민

KIST 물질구조제어연구단

Electrostrictive dielectric elastomers have garnered attention as promising candidates for next generation compact actuators, sensors, artificial muscles and micro robotics, owing to their attractive properties such as large electromechanical strain, fast response, high power to mass ratio, facile proccessibility, and affordability. However, unlike other electroactive materials such as carbon nanotubes, ionic polymer-metal composites, and conductive polymers, dielectric elastomers demonstrate large actuation only at high electric fields (above 50 V/mm), thus posing the greatest obstacle for real applications. The present work demonstrates that introduction of dielectric mismatched nanodomains to a dielectric elastomer results in an unexpected ultralarge electrostriction coefficient, enabling a large electromechanical strain response at a low electric field. This strong electrostrictive effect is attributed to the development of an inhomogeneous electric field across the film thickness due to the high density of interfaces between dielectric mismatched periodic nanoscale domains. In addition, it demonstrates that introduction of conducting fillers to a dielectric elastomer helps to reduce the operational voltage. The present work offers a promising pathway to design novel high performance dielectric elastomers as well as to understand the underlying operational mechanism of electroactive nanostructured multiphase electrostrictive systems.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-3**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 10:50, 좌장: 강영종

Molecular Chimeras of Polypeptides Block Synthetic Polymers as a Biocompatible Anticancer Drug Delvery System

김일

부산대 고분자공학과

A potential way of combining advantages of synthetic block copolymers and peptide β-structures lies in the creation of “molecular chimeras” or “hybrids”. These chimeras are potentially attractive in that they might inherit pros of both sides, namely the solubility, melt processability, or rubber elasticity of the synthetic block, and the hierarchical structure formation, mutual recognition, biological activity, or biodegradability from the peptide block. Intrinsically they may stabilize the interface between synthetic polymer systems and biosystems, thus making both sides compatible to each other. We have aimed to develop a new water soluble synthetic polymer block polypeptide bioconjugate hybrid copolymers that respond to both temperature and pH, enhancing drug delivery efficiency for cancer chemotherapy. Only few research activities have been focused on dual stimuli?responsive hybrid block copolymers consisting of pH sensitive polypeptides and thermo?sensitive synthetic polymer segment. The physiologically relevant pH range is from 5.0 to 7.4, if the protonation of polymers only occurs within this pH range, they are suitable for fabricating the pH?responsive hybrid materials for biomedical applications. Most importantly, the fusogenic activity of p(His) can disrupt the enveloped membrane of acidic subcellular compartments such as endosomes, thus resulting in drug/nucleic acids reaching the cytosol to enhance the delivery efficiency. Thus, the polymeric micelle system with a p(His) core or corona could be an effective mode for the controlled drug release.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-4**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 11:15, 좌장: 강영종

Sensor and Actuator Applications of Microporous Conjugated Polymers with Intramolecular Excimer Emission

곽기섭

경북대 공과대학/고분자공학과

Since Prof. Toshio Masuda of Kyoto University for the first time synthesized a representative of diphenylacetylene polymer derivatives, poly[1-phenyl-2-(p-trimethylsilyl)phenylacetylene] [PTMSDPA] in 1991, this polymer has attracted many interests owing to unique properties. This polymer derivative was highly soluble despite of ultra-high molecular weight and, also, showed excellent chemical, physical, mechanical properties. As one of the most interesting features, this polymer emits an intense fluorescence (FL) in a visible region because of the effective exciton confinement within the main chain due to the steric hindrance and/or intramolecular electron interactions of bulky aromatic substituents such as phenyl rings. Very recently, our research group clarified the idea that the FL emission of disubstituted acetylene polymer derivatives originates from intramolecular excimer due to the face-to-face stacking of the side groups. We have focused our interests on the origin of the FL emission in order to expand our knowledge to developments of novel sensor and actuator applications. It was found that the intramolecular phenyl-pheyl stack structure of PTMSDPA in film was variable in response to various external stimuli such as heat, pressure, chemicals, and so on. Base on these facts, we have developed various potential applications such as piezochromic fluorescence, viscosity sensor, protein detection, and environment-specific responsive actuator. The details will be presented in the symposium.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-5**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 곽기섭

Functional Organics via Self-assemblies of Block Copolymers or Liquid Crystals

조병기

단국대 화학과

최근, 본 연구실에서 수행된 연구 중 하나로, PS-PLA 블록공중합체의 자기조립 구조형성 후, PLA 부분을 선택적으로 에칭하여 나노다공성 재료를 제조하였다. 제조된 나노 다공성 구조의 경우, 벽면이 음이온 특성의 carboxylate 그룹으로 구성되어 있어, 수용성 양이온 dye 인 rhodamine-6G 를 잘 흡착하였고, 반면 또 다른 수용성 음이온 dye 인 calcein 의 경우 거의 흡착하지 않음을 확인할 수 있었다. 또한, 14 nm 의 기공 지름으로 인하여, 이보다 작은 particle 들만 기공 안으로 침투하는 현상을 관찰하였다. 이 같은 현상은 크기가 다른 금 나노입자의 dye quenching 실험을 통해 규명하였다. 본 연구결과와 더불어, 클릭반응을 통해 합성한 디스크 분자의 수소결합을 통한 액정화합물 제조에 대해서도 논하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-6**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 12:05, 좌장: 곽기섭

Monosaccharide-Responsive Release of Insulin from Polymersomes of Boroxole-Containing Block Copolymers under Physiologically Relevant Conditions

김경택

울산과학기술대 나노생명화학공학부

Polymers containing organoboronic acids have recently gained interest as sugar-responsive materials owing to the reversible binding of saccharides to boronic acids, which triggers a change in the physical and chemical properties of these polymers, such as theri water solubility. In particular, the ability of these polymers to bind glucose has attaracted considerable attention because of the promise of these materials for the development of sensors and drug delivery systems for glucose-related human diseases, such as diabetes. Boronic acid-diol conjugates, however, easiliy hydrolyze in aqueous solutions at neutral pH, so boronic acid-containing polymers have been mainly used as sugar-responsive materials under high pH conditions (>9) that are incompatible with in vivo studies and applications.In this presentation, we will discuss our first synthesis of the boroxole-containing styrenic monomer and its controlled radical polymerization via the reversible addition-fragmentation and chain transfer (RAFT) method. Synthesized poly(styreneboroxole) (PBOx) showed binding to monosaccharides in phosphate buffer at neutral pH (pH 7.4), which was quantitatively studied using Wang's competitive binding assay. By virtue of a controlled radical polymerization, we synthesized a series of sugar-responsive block copolymers that self-assembled to form polymersomes in water. We demonstrate that the polymersomes of these block copolymers could encapsulate water-soluble guests such as insulin, which could then be released from the polymersomes only in response to the presence of monosaccharides in aqueous solution under physiological pH conditions.We also discuss our recent development of a new class of sugar-responsive block copolymers that are based on a sequence-specific copolymers.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY3-7**

발표분야: Smart Responsive Polymers: Synthesis and Applications

발표종류: 심포지엄, 발표일시: 금 12:30, 좌장: 곽기섭

Stimuli-Responsive π-Conjugated Polymers and Carbon Nanotubes for Molecular Actuators, Sensors, and Novel Conduits

송창식

성균관대 화학과

Electronic properties of π-electronic materials, such as π-conjugated polymers 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 huge 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-electronic materials, especially by designs at the molecular level, in the context of molecular (polymer) actuators, sensors, and energy-related materials. In the first part, I will propose novel molecular structures for π-conjugated polymer actuators, and discuss their synthesis and interesting properties. In the second part, single-walled carbon nanotubes, another π-electronic material, will be modified for sensing a biologically important species, harvesting photo-energies, and discovering a novel phenomenon (thermopower wave)

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND1-1**

발표분야: Recent Trends in Organosilicon Polymers and Nanocomposites

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 유효종

Quantum well polymers and silicon quantum dot nanocomposites

정현담

전남대 화학과

A new kind of organic-inorganic hybrid polymer, poly(tetraphenyl)silolesiloxane, was invented and synthesized for realization of its unique charge trap properties. The organic portions consisting of (tetraphenyl)silole rings are responsible for negative charge trapping, while the Si-O-Si inorganic linkages provide the intrachain energy barrier for controlling electron transport. Hydrogen terminated silicon quantum dots were grafted with polystyrene chains through thermal induced surface initiated polymerization. The resultant silicon quantum dot nanocomposites provide thermally robust positive charge trapping property as confirmed by C-V hysteresis with negative flat band shift.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND1-2**

발표분야: Recent Trends in Organosilicon Polymers and Nanocomposites

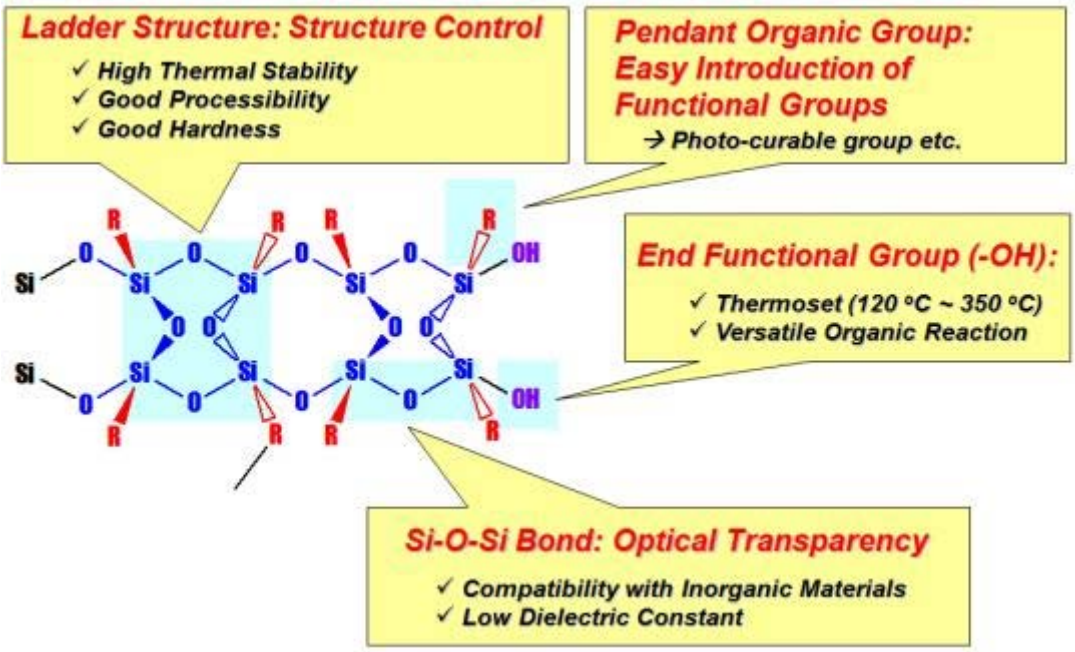
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 유효종

사다리형 실세스퀴옥산 소재의 구조와 물성

황승상

KIST 물질구조제어 연구단

Si-O-Si 결합으로 이루어진 실록산의 구조는 치환기의 개수에 따라 4 가지 종류가 가능한 데, 그 중 (RSiO3/2)n 으로 표시되는 실세스키옥산 소재는 가수분해 중합방법을 이용하여 합성되며, 크게 트리알콕시실란(RSi(OR)3)을 이용하는 방법과 트리클로로실란(RSiCl3)을 이용한 가수분해 중합법이 현재까지 널리 알려져 있다. 이렇게 합성된 폴리실세스키옥산은 통상적으로 고규칙성의 사다리형 구조(perfect ladder structure)외에 6,8,10,12 량체와 같은 바구니 구조(cage structure) 및 저 분자량의 불규칙적 구조(random, branched structure)의 혼합체로 구성되어 있다. 이러한 구조적 불균일성으로 인하여 기계적, 물리적 특성이 분자합성 설계 시에 예상하였던 기대에 미치지 못하게 된다. 이의 극복을 위하여 본 발표에서는 실세스퀴옥산 소재의 구조제어에 관한 최근의 연구를 소개를 하고자 하며, 특별히 사다리형 구조로 제어된 소재를 바탕으로 그 기능성과 다양한 응용성에 대하여 토의하고자 한다.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND1-3**

발표분야: Recent Trends in Organosilicon Polymers and Nanocomposites

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 유효종

Functionalized Hollow Polysilsesquioxane Spheres

하창식

부산대 고분자공학과

Hollow micro/nanostructured materials have attracted increasing interest for their potential applications as nanoparticle collectors, efficient catalysts, and drug-delivery carriers because of their empty interior. However, very few studies have examined organic-inorganic hybrid materials with hollow structures, though this type of organic-inorganic molecular-level hybrid polymers has many unique properties, which traditional composite materials do not exhibit. Recently we have investigated functionalized hollow polysilsesquioxane (PSQ) particles with a general formula of $[RSiO_{1.5}]_n$ for PSQs, where R is an organic group. In this talk, a few functionalized PSQ hollow spheres will be briefly overviewed with their various applications.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND1-4**

발표분야: Recent Trends in Organosilicon Polymers and Nanocomposites

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 한준수

실리콘 기반 방열 나노복합재료의 열전도 및 열적 특성

심상은

인하대 화학공학과

실리콘 고무는 다른 일반적인 고분자 재료 중 저온 및 고온에서의 열적 안정성이 동시에 뛰어난 재료이다. 이러한 장점을 이용하여 실리콘을 기반으로 한 grease, adhesive, gel, phase change materials (PCMs) 등과 같은 다양한 종류의 Thermal Interface Materials (TIMs)들이 개발되어져 왔으며 현재 전자제품의 방열성이 필요한 부분에서 널리 적용되어지고 있다. 특히 최근에는 LCD 및 LED 디스플레이 소자에서 방열 성능이 더욱 중요해지고 있어, 실리콘 기반의 방열재료에 대한 관심이 고조되고 있다. 본 발표에서는 현재 방열시장의 개요 및 방열재료 개요, 국내외 기업의 연구성과를 소개하고, 실리콘 기반에 흑연, 탄소나노튜브, 그래핀 등과 같은 탄소소재 및 boron nitride, alumina, zinc oxide 등과 같은 세라믹 소재를 충진한 실리콘 나노복합재료의 열전도, 전기전도 특성 및 내열성에 대하여 발표할 예정이다.

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장소: 부산BEXCO

발표코드: **IND1-5**

발표분야: Recent Trends in Organosilicon Polymers and Nanocomposites

발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 한준수

Highly tunable and rapid self-assembly of siloxane block copolymers for sub-10 nm lithography and nonvolatile memories

정연식

KAIST 신소재공학과

Directed self-assembly (DSA) of block copolymers (BCPs) can generate uniform and periodic patterns within guiding templates, and has been one of the promising nanofabrication methodologies for resolving the resolution limit of optical lithography. BCP self-assembly processing is scalable and of low cost, and is well-suited for integration with existing semiconductor manufacturing techniques. This talk will deal with recent research results on the self-assembly of Si-containing block copolymers for the achievement of sub-10 nm resolution, fast pattern generation, transfer-printing capability onto nonplanar substrates, and device applications for nonvolatile memories. One of the critical challenges of DSA is long annealing time (up to several hours), resulting in a low throughput. We demonstrate an approach to achieve both ultrahigh resolution (

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장소: 부산BEXCO

발표코드: **IND2-1**

발표분야: Technology Transfer from University or Institute to Industry

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이분열

지적자산 수익화를 위한 다양한 비즈니스 모델과 우수특허 개발

민승욱

아이피큐브파트너스

연구, 제품개발, 혹은 일상생활 등을 통해 생겨난 다양한 아이디어와 발명을 통해 수익을 창출하기 위해서는 다양하고 복잡한 프로세스가 필요하다.가장 기본적으로는 특허를 통해 독점적 권리를 인정받고 이를 활용하여 제품 생산, 서비스 제공 등을 통해 수익을 창출하는 것이 가장 널리 알려진 방식이나, 특허 자체의 가치가 점점 더 중요해지고, 기업간의 특허 분쟁이 심화됨에 따라 다양한 형태의 특허 매매, 라이선스에 관련된 비즈니스가 해외를 중심으로 진행되고 있다. 본 발표에서는 국내에서도 최근 지적자산을 활용하기 위한 다양한 자본이 생겨나고 있으며, 이를 최대한 활용하기 위해 특허의 다양한 특성을 이해하고, 관련된 다양한 비즈니스 모델들에 대해서 알아본다. 또한, 국내 창의 자본의 역할과 특허를 통한 수익화를 위한 최소한의 특허의 요건 등을 제안한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND2-2**

발표분야: Technology Transfer from University or Institute to Industry

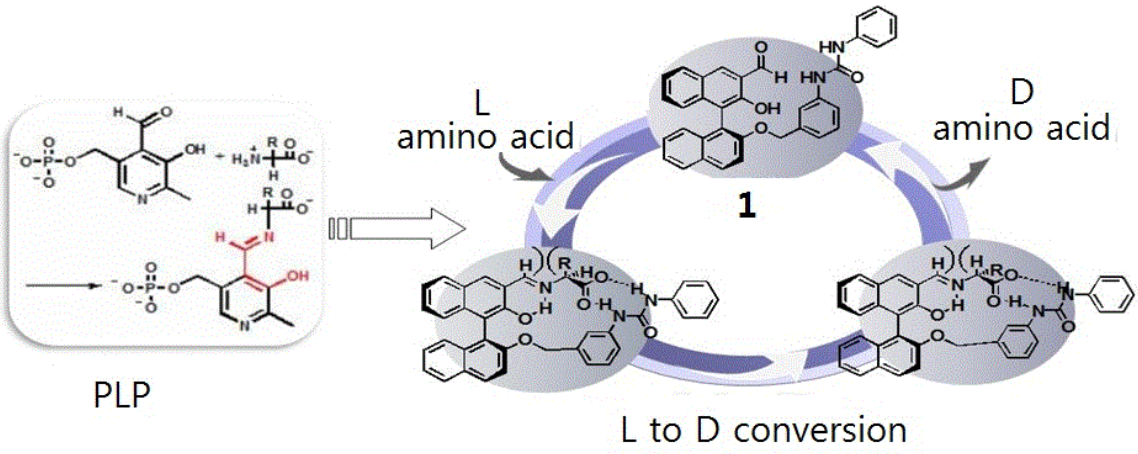
발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 이분열

The Technology of the Chirality Conversion of Amino Acids

김관묵

이화여대 화학과

The binaphthol-based chiral receptor, 1, exhibits high efficiency in enantioselective recognition of 1,2-amino acids. The receptor is also a chirality conversion reagent (CCR), as it converts the L-form to D-form of amino acids and peptides. The compound 1 has the capability to form a Schiff base like PLP. In contrast to PLP, the compound 1 deracemizes the bound amino acids due to the chirality of the binaphthyl moiety.그림 Extractive resolution coupled with racemization has been developed in order to realize economical conversion of L amino acids to D amino acids. This process includes the receptor 1, a phase transfer catalyst and a racemization catalyst. This technology is now applied in the industrial production of unnatural amino acids or nonproteinogenic amino acids, whose demands in both pharmaceutical industry and academic research are continuously increasing.References:1.Kim, K. M.; Park, H.; Kim, H.-J.; Chin, J.; Nam, W. Org. Lett. 2005, 7, 3525. 2.Tang, L.; Choi, S.; Nandhakumar, R.; Park, H.; Chung, H.; Chin J.; Kim, K. M. J. Org. Chem. 2008, 73, 5996.3.Park, H.; Kim, K. M.; Lee, A.; Ham, S.; Nam, W.; Chin, J. J. Am. Chem. Soc. 2007, 129, 1518. 4.Nandhakumar, R.; Ryu, J.; Park, H.; Tang, L.; Choi, S.; Kim, K. M. Tetrahedron, 2008, 64, 7704.



대 한 화 학 회
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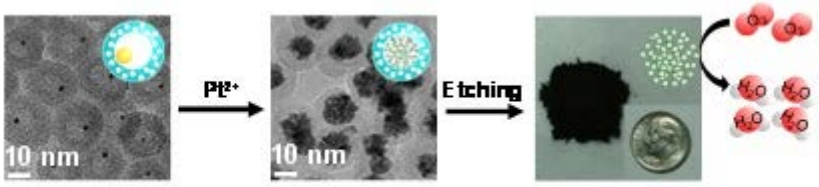
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **IND2-3**
발표분야: Technology Transfer from University or Institute to Industry
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이분열

Nanoreactor Strategy for the High-Concentration Synthesis of the Pt Nanocrystals with Enhanced Catalytic Performance

이인수 박만영[1] 이신화[1]

포항공과대 화학과 [1](주)디엔에프 나노소재연구센터

Pt and its alloys play important roles in many industrial applications, such as CO/NOx oxidation in catalytic converters, synthesis of nitric acid, oil cracking, and fuel cells. Although there has been considerable progress in the preparation of highly active Pt nanocatalysts through controlling their morphologies, the lack of a facile synthetic route has limited their practical applications. In particular, there is strong demand for a new synthetic method for the mass production of the Pt nanocatalyst with highly efficient electrocatalytic performance that is required for the commercialization of the fuel cell technology for automotive applications.In this presentation, I will discuss the novel nanoreactor approach to synthesize the Pt nanodendrites via Au-seed mediated growth inside hollow silica nanospheres. The synthetic protocol based on isolated nanoreactors is quite remarkable in terms of the product yield per unit reaction volume compared to traditional capping-agent based synthesis, which produces only a few mg of Pt nanodendrites per 1 ml of reaction suspension. The nanoreactor-based synthetic route enabled the synthesis of as much as 1.5 g of uniform Pt nanodendrites from a single reaction in a 40 ml aqueous suspension. The prepared ligand-free Pt nanodendrites exhibited greater ORR activity than commercial Pt black catalysts.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND2-4**

발표분야: Technology Transfer from University or Institute to Industry

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 이인수

Development and prospective of new PET radiopharmaceuticals: New fluorination methods

지대윤

서강대 화학과

Noninvasive imaging of molecular and biological processes in living subjects with positron emission tomography (PET) provides exciting opportunities to monitor metabolism and detect diseases in humans and in small-animal models. Measuring these processes with PET requires the preparation of specific molecular imaging probes labeled with positron-emitting radioisotopes. Recently, we have developed a remarkable effect of using tertiary alcohols as a reaction medium for nucleophilic fluorination with alkali metal fluorides. The great efficacy of this method is a particular advantage in labeling radiopharmaceuticals with [^{18}F]fluorine in high yield and purity, and in shorter times compared to conventional syntheses.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND2-5**

발표분야: Technology Transfer from University or Institute to Industry

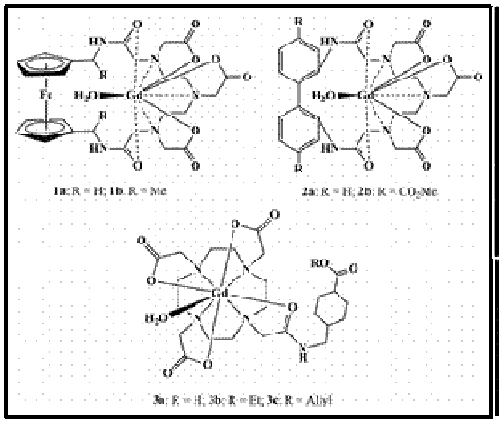
발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 이인수

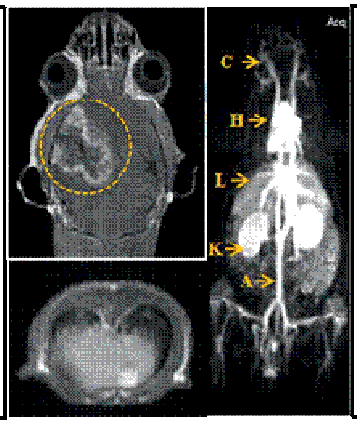
Blood-Pool and Targeting MRI Contrast Agents: From Gd-Chelates to Gd-Nanoparticles

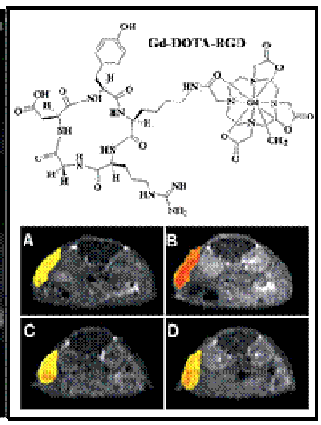
김태정

경북대 응용화학과

Magnetic resonance imaging (MRI) is a powerful and noninvasive diagnostic technique of the human anatomy, physiology, and pathophysiology on the basis of superior spatial resolution and contrast. MRI is useful in providing anatomical and functional images of the human body. A large number of MRI techniques are performed employing gadolinium III [Gd^{III}] complexes to enhance image contrast by increasing the water proton relaxation rate in the body. Despite their wide and successful application in clinic, however, conventional GdIII-based low-molecular weight contrast agents(CAs) are mostly extracellular contrast agents (ECCAs) exhibiting rapid extravasation from the vascular space. As a result, the time window for imaging is considerably reduced, thus limiting acquisition of high-resolution images. To overcome such limitations inherent to ECCAs, the necessity and the demand for the development of a new class of MRI CAs with functions including blood-pool and organ (or tumor)-targeting have risen recently. This microreview deals with our recent efforts on the design and the synthesis of new Gdchelates and Gd nanoparticles (GdNPs) for use as blood-pool and organ/tumor-targeting MRI CAs. We also consider properties such as high r_1 relaxivity and high thermodynamic, kinetic,and biostabilities.







대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND2-6**

발표분야: Technology Transfer from University or Institute to Industry

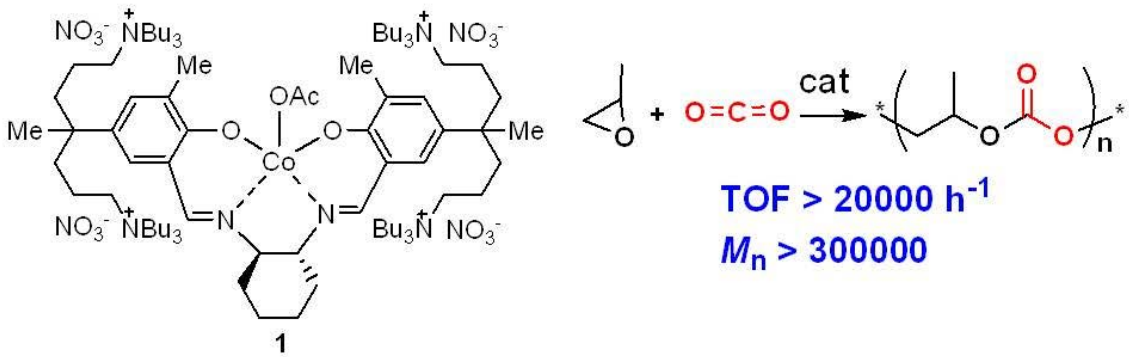
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 이인수

CATALYTIC COPOLYMERIZATION OF CO2 AND EPOXIDE: FROM FLASK TO INDUSTRIAL PROCESS

이분열

아주대 분자과학기술학과

We developed a highly active catalyst for the CO2/epoxide copolymerization. It is a cobalt(III) complex (1) prepared from a Salen-type ligand tethered by four quaternary ammonium salts.[1] The catalyst showed a high turnover frequency (TOF) above 20000 h-1 that produced a strictly alternating copolymer with a high molecular weight (Mn) exceeding 300000. The catalyst is transferred to industrial sector for commercialization and a pilot plant for continuous commercial process was constructed. Recent processes will be discussed especially in the point of commercialization of this attractive polymer. We carried out basic researches to reveal the binding mode of the active species. An efficient and economical synthetic route is developed to scale up the catalyst in a large scale (100 Kg scale). A tool to control the molecular weight and to construct various block copolymers was developed.[2]



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-1**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김명종

전자부품용 플라스틱 복합 재료를 이용한 방열기술 개발 동향

심상은

인하대 화학공학과

방열재료는 현재까지 전자제품의 반도체와 메모리소자와 같은 발열부분에 적용하여 발생된 열을 외부로 전달하여주는 역할을 한다. 전자제품에 있어서 사용시 10oC 의 온도 상승 시 제품의 수명은 1/2 로 감소하며, 1 oC 의 온도 상승 시 CPU 의 성능은 4.1%씩 감소함이 보고되어져 있다. 따라서 방열 특성은 가전제품의 안정성 확보 뿐 만 아니라 제품의 수명 연장을 위하여 필요한 성질이다. LED 조명에 있어 방열특성이 강력히 요구되어지고 있으며 패키징 재료로써 기존에 사용되는 알루미늄과 같은 금속을 고분자 복합재료로 대체하기 위하여 노력하고 있다. 또한 인쇄회로기판(PCB)에 있어서도 방열성능 구현이 대두되고 있다. 이에 본 발표에서는 LED 및 PCB 응용 분야에 중점을 두어 방열 플라스틱 소재 개발 동향 소개와 절연성이면서 동시에 고열전도성을 지닌 충진제 개발 및 이의 성능에 대하여 소개하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-2**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 김명종

The development of thermal conductive hybrid composite materials

김주헌

중앙대 화학신소재공학부

LED Chip 의 전기접속 및 방열 기능을 열화시키는 주된 원인은 Chip 과 패키지 몸체와의 접합, 패키지와 기판간의 접합, 기판과 방열판의 접합(접촉저항 기인)에 기인한 발열이며 이러한 열화에 의한 소자의 수명은 열 축적에 의한 작용온도가 약 10~20℃의 감소는 소자의 수명을 약 2 배 이상 증가시키는 것으로 알려져 있다. 이에 있어방열은 고효율 이전의 연구에서는 낮은 방열로 인해 Thermal interfacial properties 가 중요한 문제가 되지 않았으나, 고효율의 LED 에서는 높은 열 발생에 따른 장치의 노후화를 막는 문제가 중요한 요소가 되고 있다. 따라서 본 발표에서는 이러한 LED 를 포함한 전자 소재 내에서의 열 축적의 방지 및 효과적인 열 방출을 위한 Thermal interface Materials (TIM)의 최근 연구 동향 및 발전 방향에 대해 기술하고 이를 통하여 향후 개발 방향과 가능성에 대해 살펴보고자 한다

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-3**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 김명종

Behaviors of Thermal Conductivities in Multicomponent Polymer Composite Sheets Including Core-Shell Particles with Nanoporous Shell Layer

김상우

KIST 청정에너지연구센터

In the high-power light-emitting diodes display and multi-functional electronic devices, there are critical issues such as heat dissipation and electromagnetic interference which cause a program to malfunction or to health hazards. To solve these issues, multi-component composites with high thermal performance have recently been studied by many researchers. In this study, thermal conductivities of multi-component polymer composites of core-shell particles with a nanoporous nanostructured shell layer were investigated. Soft-magnetic FeCr core and alumina shell particles were fabricated by a supercritical fluid technology combined with sol-gel processing and subsequent heat treatment. As-prepared core-shell particles and additional alumina powders were blended with a polyolefin binder solution, and then were tape-casted onto the Mylar film. Heat-spreadable composite sheets consisting of the core-shell particles with a mesoporous ?-Al2O3 shell were fabricated and their thermal conductivities were measured. The multi-component nanocomposites showed much higher thermal conductivity compared to that of the simple mixture composites of the FeCr-alumina. Thermal conductivities of three-component composite sheets including core-shell particles with nanostructured shell layer was discussed from the results of a modified thermal conductivity theory and microstructural analysis.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-4**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 양철민

자동차 샤시 시스템의 Electric Control Unit 의 방열특성

김성수

(주)만도 연구개발본부

Abstract : 자동차의 지능형, 친환경, 정보화 기술의 급속한 발전에 따라 시스템을 구동하는 방식이 기존에는 기계식 혹은 유압식으로 하였으나, 근래에는 모터로 구동할 수 밖에 없게 되었다. 또한 그 동안의 모터구동은 소형 모터로 상시 작동이 아닌 일정시간 작동하여 구동하는 시스템에 한정이 되어 적용 되었으나, 점점 중대형 모터로 상시 적용하는 시스템까지 적용이 확대되고 있는 추세이다.이에 조향 시스템도 기존 유압의 도움을 얻어 운전자에게 조향을 편리하게 제공하는 방식에서 모터의 도움으로 구동하는 방식으로 전세계 차량의 50%이상이 바뀌고 있다.모터구동 조향 시스템에서 센서 신호를 받아 모터를 제어해주는 ECU(Electric Control Unit) 내부의 발열 소자로 인해 ECU Housing 을 알루미늄으로 사용하여 방열을 해주고 있는데, 이는 알루미늄의 무게 등으로 인해 시스템 무게 증가로 이어지는 문제가 있었다.이에 본 과제는 차량 및 시스템 경량화 측면에서 고방열 플라스틱을 적용한 ECU Housing 을 개발하여 경량화에 기여하고자 하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-5**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 12:10, 좌장: 양철민

전기자동차 베터리 케이스 적용을 위한 방열소재의 열 해석

윤여성

자동차부품연구원 친환경소재부품연구센터

차세대 자동차 개발에 따라 변화하는 자동차 소재와 설계 기술은 자동차 산업의 중요 연구 테마로 추진되고 있다. 특히, 전기자동차 개발이 확대되면서 차체, 부품 등에 적용 될 수 있는 경량 소재 기술 및 공조, 배터리 등 열관리를 위한 설계 및 방열 소재 기술의 요구가 점진적으로 늘어나고 있다. 실제 소재 개발에 따른 적용성에 많은 시간과 노력이 필요하며, 개발되는 소재 각각에 대해 제품을 만들어 적용하는 것을 현실적으로 어렵다. 뿐만 아니라 소재의 개발로 그 물리적 특성에서 차이가 나타나므로 부분적인 디자인 변경에 의해 방열효과를 최적화할 필요가 있다. 기존 방열소재는 주로 알루미늄을 중심으로 금속 제품이었으나, 본 연구에서는 최근 경량화 및 방열 두가지 효과를 동시에 만족 시키기 위해 고분자 수지를 매트릭스로 열전도성 무기 필러를 사용한 복합소재로 밧데리 케이스 적용 소재로 적용 가능성을 검토 하였다.일반적인 modeling 은 열해석 혹은 유체해석 등 각각의 수치해석을 진행하나 본 연구에서는 두 가지를 복합적으로 배합하여 두 조건을 동시에 구현하여 가능한 실제 상황에 가까운 조건으로 모사하였다. 배터리 케이스는 배터리 충방전에 의한 발열과 케이스 내부를 흐르는 냉매(공냉 혹은 수냉)의 유체 흐름 등을 복합적으로 동시에 구현하였다. 본 연구에서는 배터리 케이스 소재의 열전도 특성 수준을 가이드하기 위해 다양한 조건에서 modeling 을 수행하였으며, 금속 대체 소재의 선정 및 제조에 대한 기초 자료를 마련하고자 하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND3-6**

발표분야: Thermal Management Materials

발표종류: 심포지엄, 발표일시: 금 12:40, 좌장: 양철민

IT부품 분야의 방열소재 응용: LED Application

이혁수

LG이노텍 부품소재연구소

최근 기후변화 및 에너지 환경 규제에 대응하기 위하여 전세계적으로 신재생/친환경 에너지원에 대한 관심이 증가되고 있다. LED 는 반도체공정기술과 광/IT 기술이 융합된 21 세기 광원으로, 기존의 광원 대비 월등한 고효율?장수명의 구현이 가능하며 에너지절감 효율이 최고 90%에 달하는 반영구적 광원이다. 현재 일반적으로 생산되는 LED 의 경우 열로의 변환비율은 약 75~85% 정도이며 열에 의한 칩의 온도상승은 광효율의 감소뿐만 아니라 장기적으로는 신뢰성에 많은 문제를 야기하여 LED 의 수명을 감소시키는 원인을 제공한다. LED application 의 지속적인 성장을 위해서는 우수한 방열/내열 소재 및 방열구조의 개발이 요구되고 있다. LED PKG, LED BLU 그리고 LED 조명의 trend 를 살펴보고 해결되어야 할 Thermal Issue 들에 대해 논의하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR1-1**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 정옥상

Fascinating Metal-Oxygen Intermediates in Coordination Chemistry

남원우

이화여대 화학과

Dioxygen is essential in life processes, and enzymes activate dioxygen to carry out a variety of biological reactions. One primary goal in biomimetic research is to elucidate structures of reactive intermediates and mechanistic details of dioxygen activation and oxygenation reactions occurring at the active sites of enzymes, by utilizing synthetic metal-oxygen complexes. A growing class of metal-oxygen complexes, such as metal?superoxo, ?peroxo, ?hydroperoxo, and ?oxo species, have been isolated, characterized spectroscopically, and investigated in various oxygenation reactions. During the past decade, we have been studying the chemical and physical properties of various reactive intermediates in oxygenation reactions, such as high-valent iron(IV)- and manganes(V)-oxo complexes of heme and non-heme ligands in oxo-transfer and C-H activation reactions, non-heme metal-peroxo complexes in nucleophilic reactions, and non-heme metal-superoxo complexes in electrophilic reactions. The effects of supporting and axial ligands on structural and spectroscopic properties and reactivities of metal-oxygen adducts have been extensively investigated as well. In this presentation, I will present our recent results on the reactivities of various metal-oxygen intermediates in electrophilic and nucleophilic oxidation reactions. The synthesis and structural and spectroscopic characterization of mononuclear nonheme metal-dioxygen intermediates will be discussed as well.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR1-2**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

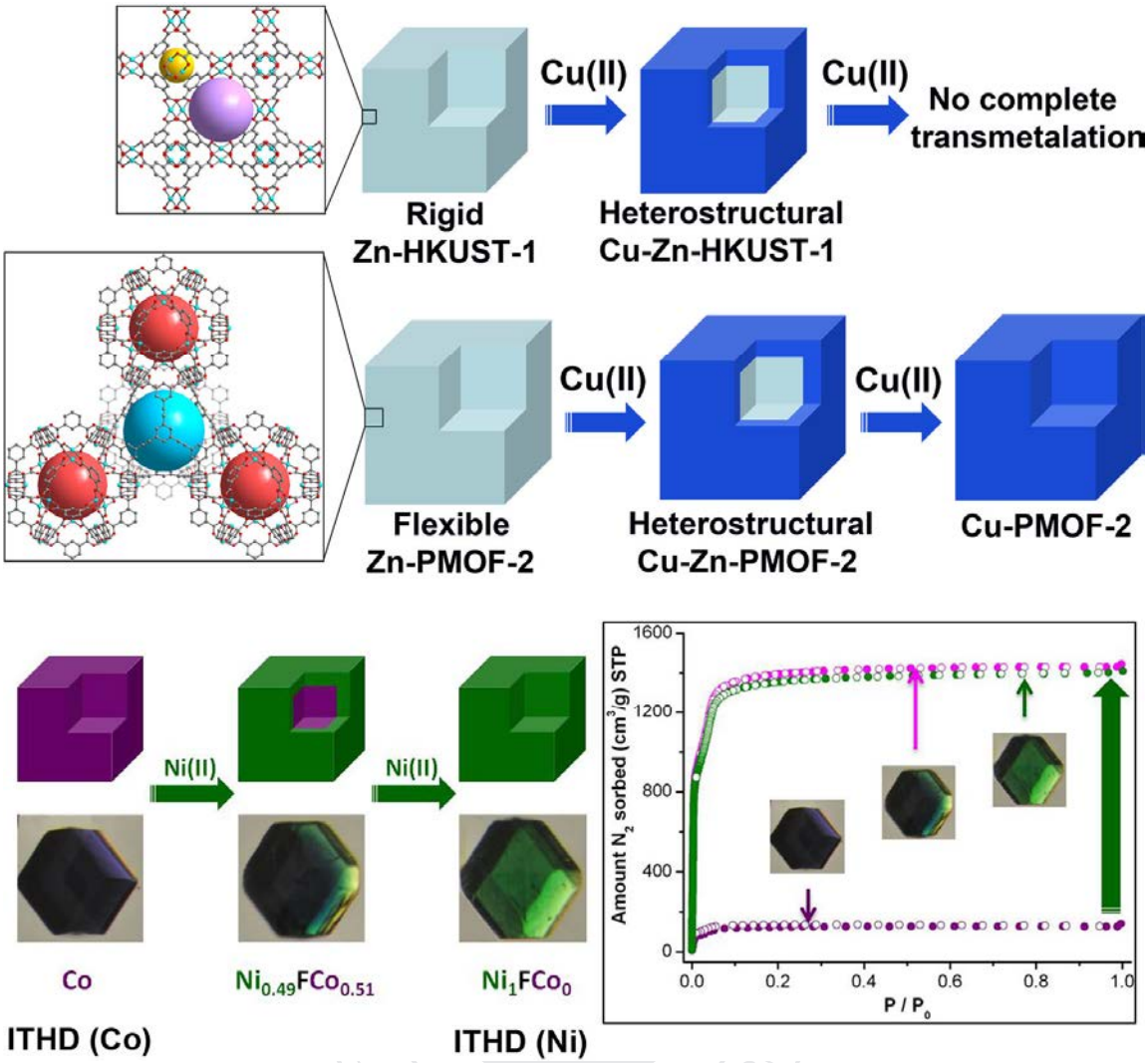
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 정옥상

Core-shell Heterostructures via Selective Transmetalations of Framework Metal Ions in Metal-organic Frameworks

나명수

울산과학기술대 친환경에너지공학부

The transmetalations (the replacements of metal ions) were investigated in metal-organic frameworks (MOFs), which have different framework stabilities depending on the framework metal ions and the ligand rigidities. By simply controlling the soaking time, not only could homogeneously transmetalated crystalline framework structures be prepared via the thermodynamically controlled complete replacement of the framework metal ions but also selectively transmetalated core-shell heterostructures were formed via kinetically controlled replacement that was mainly restricted to the external shell region of the crystal. The transmetalated MOFs showed significantly improved framework stabilities compared with the parent MOFs. Although the frameworks are partially transmetalated, the framework stability of not only the external shell region but also of the internal core region was significantly affected.



KOREAN CHEMICAL SOC

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR1-3**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 정옥상

BODIPY and zinc-based fluorogenic compounds for molecular recognition

D.G.Churchill

KAIST 화학과

In this presentation, the synthesis and utility of certain BODIPY and non-BODIPY chemosensors will be discussed bearing (*i*) thienyl/furyl rotor attachments where probing is centered at the aromatic ring chalcogen atom, and (*ii*) arene rotor attachments where the heteroatom is external to the ring and used in sensing or in formation of alternate fluorophore skeletons. While we will go through a variety of results, some newer results are listed below: (A) Bis-arylsulfide BODIPY systems were prepared and studied for multiple *Oxygen*-atom sensing (at 522 nm) at the *meso* group position; 2- or 3-atom loading was optimal (50-fold, “turn-on”). Neuronal studies showed greater H_2O_2 sensitivity than 2’,7’-dichlorofluorescein diacetate. Mercury detection was also examined with this class and there was found to be an Hg^{2+} "AND" superoxide correspondence. The novel 1,3,6-trimethyl BODIPY was discovered as a biproduct under Lindsey conditions. (B) In related work, a novel fluorescent difluoroboroazaoxobenzazulene dye was synthesized from commercially available substrates in “one pot;” it was characterized structurally and spectroscopically, derivatized, and finally compared to a related BODIPY system that demonstrates “turn-on” H^+ (42-fold) and F^- (~5-fold) responses. (C) Fluorescence 'OFF-ON' behavior with addition of biological phosphate and Zn^{2+} was studied with $Zn_2(slys)_2Cl_2$ [H_2slys = 6-amino-2-{(2-hydroxybenzylidene)amino}hexanoic acid], a fluorescent water soluble complex, using various spectroscopic tools (*e.g.*, ^{31}P NMR, UV-Vis, emission and CD spectroscopy) at the mM level. Adduct-dependent fluorescence intensity changes can be interpreted as a two-input (cation / anion) implication molecular logic gate system. A displacement study of PPi (versus diphosphate and triphosphates) from the dizinc complex is also reported. Related work also involved assays with the proteins implicated in Parkinson’s Disease aetiology. Copper analogues of the zinc species were also used in substrate recognition and intriguing crystal packing effects in the solid state.

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장소: 부산BEXCO

발표코드: **INOR1-4**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 이심성

A Versatile Synthetic Platform Based on Bicyclo[4.1.0]heptenes

정영근

서울대 화학부

Bicyclo[4.1.0]heptenes, which are readily accessible molecules via the transition metal-catalyzed cycloisomerization of 1,6-enynes, and have served as useful building blocks in organic synthesis. These molecules can undergo a variety of ring-opening reactions given that the release of the cyclopropyl ring strain may serve as a thermodynamic driving force for reactions, and the double bond within the skeleton can afford the kinetic opportunity to initiate the ring-opening via a coordination to a metal species. Even though the chemistry of the cyclopropyl group has been widely explored in organic chemistry, less attention has been paid to the chemistry of bicyclo[4.1.0]heptenes. However, during the past 5 years, we have been engaged in the exploration of the chemistry of bicyclo[4.1.0]heptenes. The chemistry developed in our laboratory will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR1-5**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 이심성

Construction and Solvent Reservior of Kagome-Type Coordination Polymers

정옥상

부산대 화학과

Self-assembly of CuX2 (X = 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 (Cu6L6) and triangular (Cu3L3) motifs. Notably, two slightly different kinds of triangles exist in the two-dimensional (2D) infinite structure in the solid state. The nano-sized hexagons with diagonal distance Cu???Cu = 25.172(1) ? for [Cu3Cl6L2] and 25.405(1) ? for [Cu3Br6L2] are occupied by six ethanol molecules (6EtOH@[Cu3Cl6L2]) and by a mixture of three ethanol and three methanol molecules (3MeOH?3EtOH@[Cu3Br6L2]) indicating that the hexagon is an effective reservoir for small alcohol molecules. The interlayer distances are very short (3.606(1) ? for 6EtOH@[Cu3Cl6L2]; 3.560(1) ? for 3MeOH?3EtOH@[Cu3Br6L2]), and are comparable to that of graphite (3.35 ?). In the present study, the temperature-dependent morphology change of the crystals was monitored in order to confirm the solvent-desorption and decomposition procedures.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR1-6**

발표분야: Recent Advances in Coordination and Organometallic Chemistry

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 이심성

Quantum Magnets

홍창섭

고려대 화학과

Single-molecule magnets (SMMs) and single-chain magnets (SCMs) have been intensively explored owing to their fundamental interest and potential applications in magnetic devices. To achieve such anisotropic materials, it is of utmost importance to control molecular structures into low-dimensionality. Recently, a new group of lanthanide-based SMMs has attracted much attention since pioneering works reported observations of slow relaxation in lanthanide ion complexes of [Pc2Ln]- (Pc = phthalocyanide, LnIII = Tb, Dy, Ho). Unlike SMMs composed of paramagnetic metal ions with d orbitals, lanthanide ion SMMs are based on 4f orbitals and, as a result of spin-orbit coupling, their (2J+1)-fold degenerate levels can be split under the ligand field to give separated Kramers doublets. In this presentation, I will introduce synthetic efforts and exotic magnetic phenomena of 3d-4d and 4f-based quantum magnets. These materials were fully characterized by means of various techniques to give understanding of the properties at a molecular level. Detailed results will be discussed in my talk.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-1**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

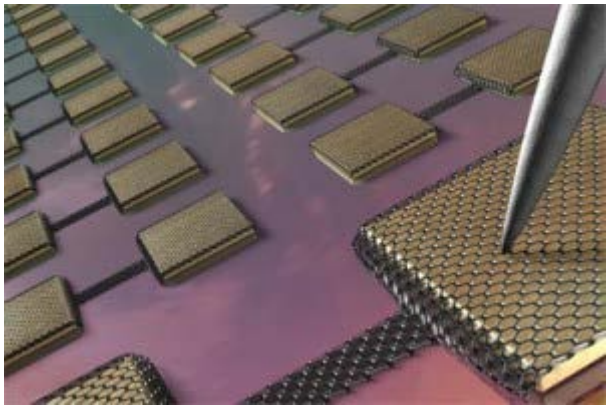
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 오준학

Graphene and Boron Nitride for Atomically Thin Circuitry

Jiwoong Park

Cornell University

In the past few years, the science and application of graphene, a hexagonal crystal entirely made of carbon atoms, has experienced a revolutionary change, mainly due to the development of large scale growth methods based on chemical vapor deposition (CVD). This enabled production of single-atom-thick conducting films in meter scale. However, it still remains difficult to characterizeand process graphene films, while maintaining many or their excellent properties. Namely, the materials science and engineering of graphene is still in its infancy.First, these CVD graphene films are polycrystalline as grown. We recently reported the first atomic-resolution imaging of individual grain boundaries in graphene membranes as well as a dark-field transmission electronmicroscopy (TEM) technique that rapidly characterizes graphene grain structures. Using these new synthesis, fabrication and TEM characterization methods, our group can now investigate the structure of grain boundaries and probe their effects on the mechanical, electrical, and chemical properties of CVD graphene.In addition, CVD graphene produces bilayer regions with different stacking structures. We showed that the angle dependent interlayer interaction leads to fascinating electrical and mechanical properties of bilayer graphene in different configurations (vertical junctions). Finally, we used some of these newly developed capabilities in order to demonstrate atomically thin circuitry entirely made of graphene (conductor) and hexagonal boron nitride (insulator), which presents exiting new directions for these materials.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-2**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 오준학

Reversibly Light-Modulated Dirac Point of Graphene Functionalized with Photochromic Molecule

신현석

울산과학기술대 에너지공학부

Graphene has been functionalized with spiropyran (SP), a well-known photochromic molecule. It has been realized with pyrene-modified SP which has been adsorbed on graphene by ?-? interaction between pyrene and graphene. The field-effect transistor (FET) with SP-functionalized graphene exhibited n-doping effect and interesting optoelectronic behaviors. The Dirac point of graphene in the FET could be controlled by light modulation because spiropyran can be reversibly switched between two different conformations, a neutral form (colorless SP) and a charge separated form (purple colored merocyanine, MC), on UV and visible light irradiation. The MC form is produced during UV light irradiation, inducing the shift of the Dirac point of graphene toward negative gate voltage. The reverse process back to the neutral SP form occurred under visible light irradiation or in darkness, inducing a shift of the Dirac point toward positive gate voltage. The change of the Dirac point by UV and visible light was reproducibly repeated. SP molecules also improved the conductance change in the FET device. Furthermore, dynamics on conversion from MC to SP on graphene was different from that in solution and solid samples with SP-grafted polymer or that on gold nanoparticles.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-3**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 오준학

Bio-analytical Platform Technology for Drug Discovery based on Graphene Oxide

민달희

서울대 화학과

To date, various nanomaterials have been harnessed as critical components of bioanalytical systems such as gold nanoparticles for sensing DNA-related biochemical events. To design “good” bioanalytical systems using new nanomaterials, one should be able to understand and fully utilize chemical/physical properties to detect molecular changes during certain biochemical transformations in a biological system. Moreover, the new system should overcome limitations of conventional assay methods?detection limits, cost issues, labors, efficiencies, quantitativeness, reproducibility, etc. In this talk, I will introduce recent efforts to utilize “graphene oxide” for the development of bioanalytical systems and biotechnological tools. We have developed convenient and sensitive biosensors for the activity assays of helicase, nuclease, methyl transferase and phopholipase based on graphene oxide, which are compatible with high throughput screening. In addition, I will discuss on the efforts towards successful interfacing of graphene for biosystems-for example, study on responses and behaviors of cells towards graphene oxide and encapsulation of mammalian cells with graphene oxide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-4**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 신현석

Single Ferroelectric-Domain Photovoltaic Switch

조문호

연세대 신소재 공학부

Bistability of ferroelectric polarization states serves as a basis for solid-state memory. It can also yield interesting photovoltaic effects in such a way that the directional photocarrier motion follows the inherent potential gradient imposed by the polarization vectors of ferroelectrics that are electrically switchable. Therein, the defining characteristic of such coherent switching between of the polarization states is realized by single-domain switching. Here we provide visual evidence for such a coherent photovoltaic switching of lateral $BiFeO_3$ channels by a scanning photocurrent imaging that are spatially and spectrally resolved. Direct comparison of the sequential photovoltaic current images at different remanent polarization states of single-domain $BiFeO_3$ channels with those on multi-domains reveals that the switching characteristics is determined both by the internal polarization vector of the domain and oxygen vacancy migration at the domain walls. Our study suggests general implication for the design rules of the ferroelectric photovoltaic cells, which can be tuned by domain engineering and nano-ionic transport.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-5**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 신현석

3D nanoarchitectures based on nanorods, nanotubes and graphene for electronic and optoelectronic applications

박원일

한양대 신소재공학부

Compared with the discovery of a totally new material, hybrid materials could present substantial opportunities for achieving new types of materials with versatile and tailor-made properties. In particular, nanometer-scale hybridization may enable unique and fascinating properties and high-performances superior to those of their counterpart individual components and/or bulk materials. Here, I will present a controlled synthesis of 3D nanoarchitectural systems based on nanorods, nanotubes and graphene as emerging building blocks for future electronics and photonics. The first type of 1D-2D hybrids can be achieved by growing regular arrays of ZnO nanorods on 2D graphene layers transferred to the transparent and/or flexible substrates. The hybrid nanostructures exhibited the outstanding electrical conductivity, optical transparency, and mechanical flexibility, which, combined with new optical functions inherited from the ZnO nanorods, suggests a wide spectrum of applications. The second type of 1D-2D hybrid can be fabricated by mounting 2D graphene sheets directly on the top of the nanorods/pillars to develop novel light emitting diodes, laser diodes and sensors.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR2-6**

발표분야: Optical, Electrical, and Chemical Properties of Low-Dimensional Nanostructures and Their Applications

발표종류: 심포지엄, 발표일시: 목 16:35, 좌장: 신현석

Organic Semiconductor Nanowires: Synthesis, Photophysics, and Applications

오준학

울산과학기술대 나노생명화학공학부

Organic semiconductor nanowires have attracted great interest recently as they are promising building blocks for various electronic and optoelectronic applications such as light-emitting diodes, field-effect transistors, photoswitches, sensors, solar cells, nanoscale lasers, optical waveguides, and memory devices. In particular, organic single-crystalline nanowires typically show better performance compared with their bulk counterparts due to the lack of grain boundaries that act as an energetic barrier for charge transport. Their one-dimensional, intrinsically defect-free and highly ordered nature allows a deeper understanding of the fundamental mechanisms of charge generation and transport, while enabling a bottom-up fabrication of optoelectronic nanodevices. Herein, I would like to report the synthetic methodologies, photophysics, charge-transport behaviors and optoelectronic applications of organic semiconductor nanowires, mainly focusing on n-channel molecular semiconductors.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS1-1**

발표분야: Physical Chemistry Approach for Biological Phenomena

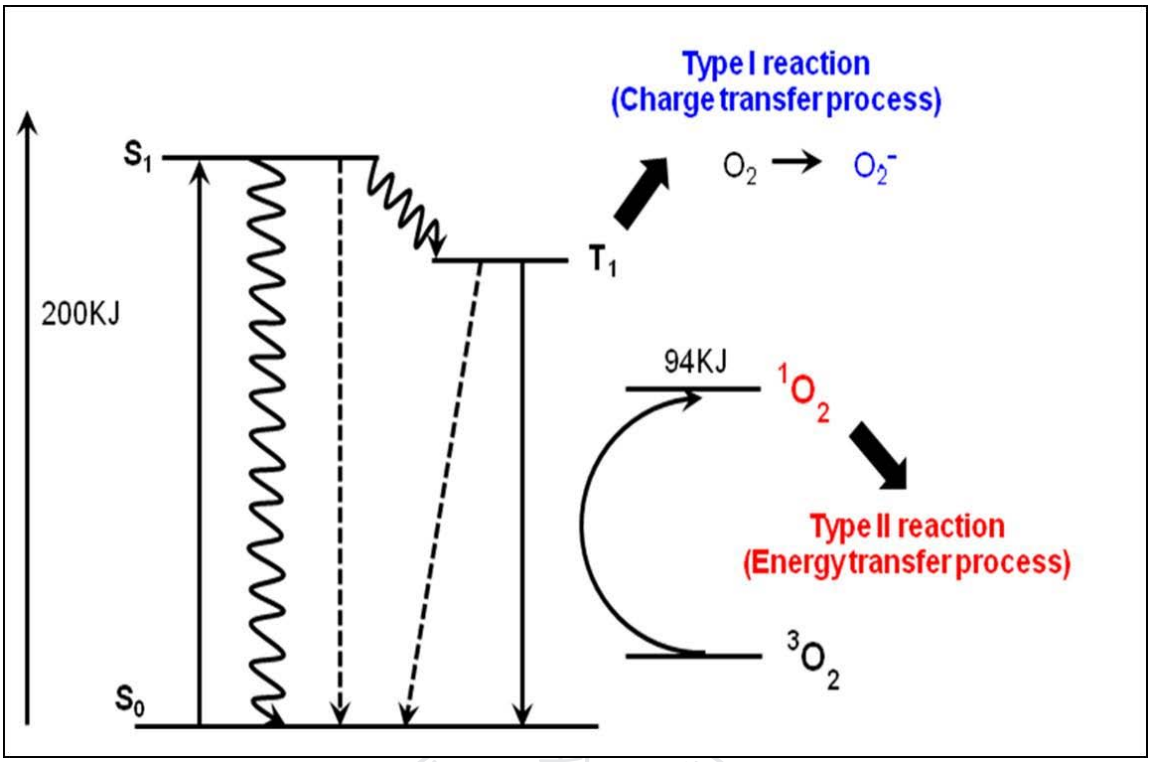
발표종류: 분과기념강연, 발표일시: 목 09:00, 좌장: 주태하

Photo-Induced Reactive Oxygen Species and Their Biophysical Applications

김용록

연세대 화학과

Reactive oxygen species (ROS) have been a long time subject in chemical, environmental, and bio-medical science due to their strong reactivity and selectivity, and the involvement with metabolism of cell and organs. There are many applications of ROS such as photodynamic cancer therapy, decontamination of blood product, water disinfectant, drug delivery system, and stereo-selective synthesis of drug in life science area. Investigation on the photosensitizers with high efficiency of ROS generation has always been in a great demand. Photophysical factors determining the efficiency of transient ROS generation, particularly for the singlet oxygen that is known to be one of the most critical species, are investigated in terms of the molecular structure and electronic property. Based on the photophysical parameters, the fabrication strategy for the multifunctional composite materials which generate ROS is established for specific medical and environmental applications. In this presentation, various multifunctional composite materials that are recently fabricated will be introduced along with their photophysical parameters and the targeted application efficiencies regarding of the biophysical aspects.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS1-2**

발표분야: Physical Chemistry Approach for Biological Phenomena

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 이남기

New fluorescent materials for biological imaging applications

김성근

서울대 화학부

A group of new, highly fluorescent compounds was generated from a photochemical reaction of originally non-emitting compounds. UV irradiation of trans-resveratrol and its sugar derivatives leads to its multi-step photochemical transformation to a new compound (called “resveratrone”) and its corresponding sugar derivative, which have never been identified to date or registered in the CAS. We isolated these elusive compounds by HPLC and elucidated their chemical identities using mass spectrometry, NMR and FT-IR spectroscopy, and quantum calculations. Resveratrone has a high fluorescence quantum yield (0.49), a large Stokes’ shift (150 nm), and a large two-photon absorption cross section (132 GM), while its sugar derivative retain all these properties yet are soluble in aqueous environment, which may prove to be a vital trait as an ideal fluorophore in bio-imaging, multi-color labeling, and two-photon microscopy applications. As a demonstration, we present images of various life forms in vitro and in vivo along with the cytotoxicity test results of these compounds.

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장소: 부산BEXCO

발표코드: **PHYS1-3**

발표분야: Physical Chemistry Approach for Biological Phenomena

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 이남기

Force-Based Atomic Force Microscopy for Bioanalysis and Single Molecule Manipulation

박준원

포항공과대 화학과

Dendrons have been applied to AFM probes and substrates to control spacing between the immobilized biomolecules on them. It was observed that use of thus-prepared probe and substrate allowed mostly one to one DNA interaction during the force measurement. The approach was extended to map individual prostate-specific antibodies captured on a microarrayed spot, and used to calculate the PSA concentration in solution. As a new application, picking a biomolecule such as DNA and proteins with the AFM tip was examined.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS1-4**

발표분야: Physical Chemistry Approach for Biological Phenomena

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 이남기

Application of Fluorescence Polarization to Single-biomolecule Imaging

이종봉

포항공과대 물리학과

Polarization/anisotropy in emission from a fluorescent molecule can be used to study rotational dynamics of biomolecules. Even though the emission from a free fluorophore in solution is easily depolarized since most of small fluorophores in biological relevant solutions have faster rotational diffusion rate than the rate of emission, the fluorophores immobilized on macromolecules such as proteins and nucleic acids can be polarized in response to the dynamics of the macromolecules. I will present two applications of biomolecule imaging using fluorescence polarization: 1) Rotational dynamics of proteins on DNA. 2) A simple imaging method that uses an interaction between the polarization of the excitation light and the transition dipole moment of a fluorescent molecule to determine dipole directions of two fluorescence emitters located within the diffraction-limited spot.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **PHYS1-5**
발표분야: Physical Chemistry Approach for Biological Phenomena
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 김우연

Developing protein modeling methods for practical applications

석차옥

서울대 화학부

We have been developing computational methods for protein structure prediction, protein-ligand docking, and protein-protein docking. Although numerous computer programs have been developed for such purposes, accurate prediction is still not within our grasp. In general, reliable predictions are possible only when experimental structures of close homologues are available. Despite this fact, there exist a range of problems that the current methods can provide useful prediction results, and more and more researchers are using prediction methods for such reasons. More accurate and effective prediction methods will extend the applicability range of the methods and may provide breakthroughs in certain application areas. To promote advancement in the prediction areas, community-wide experiments CASP (Critical Assessment of techniques for protein Structure Prediction) and CAPRI (Critical Assessment of PRediction of Interactions) have been held by assessing blind prediction results of participating groups on common prediction problems. In this presentation, our outstanding results in recent CASP and CAPRI experiments will be discussed. A key feature of our method is a proper combination of physics-based energy and bioinformatics-derived properties. I will also show free web servers developed for wide users in the field.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS1-6**

발표분야: Physical Chemistry Approach for Biological Phenomena

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 김우연

Novel Chemical Kinetics for Description of Chemical Noise in Dynamically Heterogeneous Biological Reaction Systems: Quantitative interpretation of mRNA level fluctuation in a living cell

성재영

중앙대 화학과

We introduce a novel chemical kinetics for a quantitative description of chemical noises in dynamically heterogeneous biological reaction systems. In the first part of this talk, we will discuss the renewal chemical kinetics recently proposed for biopolymer reactions composed of arbitrary non-Poisson elementary processes, which could provide a successful quantitative explanation on the dependence of the randomness in single enzyme turnover times on substrate concentrations. In the second part we will discuss the number fluctuation of product molecules for an elementary biopolymer reaction with a dynamically heterogeneous rate coefficient. A simple but general model of transcriptional rate fluctuations will be proposed, which provides an excellent quantitative interpretation for the counting statistics of the mRNA expressed from 20 E. Coli promoters, measured by using single-molecule fluorescence in situ hybridization (smFISH).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-1**

발표분야: Recent Trends in Physical Chemistry

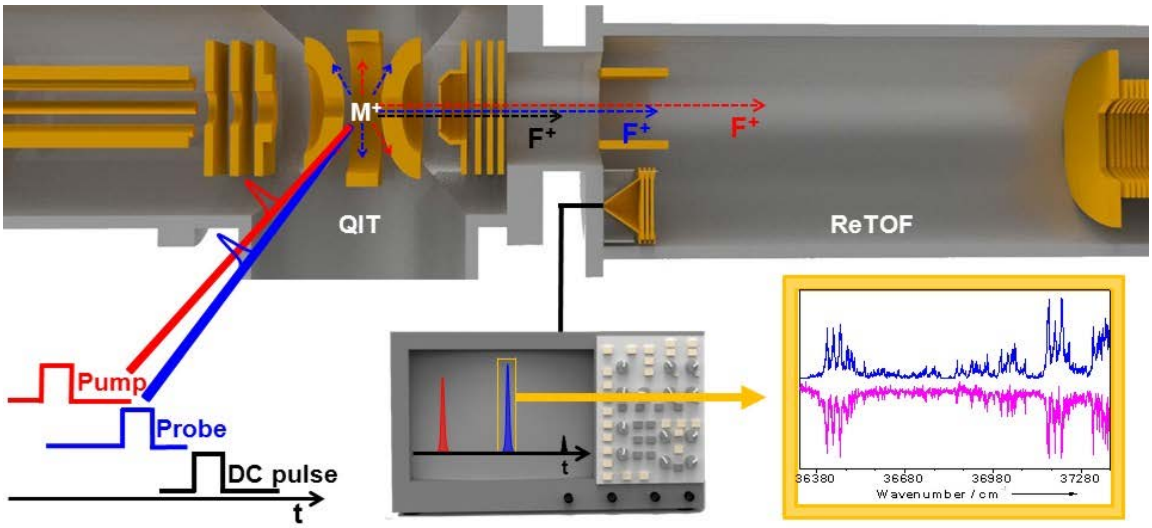
발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 주태하

Ultraviolet-ultraviolet hole burning spectroscopy of crown ether complexes with alkali metal cations stored in a cold quadrupole ion trap

김남준

충북대 화학과

We developed a new technique of ultraviolet-ultraviolet (UV-UV) hole burning (HB) spectroscopy that can be applied to ions stored in a quadrupole ion-trap (QIT). Although UV-UV HB spectroscopy has been extensively used to obtain conformationally selective electronic spectra of neutral molecules produced in a supersonic jet, it has never been applied to ions in an ion trap due to the difficulty in distinguishing the ions produced by the pump laser from those by the probe laser. However, we found that some photofragment ions do not get trapped but escape from the ion trap right after the irradiation of the pump pulse and thus can be detected separately from those produced by the probe pulse by using a reflectron time-of-flight mass spectrometer next to the ion trap. Using this method, we obtained the UV-UV HB spectra of dibenzo-18-crown-6 complexes with alkali metal cations and confirmed the presence of only single conformational isomers for all of the complex ions in the cold QIT. We also investigated the ejection mechanism of photofragment ions from the QIT. To understand the ejection mechanism, we measured the dependences of the ejection process on the rf amplitude, time delay between the laser pulse and extraction direct current (DC) pulse, and buffer gas pressure in the QIT. We suggested that the photofragment ions undergo unstable oscillatory motion upon their generation inside the QIT due to their larger values of the Mathieu parameter qz than that of the stability boundary. The fragment ions increase their oscillation amplitudes by taking up energy from the rf field and are eventually ejected out of the QIT. The lower limits of the qz value necessary for the ejection of K+, Rb+, and Cs+ ions from the QIT are determined to be larger than the stability boundary.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-2**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 류순민

Nanoparticle-plasmonics for Single-Molecule Reaction kinetics and Optical Nanoscopy

김지환

고려대 화학과

I will introduce my group's recent effort on nano-plasmonics and its application to single-molecule kinetics and optical nanoscopy. First, I will demonstrate the use of well-defined gap-plasmons to locally drive a photochemical reaction, and follow the reaction kinetics of individual product molecules using the surface-enhanced Raman scattering (SERS). Secondly, as a further application of nano-plasmonics, I will demonstrate the use of infrared near-field microscopy to identify two different stacking structures, the rhombohedral (ABC) and the Bernal (ABA) form, of multilayer graphenes at 10 nm spatial resolution.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-3**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 류순민

Surface Reaction between Adsorbed Molecules and Substrate: Tautomerism and Oxidation

이한길

숙명여대 화학과

First, we confirmed the coverage dependent variation of tautomerism (thiol- and thioketo form) for 2-mercaptothiazoline molecule adsorbed on the Ge(100) surface in UHV condition using CLPES measurement and DFT calculation method. CLPES revealed that two distinct adsorption structures simultaneously exist at both lower (0.15 ML) and higher (0.55 ML) coverage with a different predominance. We have also modeled the adsorption structures and geometric configurations of the bonding states of 2-mercaptothizoline on the Ge(100) surface using DFT calculation methods. We will systematically demonstrate the existence of tautomerism (thiol- and thioketo form) for 2-mercaptothiazoline molecule adsorbed on the Ge(100) surface varying with its coverage using CLPES in conjunction with DFT calculation method.Second, the catalytic effect of oxidation reaction from aniline to Azobenzene between a graphene oxide (GO) and reduced graphene oxide (rGO) films was compared and investigated using SEM, AFM, Raman spectroscopy, and CLPES. We confirmed that oxygen carriers present on GO film acted as a heterogeneous catalyst, which facilitated the oxidation reaction from aniline to Azobenzene, as we monitored the surface morphological change using SEM and AFM and variation of electronic properties using core level spectra and Raman shift induced by aniline exposing. We will demonstrate that the catalytic effect of oxygen carriers existing on GO film effectively occurs using SEM, AFM, Raman spectra, CLPES, as well as the work function measurements.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-4**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:05, 좌장: 조범석

Vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectrometry: Structure determination of ionic molecules

권찬호

강원대 화학과

We have constructed the mass-analyzed threshold ionization (MATI) time-of-flight mass spectrometer using coherent vacuum ultraviolet (VUV) radiation generated by four wave difference frequency mixing (FWDFM) in Kr and utilized it to obtain the spectroscopic information of the azabenzene cations in the ground electronic state. Particularly, the VUV-MATI spectrometry has been revealed that it is very useful to acquire the vibrationally high-resolved spectra of pyridine, pyrimidine, and 2-methyl pyrazine that are highly important molecules for the study of biomolecular interactions and the structures. In addition, vibrational analysis in the observed spectra has been accomplished with calculating the vibrational frequencies and Franck-Condon factors at the B3LYP/cc-pVTZ levels. The details in determining the ionization energies to the ionic ground state and the structures of molecular cations are discussed in this presentation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-5**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 조범석

Non-adiabatic simulations of excitation energy transfer process in photosynthetic Fenna-Matthews-Olson complex: A dumb way of seeking cleverness

이영민

포항공과대 화학과

Applying an all-atom non-adiabatic simulation technique for complex molecular systems is nothing but a daunting task, even though it will be extremely advantageous for elucidating various physical aspects of the involved processes. Here, we will present the results of our semiclassical Poisson bracket mapping equation simulations on excitation energy transfer (EET) in the photosynthetic Fenna-Matthews-Olson complex. By inspecting the atom-specific interactions, we will show that the chromophore coupling maintained by the protein scaffold is the key factor for governing the coherence. The electrostatic modulations by the protein and the related site energy dispersion have only a limited effect. The role of thermal fluctuations in the chromophore coupling will be additionally inspected in view of EET pathway diversity. We will focus on the discussion about what we can seek out of this time-consuming simulations.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2-6**

발표분야: Recent Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 16:55, 좌장: 조범석

Ultrafast Chemical Exchange 2DIR Spectroscopy : Studies of Thermal Equilibrium Dynamics

박성남

고려대 화학과

Ultrafast 2DIR spectroscopy, which is an ultrafast analog of 2D-NMR, is an excellent experimental tool to study chemical exchange dynamics occurring on picosecond timescales by probing molecular vibrations. 2DIR spectroscopy has been applied to many molecular systems to understand thermal equilibrium dynamics, such as, hydrogen-bond exchange dynamics in aqueous solutions, ion pairing dynamics in electrolyte solutions, intramolecular vibrational energy transfer dynamics, ligand-exchange dynamics, and acid-base equilibrium dynamics. In this talk, principles and experimental details of 2DIR spectroscopy will be presented. Experimental results in our group will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-1**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 강성호

Nanoparticle-enhanced Raman analysis for environmental measurements

주상우

숭실대 화학과

Detection and analysis of pathogens and engineered nanomaterials have gained enormous attention to protect human health and the enviroments. Raman methods can offer several advantages due to distinct spectral signatures for high throughput screening of various environmentally hazardous materials by introducing novel nanostructures. Extremely strong electric fields can be formed in the gap between the noble metal nanoparticles (NPs) when they are brought closer than a few nm. The phenomenon of surface-enhanced Raman scattering (SERS) by utilizing such an enormously enhanced localized electromagnetic field has been utilized as a versatile tool to monitor the interfacial phenomena. SERS is currently enjoying a renewed interest due to their potential via a spatial confinement of plasmonic NPs to allow the detection of a trace amount of adsorbates. Our recent efforts with my students and collaborators will be discussed at the symposium to address safety issues of indoor pathogens and nanomaterials.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-2**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 09:55, 좌장: 강성호

나노물질 안전성 평가와 중금속 검출 센서 개발

양성익

경희대 응용과학대학 응용화학과

나노물질의 개발 현황과 이에 따른 인간, 환경에 미칠 수 있는 잠재적 위해성에 대한 인식이 증가하면서 나노물질에 대한 안전성 평가의 필요성이 증대되고 있다. 특히, 양자점(CdS, CdSe), 은나노, 산화아연 등 중금속을 함유하고 있는 나노물질의 경우 안전성 우려가 높은데 이는 이 들 나노물질에서 유해한 중금속이 용출될 가능성이 높기 때문이다. 이에 중금속을 함유하고 있는 나노물질의 이온 용출 시험법에 대해 소개하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-3**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 강성호

Principles and applications of time-integrated samplers for monitoring trace contaminants in the environment

권정환

아주대 환경공학과

Monitoring fluctuating concentrations of trace contaminants is one of the most challenging issues in environmental monitoring and subsequent management and regulations. Recently, time-integrated passive sampling techniques have been developed providing a very useful for measuring the time-weighted average concentrations of environmental contaminants. Although sampling kinetics depends on many factors including physicochemical properties of chemical contaminants and field conditions, a simple two-phase kinetic uptake model has been successful for explaining the accumulation kinetics and the sampling rate. Well-established examples of applying passive sampling include monitoring of polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs) in water and air. However, concerns have been raised about emerging environmental contaminants with various physico-chemical properties. For example, it is difficult to extend time-integrative sampling period for polar contaminants having less affinity toward the sampling phases. In this presentation, an overview of principles and field practice of time-integrated sampling will be presented followed by current advances to overcome troubles and to improve the applicability of the method.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-4**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 오정은

QA/QC in Environmental Analytical Chesmitry

이계호

충남대 화학과

화학분석에서 가장 중요한 사항은 정확하고 정밀한 분석 결과를 얻는 것이다. 정확하고 정밀한 분석결과를 얻기 위하여는 분석자 숙련도, 적절한 분석기기, 그리고 표준분석방법의 세가지가 균형있게 충족하여야 한다. 그런데 그동안 한국에서는 분석은 분석기기가 수행하는 것으로 인지되어 고감고 고가의 분석기기가 무분별하게 대량 구입되고 있는 실정이다. 고가 고감도의 분석기기가 너무 많이 설치되어 있는 사실에 비하여 숙련도 높은 분석자는 거의 양성되지 않고 있는 실정이다. 분석자의 사소한 실수가 국가경제에 심각한 영향을 줄 수 있다는 사실은 몇 년 전의 중국산 김치의 중금속 사건에서 찾아 볼 수 있다. 김치 중금속 분석결과에 따라 국내 김치 가공공장 900 여개가 폐업으로 하였고, 국가경제에 심각한 영향을 주었다. 그러나 언론에 발표된 김치 중금속 분석결과는 적합한 품질관리 과정을 거치지 않고 분석한 결과를 공개적으로 발표함으로서 분석결과의 신뢰도에 심각한 문제가 있었다. 정확한 분석결과를 도출하기 위한 품질관리 (QA/QC) 체계를 확립하여야 하며. 아울러 국제적 적합성을 유지하는 국제공인 시스템을 도입하여야 한다. 국제적으로 국가간의 분쟁이 예상되는 다양한 환경 시료에 대한 분석결과들이 국제적으로 상호 인정되는 국제 공인 시스템을 확립하여야 한다. 국제적으로 공인되는 분석결과를 도출하기 위한 필요 충분조건이 무엇이며, 어떻게 수행하는 지에 대하여 발표하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-5**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 오정은

식품 중 유해금속 분석결과의 신뢰도 확보

박경수 전지숙[1] 이지연

KIST 특성분석센터 [1]경희대 화학과

식품공전 시험법은 국내에서 유통되는 시험법이고, 국제적인 기준규격에 맞춘 과학적이고 객관적인 시험법이다. 그러나 식품공전 시험법은 급변하는 기술과 좀 더 효율적인 분석 방법이 반영되어야 할 필요성이 있다. 본 연구에서는 식품공전에 수록된 오래된 분석방법을 현대화된 분석법으로 개선하고, 분석결과에 대한 신뢰도를 확보하기 위하여 검출한계, 정확도, 정밀도 등 몇 가지의 유효성 검증을 확인하였다.연구 방법은 국내외 식품 중 중금속 분석법을 비교하고 각 방법에 대한 차이를 검토하였으며, 식품을 매트릭스 별로 분류하고, 대표 식품을 선정하였다. 또한, 분석 원소 별, 시료 별, 금속 함량 별, 적절한 전처리 방법, 시료 채취량 및 분석기기 등을 기술하여 적절한 시험법을 선택하였으며, 검출한계, 정확도, 정밀도 등 실험실 내외 validation 방법을 토대로 식품공전의 개선 및 현대화와 시험기관의 결과 신뢰성을 확보하였다. 내부 정도 관리는 인증 표준 물질인 NIST 8433 (corn barn)와 NIST 1566B (oyster tissue)을 가지고 앞서 확립한 분석법으로 실험하였으며, 외부 정도 관리는 FAPAS 를 이용하여 수행하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL1-6**

발표분야: Current Issues and Techniques in Quality of Environmental Measurements and Analysis

발표종류: 심포지엄, 발표일시: 목 11:45, 좌장: 오정은

Uncertainty Evaluation of Dioxin Analysis in Human Blood and Food Samples

장윤석

포항공과대 환경공학부

The aim of the present study was to estimate the uncertainty in the final measurement results for the concentration of dioxins in human blood and food samples. This was achieved by taking into account the main sources of uncertainty in the analytical processes. 'The guide to the expression of uncertainty in measurement (GUM)' was consulted during this study. First, by considering the sources of uncertainty for each step of the measurement procedure, the uncertainties in the concentration values for seventeen 2,3,7,8-substituted toxic dioxins and furans were calculated. These individual uncertainties were then combined to give the estimate of uncertainty in the total dioxin concentration. We found that, in the single human blood sample tested in this study, the concentration of dioxin was 0.0746 ± 0.0074 pg I-TEQ/g weight or 20.68 ± 2.04 pg I-TEQ/g lipid. The present work supports the hypothesis that the quality of measured analytical results can be assured by quantitatively estimating the uncertainty values associated with the measurement results.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL2-8**

발표분야: Analytical Chemistry for Bio-Technology

발표종류: 분과기념강연, 발표일시: 목 16:50, 좌장: 차상원

Unveiling aestheic complexity of natural mixture: Past, present and future

김성환

경북대 화학과

There have been many researches devoted to understand the chemical composition of natural mixture such as petroleum and humic substance. However, understanding the mixtures has not been trivial because of their extreme complexity and lack of proper analytical techniques. In Environmental and Energy mass spectrometry laboratory (EEMS Lab) at Kyungpook National University, Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) and comprehensive 2D gas chromatography mass spectrometer (2D GC-MS) have been combined to study petroleum and humic substance at a molecular level. FT-ICR MS is a powerful technique that has enabled us to study heavy and polar components of the mixtures. Resolving power of 500,000 can be routinely obtained with this technique. 2D GC-MS is a fairly recently developed technique and it is very effective in analyzing non-polar and mid-polar compounds at the same time. It is certain that combination of 2D GC-MS and FT-ICR MS will greatly broaden our knowledge on chemical compositions of petroleum and humic substance. Quantitative understanding of the mixtures is very important area of study. So far mass spectrometry is the only technique that can resolve the complexity of the mixtures. However, the quantitative study of the mixtures by mass spectrometry is difficult mainly because of the discrimination occurring during the ionization process. Therefore, mechanistic study of ionization process is currently undergoing in the EEMS Lab by combining quantum mechanical calculation and experimental data.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL2-1**

발표분야: Analytical Chemistry for Bio-Technology

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 조규봉

Electrochemical Sensing of Gasotransmitters

이영미

이화여대 화학나노과학과

In recent years, there have been an increasing interest in signaling gaseous molecules called gasotransmitters. Nitric oxide (NO), carbon monoxide (CO), and hydrogen disulfide (H_2S) are known for their important roles in vasodilation, neurotransmission, cytoprotective effect, and etc. Oxygen (O_2) is also essential for sustaining the lives of most living organisms. Due to the critical functions of these gases, many research efforts have been devoted to develop a strategy for sensing these gasotransmitters. In this presentation, we demonstrate the development of novel electrochemical microsensors and their applications for detecting one or two different gasotransmitters simultaneously in living biological samples. In fact, the electrochemical dual sensors in micro-dimensions are fabricated for the concurrent detection of either NO/CO or NO/O_2. The analytical performances (i.e., sensitivity, selectivity, detection limit, response time, stability, etc.) of these microsensors are verified. The developed sensors are employed for the real-time simultaneous monitoring of either NO/CO or NO/O_2 in living biological tissues such as rat brain and mouse kidney. Simultaneous measurement of two closely linked gasotransmitters can provide fundamental information regarding biological processes in which gasotransmitters are involved.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ANAL2-2**
발표분야: Analytical Chemistry for Bio-Technology
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 조규봉

Integrated Rotary Genetic analyzer for Viral RNA Detection

서태석

KAIST(KAIST) 생명화학공학과

In this study, a fully integrated and portable Rotary Genetic Analyzer for detection of the gene expression of influenza A virus has been developed which includes microglass bead based RNA template purification, Rotary reverse transcriptase polymerase chain reaction (RT-PCR) with real-time monitoring using a miniaturized optical fluorescence detector. A variety of influenza A viruses from animal hosts are continuously prevalent throughout the world which cause human epidemics resulting millions of human infections and enormous industrial and economic damages. Thus, early diagnosis of such pathogen is of paramount importance for biomedical examination and public healthcare screening. To approach this issue, here we propose a fully integrated Rotary genetic analysis system, called Rotary Genetic Analyzer, for on-site detection of influenza A viruses with high speed.The Rotary Genetic Analyzer is made up of four parts including a disposable microchip, thermal blocks for temperature control, a servo motor for precise and high rate spinning of the chip, and a miniaturized optical fluorescence detector. A disposable RT-PCR microchip (50 X 20 X 2 mm) consists of a solid-phase extraction based sample pretreatment unit and 1 μL of the PCR chamber. The microchip is fabricated using a patterned polycarbonate sheet with 1 mm thickness and glass coverslip with 130 μm thickness, which layers are bonded using patterned pressure sensitive adhesive film. Microglass beads with 150~212 μm diameter are introduced into the sample pretreatment chambers and held in place by weir structure for construction of solid-phase extraction system. A thermal block made from duralumin is integrated with a film heater at the bottom and a resistance temperature detector (RTD) in the middle. For the efficient performance of RT-PCR, three thermal blocks are placed on the Rotary stage and the temperature of each block is corresponded to the thermal cycling, namely 95 °C (denature), 58 °C (annealing), and 72 °C (extension).For optimization of sample dispensing, we designed dimension of microchannels. Three different samples were subsequently loaded into the sample pretreatment chamber. From the results, we could dispense an

influenza A H5N1 viral RNA sample (750 RPM for 10 sec), a washing buffer (1300 RPM for 10 sec), and an elution buffer (2200 RPM for 30 sec) by controlling the RPM. The extracted target RNA was successfully amplified confirming by gel-electrophoresis. By controlling the channel geometry, only extracted RNA sample could be moved into the PCR chamber with sealing using mineral oil dispensing and a Rotary RT-PCR reaction was performed with high speed. This fully integrated Rotary Genetic Analyzer could analyze influenza A virus subtype H1N1, H3N2, and H5N1 simultaneously in 30 min. The simple Rotary amplification system was demonstrated, and the target influenza A viruses could be amplified with high sensitivity, rapidity, and multiplicity based on the system.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ANAL2-3**
발표분야: Analytical Chemistry for Bio-Technology
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 조규봉

Mass Spectrometry and Related Methods for Micro-Omics

차상원

한국외국어대 화학과

Among various analytical methods, mass spectrometry (MS) is the major component in omics researches, especially in proteomics and metabolomics. Recent sensitivity and performance improvements in MS and new protocol developments in the sampling allow researchers to perform omics studies with smaller amounts of samples, for example, from organs to sub-organs or from tissues to homogeneous cell populations. 'Micro ?omics' is intriguing because it can provide more relevant and specific molecular portraits for a given biological phenomenon by avoiding 'averaged-out' effects. For micrometabolomics analysis, laser desorption/ionization (LDI) mass spectrometric imaging (MSI) method is a great option because there is no dilution effect and also because spatially-resolved chemical distribution information allows to assess metabolite profiles of smaller features within the sample. Here we present our LDI MSI platforms for small metabolite analysis and their applications. Especially, LDI MSI of small metabolites from Arabidopsis thaliana, one of the most important model plant systems, will be comprehensively discussed in this presentation. For tissue microproteomics analysis, laser capture microdissection (LCM) is a very useful sampling technique since LCM allows the selection of pure cell populations from the heterogeneous tissue specimens via direct microscopic visualization. In addtion, an optimized porous layer open tubular (PLOT) LC method is useful for ultratrace proteome analysis. We recently optimized a microproteomics analysis workflow which combines LCM with a sensitive nano or PLOT LC/MS method. Using this workflow, we have analyzed proteome from breast cancer epithelium and this work will be addressed in this presentation.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ANAL2-4**
발표분야: Analytical Chemistry for Bio-Technology
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 조규봉

MALDI mass spectrometry for Rapid Characterization of Biochips

한상윤

한국표준과학연구원 나노바이오융합연구단

MALDI mass spectrometry offers a unique opportunity of label-free detection of biochips. Its strength arises mainly from its capability of high-speed identification of molecules that are immobilized on the biochip surfaces and captured on the biochips by specific biomolecular interactions. In this presentation, we introduce a new scheme of matrix-free laser desorption/ionization with cation assistance for surface mass spectrometry of self-assembled monolayers of alkanethiolates on gold substrates and gold nanoparticles that provide important platforms for recent biochips and sensors. In addition, we introduce a protocol for the rapid characterization of protein chips using MALDI mass spectrometry. It is demonstrated that the microwave-assisted protein enzymatic digestion method can be successfully applied to the mass spectrometric characterization of proteins captured on the affinity surfaces of protein chips. The method was developed using a domestic microwave, completing the on-chip proteolysis reaction in minutes, whereas the previous on-chip digestion methods by incubation took hours of incubation time. It allowed the characterization of immunosensed proteins by MASCOT search using peptide mass fingerprinting. In an example of this method for protein chip applications, BSA naturally involved in fetal bovine serum was unambiguously identified on a protein chip by imaging mass pectrometry. Along with recent advances in imaging mass spectrometry, this technique will provide a new opportunity for high-speed, and thus high-throughput in the future, label-free mass spectrometric assays using protein arrays.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL2-5**

발표분야: Analytical Chemistry for Bio-Technology

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 차상원

Screening for undeclared erectile dysfunction drugs and analogues in dietary supplements by liquid chromatography hybrid ion trap-time of flight (LC-IT-TOF) mass spectrometry

김운용 강명희[1] 한상범

중앙대 약학대학 [1]서울지방식품의약품안전청 유해물질분석과

Phosphodiesterase type 5 enzyme (PDE-5) inhibitors such as sildenafil, vardenafil, tadalafil, udenafil and mirodenfilare generally prescribed for treatment of erectile dysfunction (ED). Recently, synthetic PDE-5 inhibitors and their analogues have been found in dietary supplements as adulterants.The adulterated analogues in dietary supplements may cause significant pharmacological and toxicological risks such as nausea, chest pains, fainting and irregular heart beat. Therefore, screening method for these synthetic PDE-5 inhibitors is highly required for regulation purpose and public health.Hybrid ion trap-time of flight (IT-TOF) mass spectrometer is powerful tool for screening method and gives more accurate structural information by applying MS^n analysis and accurate mass measurement of precursor and product ions. Thus, it is possible to build accurate MS^n library of the analytes. In this study, we developed an analytical method for simultaneous determination and built MS^n library of 38 PDE-5 inhibitors and their analogues by using IT-TOF. The separation was performed on Capcell PAK C_{18} UG120 (2.1 x 150 mm, 3 μm) column using gradient elution. Acetonitrile and 0.2% acetic acid wereused as mobile phase. The linearity was estimated as linear correlation coefficient (r^2) over the concentration ranged from 0.13 to 4.0 μg/mL. The linear correlation coefficients were excessed of 0.99 for all of the analytes. The intra- and inter- day accuracy and precision were 86.7 ~ 112% and 0.55 ~ 10.48%, respectively. The developed method was successfully applied to the adulterated dietary supplement.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL2-6**

발표분야: Analytical Chemistry for Bio-Technology

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 차상원

Mass spectrometric approaches to the study of membrane protein phosphorylation

박강식

경희대 의학과

Ion channels are membrane proteins responsible for regulating membrane excitability in neuron. Phosphorylation has been shown to play a major role in ion channel gating, trafficking, and cellular mechanism. We have recently applied mass spectrometric-based approaches to identify and quantify phosphorylation at specific sites on native ion channels immunopurified from mammalian brain using specific antibodies. Our previous studies have begun to show a noteworthy extent of in vivo ion channel phosphorylation in brain. Here, I show examples of the advantages of employing newly developed mass spectrometric-based approaches to explore the identification and characterization of ion channel phosphorylation in regulating the function of the channels.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ANAL2-7**
발표분야: Analytical Chemistry for Bio-Technology
발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 차상원

Single-molecule in solution: heterogeneity and dynamics

이남기

포항공과대 시스템생명공학부/물리학

Single-molecule spectroscopy has been one of the most successful physical chemistry approaches for biological problems. Currently single-molecule techniques are most essential and popular tools for molecular and cell biology area. In this presentation, I will introduce one of the popular single-molecule techniques, named alternating-laser excitation fluorescence resonance energy transfer (ALEX-FRET). Since ALEX technique has been developed, its application for biological problem has been expanded widely, including transcription, folding, enzymatic reaction, etc. The power of ALEX is to discriminate fluorescent species based on their labeling status as well as measuring FRET efficiency, which reports distance in 2-10 nm range. Here I will show two recent applications of ALEX for biological problems. First, probing protein oligomerization. Most proteins in cells have homo- or hetero-oligomeric forms as their functional units and these oligomeric states are often modulated by local environments. However, the method for directly revealing the oligomeric form of a protein is limited. Using ALEX, we directly distinguish among oligomers from monomers to tetramers and determine their quaternary structures of RecR, which is essential protein for DNA repair. Second, probing synaptic vesicle fusion. Neurons use membrane fusion of synaptic vesicles (exocytosis) to release neurotransmitters for inter-neuronal communication. This fusion process is controlled by SNARE proteins, but its detailed mechanisms are still unknown. We applied ALEX for studying vesicle fusion process at the single-vesicle level, which revealed the detailed processes of initial fusion step, i.e., docking.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO1-1**

발표분야: Synthesis and Delivery of Drugs

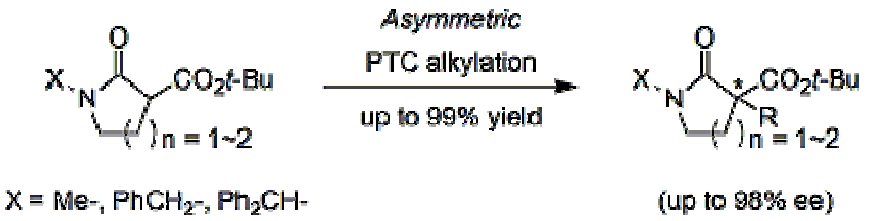
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 임태연

Construction of β-Quaternary Chiral Pyrrolidine & Piperidine Systems and Their Applications

박요한

인제대 약학대학/약학과

A new enantioselective α-alkylation of α-tert-butoxycarbonyllactams for the construction of β-quaternary chiral pyrrolidine and piperidine core systems is reported. α-Alkylations of N-methyl-α-tert-butoxycarbonylbutyrolactam and N-diphenylmethyl-α-tert-butoxycarbonylvalerolactam under phase-transfer catalytic conditions (solid potassium hydroxide, toluene, -40 °C) in the presence of (S,S)-3,4,5-trifluorophenyl-3,3′,5,5′-tetrahydro-2,6-bis(3,4,5-trifluorophenyl)-4,4′-spirobi[4H-dinaphth[2,1-c:1′,2′-e]azepinium] bromide [(S,S)-NAS Br] (5 mol %) afforded the corresponding α-alkyl-α-tert-butoxycarbonyllactams in very high chemical (up to 99%) and optical yields (up to 98% ee). Our new catalytic systems provide attractive synthetic methods for pyrrolidine- and piperidine-based alkaloids and chiral intermediates with β-quaternary carbon centers. As the applications of the new synthetic methods, natural alkaloid, (+)-isonitramine was synthesized in 12 steps (98% ee and 43% overall yield) from δ-valerolactam and β-quaternary chiral pyrrolidine and piperidine derivatives were synthesized for anticancer activity researches.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO1-2**

발표분야: Synthesis and Delivery of Drugs

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 임태연

Green synthesis of gold and silver nanoparticles by using natural products and their applications

박유미

인제대 약학대학

The most common synthesis of metallic nanoparticles has utilized chemical reducing agents to reduce the corresponding salts to create uniform suspensions. Currently, sustainability initiatives that use green chemistry to improve and protect our global environment are becoming focal issues in many field of research. Instead of using toxic chemicals for reduction and stabilization of metallic nanoparticles, the use of various biological entities has received considerable attention. Among the many possible natural products, polysaccharides and biologically active plant products represent excellent scaffolds for this purpose. Polysaccharides have hydroxyl groups, a reducing ends, and other functionalities that can play important roles in both the reduction and the stabilization of metallic nanoparticles. Among the various categories of compounds in plants that have potent biological activities, phytochemicals are emerging as an important natural source for the synthesis of metallic nanoparticles. Polysaccharides and phytochemicals possess their own biological activities which together with the intrinsic biological activities metallic nanoparticles often show synergistic effects as nanocomposites. In this talk, the immobilization of ginsenoside Rg3 on gold nanoparticles (AuNPs) will be discussed. Recent publications reported that the tethering anticancer drug on AuNPs enhances its anticancer activity. In addition glycosaminoglycans (chondroitin sulfate and acharan sulfate) and plant extracts were used as a reducing/stabilizing agent for the synthesis of silver nanoparticles (AgNPs). Surface plasmon resonance band, HR-TEM and AFM images indicated that the formation of AgNPs were successful. The newly prepared AgNPs exhibited remarkable enhancement in antibacterial activities against Pseudomonas aeruginosa, Escherichia coli and Enterobacter cloacae when compared with controls. At in vivo rat model of wound healing activity, chondroitin and acharan sulfate-reduced AgNPs showed the comparable

wound healing activity to that of commercially available silver sulfadiazine. Also several plant extracts will be introduced for the green-synthesis of AuNPs and AgNPs.

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO1-3**

발표분야: Synthesis and Delivery of Drugs

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 임태연

Nanoformulations for improving oral bioavailability of poorly absorable drugs

김민수

인제대 제약공학과

Recently, nanoscience and nanotechnology have been attracted significant attention in modern society. Nanoparticles have attracted intensive interest in many different fields, including semiconductor, chemicals, biology and drug delivery. Especially, nanoparticulate drug delivery systems are claimed to have a faster onset of action, enhanced bioavailability, targeted delivery, predictable therapeutic response and greater efficacy/safety. Nanoparticles can be produced by the top-down (wet milling and high pressure homogenization) and bottom-up (antisolvent precipitation, solvent evaporation and supercritical fluid process) approaches. During the recent years, nanonization processes that use supercritical fluids have received increasing attention from the scientific community. Indeed, supercritical fluids are characterized by a continuously adjustable solvent power/selectivity obtained by varying pressure and temperature. In this presentation, nanodrug particles and nanoformulations for drug delivery will be introduced and discussed for its usefulness in drug development and also two studies are going to be shown for pharmaceutical application using a novel nanotechnology. One study is on the development of new dosage form for poorly absorbable API using a novel nanoformulation and the other is on the development of a novel supercritical fluid technology as platform technology for the production of particles with a controlled size and size distribution in the micrometric as well as in the nanometric range.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO1-4**

발표분야: Synthesis and Delivery of Drugs

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 임태연

Discovery of new Biomarkers and Therapeutic targets for respiratory diseases

임태연

한양대 공과대학 생명공학과

천식은 잘 알려진 질환으로 생각하기 쉽지만 아직까지 원인치료제가 없는 질환의 하나다. 굉장히 많은 수의 단백질과 유전자가 질환의 발생과 악화에 관련되어 있을 것이라고 생각되고 있지만, 이전까지의 방법으로는 연구의 한계가 있을 수밖에 없다. 따라서 본 연구자는 질환과 관련이 되어있을 많은 유전자 및 단백질을 편견없이 연구하기 위하여 단백체 및 전사체 분석을 통하여 천식 등 호흡기 질환과 관련성이 있는 단백질 및 유전자 후보군을 질환의 바이오마커로 발굴하여왔다. 동시에 이와 같은 바이오마커를 조절하는 방법을 통하여 질환의 정도를 조절할 수 있는지 검토함으로서 새로운 신약을 개발할 수 있는 정보를 제공하고자 하는 연구를 수행하여왔다. 본 발표에서는 이렇게 발굴한 호흡기 질환에서의 바이오 마커를 DDS 등의 방법을 위하여 어떻게 질환의 치료방법으로 개발할 수 있을지에 대한 논의를 하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO1-5**

발표분야: Synthesis and Delivery of Drugs

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 임태연

Functional DNA with nanomaterials for environmental and biomedical applications

이정헌

성균관대 신소재공학부

While DNA is generally known to be a passive biomolecule containing genetic information, they have recently been recognized as a programmable and tailorable material with functional activity. First, I will introduce an effort to use gold nanoparticles and UO22+ (uranyl) specific DNAzyme for development of highly sensitive and selective colorimetric uranyl sensors. In addition, I will discuss how DNA aptamers can be delivered by plasmonic gold nanoparticles to cancer cell nucleus and released by NIR ultrafast femtosecond pulsed laser for targeted cancer therapy. These interesting functional and structural properties of DNA can provide new opportunities to develop dynamic DNA structures for potential use as enviromental analysis and drug delivery agents.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO2-1**

발표분야: Studies on the Protein Structure and Its Application

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김용학

Structure and function of sterol binding proteins in lipid homeostasis and resistance to antifungal agent

임영준

전남대 약학부

Azole drugs inhibit the biosynthesis of ergosterol, the essential component of fungal plasma membrane. Upc2, a zinc cluster transcription factor, is a regulator of ergosterol biosynthesis in yeast. In response to sterol levels in the cell, the transcriptional activity of Upc2 is regulated by the C-terminal domain. Resistance to azole drugs in Candida albican is partly due to the mutations of Upc2 gene leading to constitutive activation of the transcription factor. In order to obtain a structural insight into the regulatory mechanism of Upc2, we determined the 3 dimensional structure of the C-terminal domain of Upc2 and discovered a specific ligand for Upc2. Based on structure-guided biochemical and cell biology studies we find that Upc2 is one of the fungal nuclear receptors. In this presentation, structure and a regulatory mechanism of Upc2 will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO2-2**

발표분야: Studies on the Protein Structure and Its Application

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김용학

Structural understanding of the oxidation-induced activation process of a molecular chaperone, Hsp33

원형식

건국대 생명과학부

Hsp33 is a prokaryotic molecular chaperone of which activity is regulated by redox potential. The oxidation-induced unfolding and concomitant dimerization constitutes the activation process of Hsp33. In this study, solution structure of the reduced, inactive Hsp33 monomer from *Escherichia coli* was characterized by NMR. Although the overall conformation was observed to be similar to that previously shown in the crystal structure of the reduced, dimeric Hsp33, three specific regions around the interdomain linker, beta-strand 1 and alpha-helix 1 hardly exhibited NMR signals. Molecular dynamics simulation predicted beta-to-loop conversion of the linker strand, which contacts to the N-terminal beta-strand 1. N-terminal six-residue deletion resulted in more NMR signals observed. Thus, the inactive, reduced Hsp33 monomer in solution is suggested to exist with a dynamic conformational exchange at the linker strand and its counterpart, the N-terminal strand. Then, the N-terminal nine or more residue deletions that probably destroy the beta-strand 1 led to the formation of constitutively active dimers, without unfolding of the C-terminal redox-switch domain. It is conclusively suggested that the observed linker dynamics is a key factor handling the activation process of Hsp33.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO2-3**

발표분야: Studies on the Protein Structure and Its Application

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김용학

Molecular mechanism of CueP action in the intracellular pathogen Salmonella enterica serovar Typhimurium

하남출

부산대 제약학과

Salmonella enterica serovar Typhimurium (S. Typhimurium) has evolved to survive in the phagosome of macrophages. It was reported that CueP confers to copper resistance to S. Typhimurium under anaerobic conditions. However, the biochemical role of CueP with respect to copper resistance remains unclear, and no crystal structure of CueP or its homologue has been determined. In this study, we determined the crystal structure of CueP, revealing the V-shaped dimeric structure with a disulfide bond in each protomer. Subsequent biochemical experiments showed that CueP specifically mediates the reduction of the copper ion using electrons released during the formation of the disulfide bond. We observed that the copper ion-mediated Fenton reaction in the presence of hydrogen peroxide was blocked by CueP in vivo as well as in vitro. Consistently, the survival rate of a cueP-deleted strain of Salmonella in macrophage phagosome was significantly reduced. Based on these observations, we propose a molecular mechanism for CueP in neutralizing copper ion-mediated Fenton reaction. This study provides insight into how S. Typhimurium can survive in the phagosome of macrophages that produce hydroxyl radicals by the copper ion-mediated Fenton reaction.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO2-4**

발표분야: Studies on the Protein Structure and Its Application

발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 하남출

The study of ecotoxicology using 1H NMR-based metabolomics

김석만

부산대 화학과

Metabolomics is a part of system biology, it has shown that the great potential of finding biomarker group for disease diagnosis and toxicity assessment. Usually, NMR (Nuclear Magnetic Resonance) and chromatography-mass spectrometry are used to analyze as many metabolites with the molecular weights smaller than 1000 daltons as possible. Multivariable statistical analysis methods are used to classify different groups, and define the significantly changed metabolites to identify new biomarkers.The presentation will discuss several applications of NMR-based metabolomics study; disease diagnosis, toxicity of polymer, forensic applications and focused on environmental toxicology extensively. It includes different kinds of samples; human and animal urine, serum, tissue, cultured cell and extracts. Recent development in NMR field, researcher could measure gel or semi-solid sample with HR-MAS (High Resolution-Magic Angle Spinning) or nano-probe. In this study, tissues are used for 1D proton measurement without pre-treatment. It shows similar resolution with solution 1D spectrum and much fast total analysis time. This technique could apply serum or blood sample because those samples have high viscosity in some case.This study demonstrates the usefulness and versatility of NMR spectroscopy coupled with multivariate analysis in investigating the metabolic response to external stimuli and identifying the responsible individual metabolites and/or metabolic pathways. And these kinds of analysis could provide the information related to the environmental influences by the chemicals.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO2-5**

발표분야: Studies on the Protein Structure and Its Application

발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 하남출

Alterations in protein function and cellular mechanism by protein oxidation

김용학

대구가톨릭대 의학과/미생물학

Protein oxidation caused by reactive oxygen species (ROS) alters not only protein structure and function, but also cellular state. Cysteine oxidation is the most common posttranslational modification of protein that occurs in response to ROS generation in physiological conditions. A ROS-sensitive protein can change its structure and function and induce various cellular responses - such as alterations in growth rate and metabolism under environmental and chemical stresses. For example, *Pseudomonas fluorescens* strain KU-7 has 2-nitrobenzoate 2-nitroreductase (NbaA) which comprises a homodimeric protein with a flavin (FMN) cofactor. This enzyme transforms 2-nitrobenzoic acid (2-NBA) to 2-hydroxyaminobenzoic acid in reducing condition, but alters its substrate specificity from 2-NBA to 2,4-dinitrobenzoic acid under oxidizing conditions in which it forms the higher-order oligomers through the formation of intermolecular disulfide bonds. Furthermore, NbaA and its mutant proteins, when overexpressed in *Escherichia coli*, alter the cellular sensitivity to ROS and some antibiotics. Non-reducing/reducing diagonal electrophoresis and mass spectrometry analyses help us understanding the cellular changes in oxidative stress conditions which cause the increase in endogenous ROS levels and lead to posttranslational oxidative modifications and down-regulations of abundant proteins in cells. This presentation shows that posttranslational oxidative modification of protein is not only important for protein structure and function, but also for the induction of various cellular changes in response to oxidative stress caused by ROS generation. In such conditions, understanding protein oxidation will help us to understand functions and dysfunctions of ROS-sensitive proteins, and provide insights in endeavoring after preventions and therapies against oxidative stress-related diseases and illnesses.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN1-1**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 홍석원

Transiton Metal-Catalyzed Coupling Reactions of Propiolic Acids

이선우

전남대 화학과

We reported the decarboxylative coupling of alkynyl carboxylic acids and aryl halides using a palladium catalyst, which provides an efficient method for the synthesis of unsymmetrical and symmetrical diaryl alkynes. Aryl alkynes are important building blocks in the preparation of pharmaceutical and conjugated functional materials. The employment of alkynyl carboxylic acids as an alternative to terminal alkynes provides a very useful tool in the handling of alkynes with a low boiling point. Since we first reported the decarboxylative coupling reactions, a variety of such reactions involving alkynyl carboxylic acids have been reported by many research groups. Herein, we discuss a number of coupling reactions which are related to the decarboxylative couplings of propiolic acids including the selective coupling reaction, the multicomponent reactions and the carbonylations.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN1-2**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 홍석원

Catalytic Enantioselective Carbon-Carbon Bond Formation of Diazoesters with Aldehydes

류도현

성균관대 화학과

The chemistry of α-diazocarbonyl compounds has attracted great attention because of its extensive applications in organic chemistry since the first recorded synthesis of ethyl diazoacetate by Curtius in 1883. Recently, we developed highly enantioselective, catalytic carbon-carbon bond formation reactions of diazoesters with aldehydes. Enantioselective cyclopropanation reactions via Michael- initiated ring closure between diazoacetates and α,β-unsaturated aldehydes are highly desirable as the corresponding cyclopropanes containing two or more electron-withdrawing groups can be valuable synthetic intermediates for various applications. In the presence of chiral (S)-oxazaborolidinium cation as catalyst, catalytic synthetic approach to get the highly functionalized cyclopropane was investigated. Reactions proceeded in high yield with high to excellent diastereoselectivity and enantioselectivity. In addition, a catalytic route toward chiral α-alkyl-β-ketoesters using asymmetric Roskamp reaction of α-alkyl diazoester with aldehydes has been developed. The reaction proceeds with high to excellent enantioselectivities and this methodology was applied to a concise two-step synthesis of the natural pheromone sitophilate.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN1-3**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 홍석원

Homogeneous Catalyst Development for Atom Economical C-N Bond Formation

홍순혁

서울대 화학과

Development of useful, practical, and selective synthetic methods that generate minimal by-product is of critical importance in both academic and industrial research. The research of our group seeks to develop practical and environmentally friendly synthetic methodology using transition metal catalysts. Specifically, we have explored atom-economical catalytic C-N bond formation reactions. A few topics with this theme-Ru catalyzed amide synthesis directly from alcohols, selective sp3 C-O bond cleavage, and other C-N bond formation reactions-will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN1-4**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

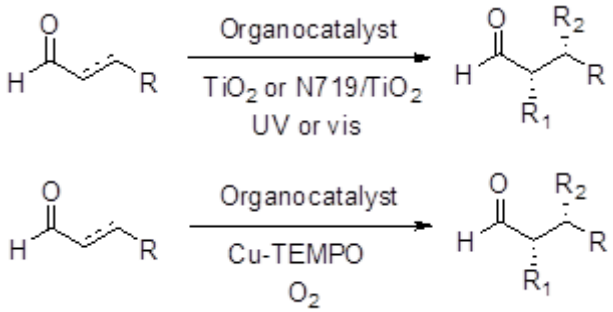
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 강은주

Merging Transition-Metal Catalysis with Asymmetric Organocatalysis

장혜영

아주대 화학과

Asymmetric enamine and iminium catalysis have been provided a wide range of enantiomerically enriched organic compounds which are the key structure for pharmaceuticals and natural product synthesis. In the context of expanding the scope of enamine and iminium organocatalysis, various transition metal complexes have been introduced to asymmetric organocatalytic reactions, rendering unexpected bond formations with high levels of stereoselectivity. In this presentation, our recent accomplishments regarding asymmetric organophotocatalytic reactions using TiO_2 and N719/TiO_2 photocatalysts, and multistep organocatalytic reactions involving copper complexes will be presented.References1) H.-S. Yoon, X.-H. Ho, J. Jang, H.-J. Lee, S.-J. Kim, H.-Y. Jang, Org. Lett. 2012, 14, 3272.2) X.-H. Ho, H.-J. Oh, H.-Y. Jang, Eur. J. Org. Chem. 2012, ASAP.3) X.-H. Ho, M.-J. Kang, H.-Y. Jang, Catal. Sci. & Technol. 2011, 1, 923.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN1-5**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

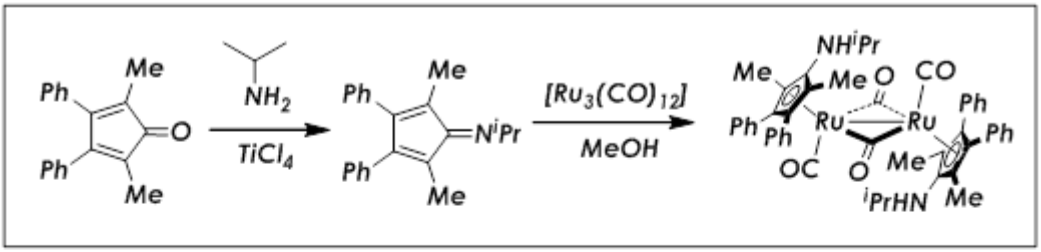
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 강은주

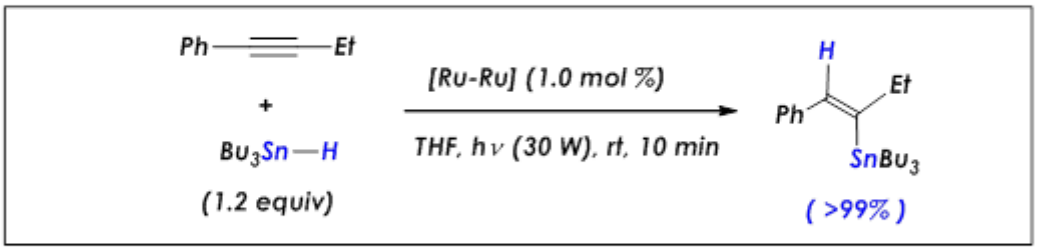
Catalysis with Diruthenium Complex and Fluorescent Light

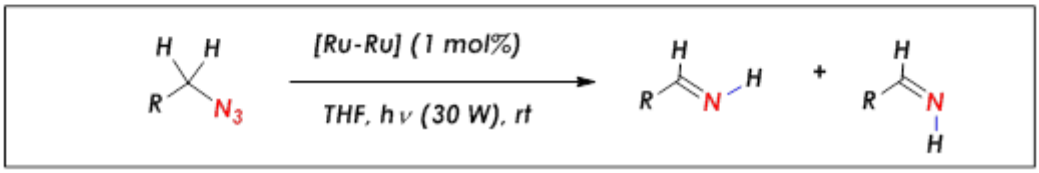
박재욱

포항공과대 화학과

Recently, our group reported the synthesis of an isolable diruthenium complex and its utilities for the chemoenzymatic dynamic kinetic resolution of secondary alcohols and the chemoselective hydrosilylation of aldehydes under photolytic conditions using household fluorescent light.[1,2] In addition to these results, new findings about the activation of hydrostannanes and organic azides with the ruthenium complex under fluorescent light will be presented.References1. (a) Hyunjin Kim, Yoon Kyung Choi, Jusuk Lee, Eungyeong Lee, Jaiwook Park, Mahn-Joo Kim, Angew. Chem. Int. Ed. 2011, 50, 10944. 2. Youngshil Do, Junghoon Han, Young Ho Rhee, Jaiwook Park, Adv. Synth. Catal. 2011, 353, 3363.







대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 신승훈

Palladium-catalyzed chemical transformations of modified Morita-Baylis-Hillman adducts

김재녕

전남대 화학과

The Morita-Baylis-Hillman reaction, which involves the coupling of activated vinylic systems with electrophiles under the catalytic influence of a tertiary amine, gives rise to adducts (Morita-Baylis-Hillman adducts) with a new stereocenter and has proven to be a very useful carbon-carbon bond-forming method in the synthesis of highly functionalized molecules. Palladium-catalyzed chemical transformations of Morita-Baylis-Hillman adducts started very recently, but have already provided many interesting results. In the presentation, I would like to share our recent results on the palladium-catalyzed chemical transformations of modified MBH adducts. The results involved the following basic and important concepts: chelation-controlled 5-*exo* carbopalladation, C(sp^3)-H activation, formal δ-carbon elimination/decarboxylation, and activation of aryl C-H bond.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN2-2**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 홍승우

Synthesis of Organic Materials via Solid State Grinding

허남회

서강대 화학과

Synthesis of organic materials via solid state grinding will be presented. The grinding method utilizes mechanical forces to accelerate chemically driven reactions, which is performed by grinding the solid reactants using a mortar and pestle. For example, simple grindings of solid hydrazines and carbonyl compounds produced azine derivatives, which provide excellent selectivities over 97% towards azine formation as compared with conventional solution-based methods. Another important example is that the imines can be isolated as the sole products in greater than 97% yields simply by grindings of carbamates and aldehydes. The grinding methodology does not require any solvent and/or additives, which provides an environmentally benign process for preparing various organic materials and could be exploited for industrial applications.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN2-3**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 홍승우

Tandem Olefin Metathesis 반응과 전자재료로의 응용

최태림

서울대 화학부

Tandem olefin metathesis 반응을 이용하여 다양한 다중 고리화합물을 만들 수 있는데, 여기서는 small ring 과 large ring 이 fused 되어있는 bicyclic compound 의 효율적 합성과 이에 응용된 tandem olefin metathesis polymerization 의 concept 을 소개한다. 더 나아가 이 고문자 물질의 Diels-Alder 반응으로 복잡계 물질들의 획기적 합성법을 제시한다. 마지막에는 유사 반응을 이용하여 단분자 wire 의 합성법을 소개하고, 이의 미래 재료로의 가능성을 제시하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN2-4**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 손정훈

Targeting protein-protein interactions using chemical tools

임현석

포항공과대 화학과

Protein-protein interactions (PPIs) are fundamental to most biological processes, and disregulation of PPIs is linked to various disease states. Therefore, molecules that can modulate these interactions would be valuable research tools to uncover molecular functions of target proteins and could be potential therapeutic candidates. However, discovering such molecules is among the most difficult challenges in chemical biology and drug discovery due to the fairly large and flat protein interfaces. Typical small ‘drug-like’ molecules may not be suitable to effectively cover such extended protein contact areas. Thus, there is an urgent need for the development of different types of molecules to target protein interfaces. In this talk, I will present our efforts to develop such molecules, which could serve as excellent sources of modulators of PPIs.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN2-5**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 손정훈

Neopentyl Glycol (NG) Class Amphiphiles for Membrane Protein Crystallization

채필석

한양대 생명나노공학과

Integral membrane proteins (IMPs) play critical roles in biology. Understanding of these bio-macromolecules is, however, extremely challenging, mainly due to difficulties of handling and analyzing these proteins in an aqueous solution. Bringing such proteins into aqueous solution generally requires the use of an amphiphilic agent to overcome the intrinsic incompatibility between the large lipophilic surfaces displayed by IMPs in their native forms and polar solvent molecules. Conventional detergents are popularly used for the purpose, but the resulting protein-detergent complexes (PDCs) are often not optimal for membrane protein structure determination. Therefore, we have developed novel classes of amphiphiles to improve upon the properties of conventional detergents. Among these agents, NG class of amphiphiles is particularly promising because they displayed favorable properties in many diverse membrane protein applications. As a result, NG amphiphiles have contributed to help obtain several new crystal structures of membrane proteins including G-protein coupled receptors such as β_2 adrenergic receptor and muscarinic acetylcholine receptors. These results raise the prospect that NG class amphiphiles will prove to be generally useful tools for structural biology of membrane proteins.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI-1**

발표분야: Medicinal Ventures in Korea

발표종류: 분과기조강연, 발표일시: 목 14:30, 좌장: 김재승

A 40 year-journey in search of selective antiviral chemotherapy

Erik De Clercq

Rega Institute for Medical Research, Belgium

My search for a selective antiviral chemotherapy started more than 40 years ago with interferon inducers, then shifted to nucleoside analogs with the discovery of BVDU (brivudin), a highly selective anti-HSV-1 and anti-VZV agent, and to dideoxynucleoside analogs such as d4T (stavudine), as anti-HIV agents. The search culminated in the discovery of acyclic nucleoside phosphonates (ANPs: cidofovir, adefovir, tenofovir) (in collaboration with the late Antonin Hol?), a key class of compounds active against HIV, hepatitis B virus (HBV), and DNA viruses at large; the best known of these compounds is tenofovir, now approved for the treatment of HIV and HBV infections and for the prevention of HIV infections. Along the way, the principle of the non-nucleoside reverse transcriptase inhibitors (NNRTIs) was established. This work, initiated in collaboration with the late Paul A.J. Janssen, eventually led to the identification of rilpivirine as perhaps the "ideal" NNRTI.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI-2**

발표분야: Medicinal Ventures in Korea

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김재승

CrystalGenomics: from Protein Structure to New Drug

노성구

크리스탈지노믹스(주)

CrystalGenomics Inc. is a clinical stage biopharmaceutical company with protein structure based drug discovery and clinical development capabilities, headquartered in Seoul, Korea with a US presence for multi-national clinical management (CG Pharmaceuticals, Inc.) in Emeryville, California and publicly traded on KOSDAQ exchange (Korea).CrystalGenomics is dedicated to the discovery and development of novel pharmaceuticals in areas of infectious disease, cancer, and inflammatory diseases. The company's capabilities have been validated thru prestigious publications including a cover page on nature for scientific accomplishment (2003), R&D collaborations with prominent pharmaceutical companies including AstraZeneca (2010), and a joint venture deal with ProQuest Investments involving a very early stage asset (2008).The Company's lead development candidate is a next generation NSAID, CG100649 with a novel mechanism of suppressing COX-2 as well as carbonic anhydrase enzymes for improved cardiovascular, gastrointestinal, and renal safety profiles which is in preparation of Phase 3 study for osteoarthritis. Additionally, its novel HDAC inhibitor, CG200745 for cancer is in Phase 1, and a novel antibiotic candidate, CG400549 for MRSA infection, is in Phase 2a Study in the US.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI-3**

발표분야: Medicinal Ventures in Korea

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 남기엽

Clinical Development of Tanibirumab, anti-KDR Neutralizing Fully Human Antibody and its Next Generation Therapeutics

유진산

파멥신

I will present our preclinical and phase I clinical study update of anti-KDR neutralizing fully human IgG1, Tanibirumab which has cross-species cross reactivity. I will also talk about our recent progress from dual target neutralizing multifunctional Ig like next generation protein therapeutics, DIG-KT (KDR & Tie2) from DIG-bodies platform, and PIG-KM (KDR & cMET) from PIG-bodies platform.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI-4**

발표분야: Medicinal Ventures in Korea

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 남기엽

New drug development pipelines in Oscotec

김세원

(주)오스코텍 연구소

Oscotec was found in 1998 and our main research area is new drug development targeting osteoporosis, arthritis and cancers. We have three R&D centers at Pangyo, Chuncheon and Boston USA. Boston R&D center belongs to Genosco which is US subsidiary of Oscotec. OCT-1547, the first new drug candidate of Oscotec, is in the Phase I clinical trial under the approval of US FDA. Currently our main areas of interest are several kinase inhibitors such as FLT3 (for acute myeloid leukemia), SYK (for rheumatoid arthritis) and LRRK2 (for Parkinsonism). Recent R&D results of these pipelines will be introduced.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI-5**

발표분야: Medicinal Ventures in Korea

발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 남기엽

Introduction of Medifron_DBT and Attacking Alzheimer's Disease

김영호 이지우[1] 서영거[2]

메디프론디비티 중앙연구소 [1]서울대 약학대학 약학과 [2]서울대 약학대학 제약학과

Medifron_DBT Inc. is a Korean biotechnology company focused on the discovery and development of the New Drugs for human central nervous system diseases. Medifron_DBT has developed especially in therapeutic areas with unmet medical needs such as Alzheimer's disease and neuropathic pain since 2001.Now the Company has leads and candidates act as beta-amyloid aggregation and toxicity inhibitors and RAGE modulators for Alzheimer's disease. Company has made contract 'licensing and collaboration' with Hoffmann La Roche for RAGE modulators year 2010. DaeWoong Pharmaceutical company and Medifron_DBT has collaboration activity for beta-amyloid aggregation and toxicity inhibitors since 2008.For the attacking Alzheimer's disease, we need disease modifying ability and better efficacy drugs. We have beta-amyloid targeted compound called AlzMedex-PM which has beta amyloid aggregation and toxicity inhibiting activity and plaque solubilization activity. Another anti-AD drug called AlzMedexR-PM which has RAGE-abeta interaction inhibiting activity.In-vivo efficacy studies on the disease mouse model, Double Transgenic Mouse (APPswe/PS1dE9) showed strong efficacy for disease modification including effects of lowering abeta peptides and memory recovery. The result of in-vivo studies showed strong evidences for disease modifying ability of those drugs.As of October, 2012, AlzMedex-PM is at the stage of human phase I single dose ascending completion. Primary GLP studies for toxicity and systemic PK studies were done with successful results.This work was supported by National Research Foundation grant funded by the Korea government (MOHW and MEST) as a part of Korea Alzheimer's Disease Center and Global Drug Candidate Development Program for Neurodegenerative Diseases.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT1-1**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 최남순

고분자 코팅에 의한 Ni-기반 양극 소재의 전기화학적 특성 향상 연구

정경윤 김광범[1] 장원영 김동현[1] 조병원

KIST 에너지융합연구단 [1]연세대 신소재공학과

리튬 이차전지는 주로 모바일 IT 기기의 전원으로 사용되어졌지만 전기자동차(EV) 및 하이브리드 전기자동차(PHEV) 등 친환경 자동차 분야로 인하여 광범위하게 연구되어지고 있다. 그러나 최근의 리튬 이차전지는 전기자동차(EV) 및 하이브리드 전기자동차(PHEV)의 요구조건인 고출력, 내구성, 안정성적인 측면을 만족하기엔 무리가 있다. 이러한 요구조건을 만족하기 위해서 Ni-기반의 양극 활물질이 후보 물질로 채택되었는데 이는 Ni-기반의 양극활물질이 200mAhg-1 의 고용량을 나타냄으로써 기존의 LiCoO2 양극활물질보다 더 높은 에너지 밀도를 가질 수 있기 때문이다. 또한 희유금속으로 가격이 비싼 코발트(Co) 사용량을 줄임으로써 가격적인 측면에서도 유리하기 때문에 Ni 기반의 여러 가지 조성의 화합물들이 연구되어 지고 있다. 그러나 이러한 Ni-기반의 양극 활물질의 경우, 사이클이 진행됨에 따라 발생하는 큰 용량 감소 및 열적 불안정성적 측면이 이들의 상업화를 막고 있다. 이러한 문제들이 발생되는 요인들 중 하나는 양극 활물질 입자 표면에서 Ni 이온이 가지는 반응성과 관련이 있는데 즉, 전극과 전해질 사이에서의 발생하는 부반응이 양극 활물질의 사이클 진행에 따른 용량 감소 및 열적 특성 저하와 같은 전극의 열화 현상을 나타낸다. 이러한 문제들을 극복하기 위해서 양극 활물질에 이종 원소(Co, Al, Mn, Zr, …)를 도핑하거나 양극 활물질 표면을 개질(ZrO2, Al2O3, AlF3, …)하는 등 여러 방법들이 연구되고 있다. 이러한 도핑 및 표면개질 처리는 사이클에 따른 양극 활물질의 용량 감소 억제 및 열적 안정성 향상 등의 효과를 보여준다. 이러한 도핑 및 표면개질 등의 효과를 확인하기 위해 sol-gel 법을 이용하여 LiNi0.8Co0.15Al0.05O2 양극활물질을 합성한 뒤 전도성 고분자로 양극활물질 표면을 개질하였다. 이러한 양극활물질 입자 표면의 전도성 고분자 개질이

나타내는 효과에 대한 분석은 X-ray Diffractometer (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Raman Spectroscopy, Multichannel Battery Tester 등을 이용하여 알아볼 것이다.

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT1-2**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 09:35, 좌장: 최남순

Magnesium Battery : Challenges & Opportunities

홍승태

대구경북과학기술원(DGIST) 에너지시스템공학

A prototype for a rechargeable magnesium battery was reported in 2000 by Aurbach group, which comprised a Chevrel phase MgxMo6S8 and thin Mg foil as the positive and the negative materials, respectively. The key to the success of the system was the electrolyte which enabled the reversible dissolution/deposition of magnesium from/onto the magnesium foil. But it has a limited electrochemical window of ~2V. The energy density of the cell was about 25% of the lithium ion batteries. However, the magnesium battery system has a potential to provide a comparable or even higher energy density than lithium ion batteries because, in principle, the magnesium anode and the positive materials could provide more than two times of capacities even with about one volt lower in the cell voltage. It could be possible only if higher energy density positive materials and electrolytes with wider electrochemical potentials are developed. During the last decade a lot of materials have been claimed to show reversible magnesium intercalation. However, many of the results are to be carefully examined again because of unknown side reactions occurring during the test, mainly due to the underdevelopment of proper electrolytes. No dramatic improvement in electrolytes has been made in terms of electrochemical window and versatility. At this symposium, a concrete analysis of the previously reported materials will be given, focused on positive materials. Some of new materials showing a reversible magnesium intercalation will be discussed, demonstrating a promising opportunities in this new field.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT1-3**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 최남순

Nanostructuring of Si-based Bulk Materials Anodes for High-Peformance Lithium-Ion Batteries

박수진

울산과학기술대 에너지공학부

For practical application, advanced lithium-ion battery systems are vital to meeting the continuous energy demands and leveling the intermittent and cyclic nature of these energy sources. Creation of nanostructured electrode materials represents one of the most attractive strategies to dramatically enhance battery performance, including capacity, rate capability, cycling life, and safety. Here, we present nanostructuring of silicon-based anode materials for lithium-ion batteries. We employed commercially available bulk Si or SiO powder to produce three-dimensional porous Si-based anode materials, by combining a metal deposition and metal-assisted chemical etching process. The Si-based electrodes having porous structures accommodate large volume changes during lithium insertion and extraction. These materials showed a highly stable cycling performance over 100 cycles. The synthetic route described herein is simple, low-cost, and mass producible (high yield of >50% in over tens of gram scale per batch), and thus, provides an effective method for producing high-performance anode materials. Also, we present a simple route for synthesizing Si-SiO-SiO2 three-component particles, consisting of Si/SiO core and crystalline SiO2 shell, from commercially available SiO bulk particles via a thermal annealing process in the presence of sodium hydroxide (NaOH). The Si and SiO act as active materials in LIBs, while the crystalline SiO2 serves as a buffer material. The combination of high specific capacity of the Si and highly stable cycling performance of the SiO exhibits high-performance electrochemical properties, including a high reversible capacity of 1280 mAhg-1 and an excellent cycle retention of 99.5% at 0.2C after 200 cycles, compared to that at 0.1C rate.

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장소: 부산BEXCO

발표코드: **MAT1-4**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 10:25, 좌장: 최남순

Bio-inspired Materials for Rechargeable Batteries

최장욱

KAIST EEWS

While the development of advanced electrode materials and structures is leading Li ion battery technology these days, the development of outstanding separators also improves the cell performance remarkably. Inspired by mussels' exceptional wet-resistant holdfast onto versatile substrates, in this study, we coated polyethylene (PE) separators with mussel inspired polydopamine layers. After the polydopamine coating, PE separators become hydrophilic and thus bring various advantages in the cell operations: 1) the enhancement of power performance, 2) the adaptability with a wider range of electrolyte, particularly polar solvent for low temperature operations, 3) homogeneous Li ion flux that makes the cell operation more stable, especially for larger-scale cells and Li metal anodes. 4) the improved resistance against thermal shrinkage. While bringing a number of advantages, the coating process does not sacrifice original advantages of PE separators at all. This study suggests that mussel-inspired materials can contribute significantly to the improvement of emerging energy storage technology.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT1-5**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 홍승태

Antisite Defects and Cation Ordering in Olivine-Phosphate Cathodes

정성윤

KAIST EEWS 대학원

In a number of Li intercalation compounds in which an ordered array of Li is usually maintained, the control of point defects including cation disordering is of major significance for application to electrodes in rechargeable cells. Furthermore, as the chemically different environment induced by point defects leads to breaking of the ordered arrangement of atoms in crystals with a complex structure, mass and charge transport behaviors are also considerably affected by the presence of the defects. A variety of investigations on Li vacancies and cation intermixing have been reported for layered oxides. In contrast, few experimental details revealing the atomic-scale point defects in olivine-type lithium metal phosphates, LiMPO4 (where M = Fe, Mn, Ni, Co), available in the literature, while these phosphates have attracted a great deal of attention as alternative cathode materials in Li-ion cells over the past decade. Proper control and direct identification of their distribution in the lattice on the basis of crystal chemistry will be crucial steps toward enhancement of effective Li mobility during the intercalation reaction in olivine phosphates. In this presentation, the observations of a variety of lattice defects in ordered olivine LiFePO4 crystals after rapid phase transformation during crystallization are presented, showing notable distribution behaviors of the defects. For this direct observation, in siu and ex situ HREM and HAADF-STEM is utilized. This analysis suggests that the lattice defects in LiFePO4 can be adjusted for improved Li ion transport.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT1-6**

발표분야: Next Generation Batteries

발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 홍승태

Advanced polymers for high performance silicon anodes in Li-ion batteries

최남순

울산과학기술대 친환경에너지공학부

Electrode designs, which can accommodate severe volume changes (ca. 400%) of silicon anode materials upon lithium insertion, are the main prerequisite for high-performance lithium ion batteries. Among various techniques investigated for this purpose, a robust polymeric binder is a promising means to inhibit mechanical fracture of silicon negative electrodes during cycling. Lithium ion batteries (LIBs) are one of the most promising energy storage devices owing to their high power and energy densities. For LIBs, silicon is a exciting candidate anode material owing to its high theoretical specific capacity of 4200 mAhg-1 for Li 4.4 Si, low electrochemical potential between 0 and 0.4 V versus Li/Li + , and small initial irreversible capacity compared with other metal- or alloy-based anode materials. Nevertheless, the practical application of silicon to LIBs is still quite challenging because silicon suffers from severe volume changes (ca. 400%) during Li + insertion and extraction processes, which breaks electrical contact between the silicon particles and results in degradation of electrodes and rapid capacity loss. Herein, we present an innovative thermally cured polymeric binder as a technological solution for lithium ion batteries with silicon-based electrodes.

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장소: 부산BEXCO

발표코드: **MAT1-7**

발표분야: Next Generation Batteries

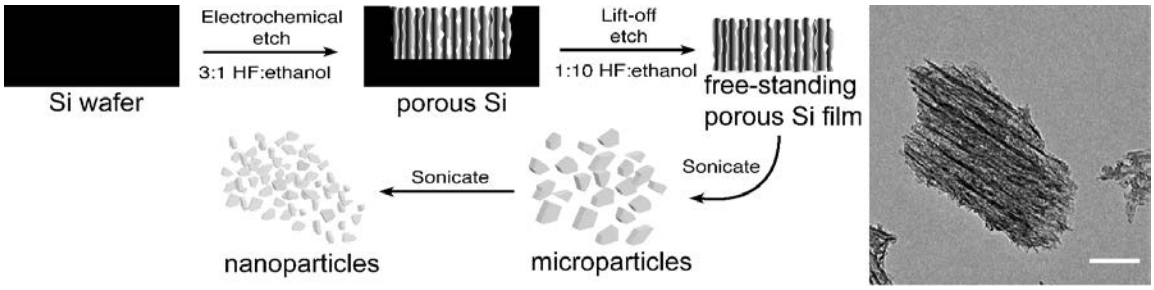
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 홍승태

Micro- and Nanoparticles of Porous Silicon as in-vivo Diagnostic and Therapeutic Agents

Michael J. Sailor

University of California, San Diego

The unique combinations of material properties that can be achieved with nanomaterials provide new opportunities in medicine. This presentation will describe self-destructing inorganic nanoparticles and microparticles based on a non-toxic porous silicon scaffold. The material allows a modular approach to the design of imaging or therapeutic agents, which includes features such as: intrinsic photoluminescence; singlet oxygen sensitization; capacity for a wide range of payloads such as magnetic nanoparticles, large proteins, or oligonucleotides; tunable degradation rates; and large external surface to provide multivalent targeting. Porous silicon is a nanostructured material prepared by oxidation of single crystal silicon in the presence of HF (Figure 1). The electrochemical preparation conditions allow the precise tuning of pore diameter and pore wall thickness, which impact both the degradation and drug release properties. Luminescent nanoparticles constructed from silicon offer a non-toxic alternative to Cd-based quantum dots, and porous silicon nanoparticles have been shown to be biodegradable and to safely image tumors and organs in live animals. The addition of a targeting ligand that selectively interacts with tissues can improve the efficacy of imaging or drug delivery. These effects can be further enhanced if the nanoparticle contains more than one copy of the targeting ligand, enabling multivalent interactions with the targeted tissue. The use of the magnetic, photoluminescence, and reflective optical characteristics of porous silicon particles for in-vitro and in-vivo sensing and imaging will be highlighted. Figure 1. Preparation of micron- and nanometer-size porous Si particles by ultrasonic fracture. At the right is a porous Si nanoparticle containing iron oxide nanoparticle inclusions. Scale bar is 50 nm.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-1**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 정현담

Graphene Synthesis and Applications: Status and Prospect

홍병희

서울대 화학부

Graphene has been attracting tremendous attention owing to its fascinating physical properties including quantum electronic transport phenomena, ultrahigh mobility, superb elasticity, thermal conductivity and mechanical strength. There have been many efforts to utilize these outstanding properties of graphene for macroscopic applications such as transparent conducting films useful for flexible/stretchable electronics. However, the scale and the quality graphene need to be further enhanced for practical applications by developing more efficient synthesis, transfer and doping methods. In this talk, the recent advances in graphene synthesis and applications will be reviewed, and the future directions of graphene applications particularly for flexible electronics will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-2**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 오제민

Synthesis of Metal Oxide Nanosheets and Their Self-Assembly into Functional Systems

Takayoshi Sasaki

National Institute for Materials Science (NIMS)

We have exfoliated various layered transition metal oxides into colloidal single layers. The resulting oxide nanosheets are taken as a unique class of molecularly-thin 2D materials with enhanced optical, photochemical, electronic, and magnetic properties. By taking advantage of these features as well as their monodispersed nature, we organized the nanosheets layer-by-layer into nanostructured films by applying solution-based techniques such as Langmuir-Blodgett deposition and sequential adsorption procedure. By optimizing deposition parameters, neat tiling of nanosheets into high-quality monolayers was achieved and its repetition enabled the construction of well-ordered multilayer films. The obtained films exhibited a range of useful functionalities depending on the nanosheets and film nanoarchitectures. We demonstrated that multilayer films of Ti/Nb oxide nanosheets showed superior dielectric and insulating properties, and a monolayer film of TaO3- nanosheet greatly reduced interfacial resistivity between two materials (LiCoO2/(Li,La)TiO3), acting as the thinnest solid electrolyte. Furthermore, we showed that monolayer films of the nanosheets can work as a seed layer to promote oriented growth of various crystal films, the structure of which matches that of the nanosheet.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-3**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 오제민

Bio-Inorganic Nano-Hybrid in Advanced Drug Delivery System for Chemotherapy

최진호

이화여대 화학.나노과학과

Up to date, many researches on drug delivery carriers have been restrictively focused on biomolecules and biodegradable polymers such as plasmid, polyethylene glycol and etc. However, there are still many problems unsolved, for example, low delivery efficacy, low expression rate, formation of toxic degradation products, and etc. In the present study, a novel concept of inorganic nano-vectors with targeting and drug delivery functions will be proposed to get breakthroughs in gene- and chemo-therapy.In order to examine 2d-structured inorganic nanohybrid as nanocarrier for gene and drug delivery, an attempt has been made to prepare host-guest interaction mediated nanohybrid assemblies by intercalating the negatively charged anticancer drug, methotrexate (MTX), into the positively charged layered double hydroxides (LDHs). And eventually we found that the encapsulated drug molecules in the interlayer space of LDHs retained their chemical and biological integrity, and that the present inorganic-bio hybrids showed targeting and drug delivery functions.According to the in vitro and in vivo experiments, the passive targeting was realized by controlling the particle size of MTX- LDHs, thanks to an EPR effect, but also the active targeting could be demonstrated due to the clathrin-mediated endocytosis of such a nanohybrid drug. Since the LDH nanoparticles are partially soluble in cytosol, the drug concentration in the cell increases and as a consequence, the drug efficacy is maximized.It is, therefore, concluded that the present advanced functional drug delivery system could provide a promising integrative therapeutic action in chemo- and gene therapy.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-4**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 오제민

Nanostructured titanates as visible light photocatalysts: Designed nanostructures for controlled reactions

Makoto OGAWA

Waseda University

Titania has been attracted much attention as useful photocatalysts. In order to optimize the properties, titania based materials have been synthesized to control the morphology (for example, nanoparticles and films) and the structures. Among possible titania based materials, layered titanates are materials with versatile applications including filler, ion exchanger and photocatalyst.1-6 Surface modification of layered titanates with organic functionality by the reactions with silane coupling reagents make the materials more attractive.1 We have already reported the functionalization of layered titanate by ion exchange2 and grafting1 for possible application as filler,3 adsorbent,4 and photocatalysts.5 Here, photocatalytic applications of layered titanates are introduced to show the merits of nanostructure design.A layered titanate, K0.66Ti1.73Li0.27O3.93, was used for photooxidation of organic compounds in water and the efficiencies and the substrate selectivity was successfully modified by the ion exchange of the interlayer potassium ions.5 The immobilization of gold nanoparticles on TiO2 particulates has attracted attentions to achieve visible light-induced photocatalysis such as the oxidation of aqueous organic substrates.7 Gold nanoparticles-loaded titania seems to be advantageous because of the size and morphology-dependent light absorption of gold nanoparticles from visible to near infrared region. Gold nanoparticles were deposited in the interlayer space of a layered titanate to give nanoporous material with molecular-sieving ability. The present hybrid catalyzed the direct oxidation of benzene to phenol by visible light irradiation. Immobilization of photosensitizing dyes on layered titanate is a way to prepare visible light responsive photocatalysts.8 References1. Y. Ide and M. Ogawa, Bull.Chem.Soc.Jpn., 80(2007) 1624.2. Y. Fuse, Y. Ide and M. Ogawa, Bull.Chem.Soc.Jpn., 81(2008) 767.3. Y. Fuse, Y. Ide and M. Ogawa, Polymer Chem., 1(2010) 849. 4. Y. Ide Y. and M. Ogawa, Angew.Chem.Int.Ed.Eng., 46(2007) 8449.5. Y. Ide, Y. Nakasato and M. Ogawa, J.Am.Chem.Soc., 132(2010), 36016. Y. Ide, N.

Ochi and M. Ogawa, Angew.Chem.Int.Ed.Eng., 50(2011) 654.7. Y. Ide, M. Matsuoka and M. Ogawa, J.Am.Chem.Soc., 132(2010) 16762. 8. N. Miyamoto, K. Kuroda and M. Ogawa, J.Phys.Chem.B, 108(2004) 4268.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-5**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 황성주

Mobility enhancement of passivated MoS_2 nanosheet devices

김규태

고려대 전기전자전파공학부

The device characteristics of a few-layer MoS_2 nanosheets were measured in a configuration of passivated field effect transistors(FET). The mobility of MoS_2 nanosheets FETs was enhanced reaching up to 50cm^2 V^{-1} s^{-1} by the passivation of with the Al_2O_3 layer with a reduction of the hysteresis pattern, which is related with the reduction of the adsorption/desorption trap sites at the surface. The higher mobility with the passivation was confirmed by the comparisonal studies on the geometric effects with the simulation. In the talk, the electrical properties of diffrent situations of MoS_2 nanosheets will be compared.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-6**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 황성주

Layered Gadolinium Hydroxide as a Contrast Agent for Magnetic Resonance Imaging

이인수

포항공과대 화학과

Layered rare-earth hydroxides (LRHs) are a class of anionic clays that are composed of positively charged hydroxide layers of trivalent rare-earth ions but are otherwise structurally similar to hydrotalcite-type layered double hydroxides (LDHs). In an attempt to devise new LRH type contrast agents, we envisaged that nanosheets of LRH incorporating paramagnetic rare-earth ions, such as Gd3+, in aqueous suspension might provide a large water-accessible surface area which is able to carry high payload of MR-active paramagnetic centers. In the first part of this presentation, I will discuss the development of a method of synthesizing a layered gadolinium hydroxide (LGdH) as a colloidal suspensions and modifying the surfaces of LGdH layers to provide them with water- and bio-compatibility and acid-resistance. The well-directed characteristics of the surface-modified LGdH as a contrast agent for MR imaging with a practical applications in medicine will be also discussed. In the second part, our research efforts to employ the LGdH for coating the surface of colloidal silica with fluorescent and MR active layers. The effectiveness of the resulting silica spheres as dual imaging agents in labeling for both fluorescent and MR imaging will be demonstrated.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT2-7**

발표분야: Recent Research Trends of 2D Nanostructured Inorganic Solids

발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 황성주

Synthesis and energy application of 2D inorganic nanosheets

백승민

경북대 화학과

Recently, 2-dimentional nanosheets have attracted considerable interests due to their unique physicochemical properties which are quite different from those of bulk materials. In the emerging field of nanoscience and nanotechnology, one important goal is to synthesize novel nanostructures with enhanced properties. Inorganic nanosheets such as layered titanates and molybdenum sulfides are one of the building blocks to fabricate a wide variety of nanostructured materials. The controlled synthetic techniques, including intercalation, exfoliation-reassembling, and pillaring reactions, could give rise to a variety of new nanohybrid compounds. If the active sites in layered host lattices bear an electric charge, an electrostatic attraction between the oppositely charged hosts and guests could be a driving force in the fabrication of new hybrid materials. For example, a novel inorganic/inorganic hybrid with high photocatalytic activities could be obtained via exfoliation-restacking method as a consequence of the synergetic functionality of hybrid materials. In addition, new nanohybrids with energy storage properties will be also highlighted in this presentation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC-1**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김종원

Simultaneous separation, processing, and detection of biomolecules in silicon-based optical nanostructures

Michael J. Sailor

University of California, San Diego

Separation, concentration, and detection of the analyte are key aspects of bioanalytics. Nanostructured optical films constructed from porous silicon provide a versatile platform that can incorporate all three of these components within a 5 nL volume. This presentation will illustrate the enabling aspects of the electrochemical synthesis and optical properties of porous silicon for label-free biosensing applications. Focusing on the preparation of chemically modified porous multilayers and the optical interferometric means of monitoring these nanostructures, several examples of protein and enzyme detection will be highlighted. The ability to manipulate proteins within porous silicon nanostructures through the selective application of electric fields will be discussed. The approach uses a high surface area, highly porous optical electrode based on a carbonized porous silicon Fabry-Perot film. Application of a negative bias induces concentration of a positively charged protein such as lysozyme within the porous nanostructure to a level ~ 9600 times the free solution concentration. Diffusion and adsorption of protein within the 40nm-diameter pores can be monitored by optical interferometry, providing a means to identify the protein based on its characteristic charge, size, and diffusion characteristics. The captured protein can be held for several hours, and it is released when the sensory electrode is returned to zero bias. The released protein retains its enzymatic activity, and the optical electrode can undergo multiple adsorption/desorption cycles.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC-2**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 김종원

Electrochemical biosensors for cancer cell detection in biological fluids

심윤보 Pranjal Chandra Ye Zhu

부산대 화학과

We developed numerous methods to detect cancer cells based on (i) the interaction between anticancer drug and the cell membrane, (ii) selective signal amplification through silver ions deposition, and (iii) ultrasensitive cancer cell detection using aminophenyl boronic acid interaction with the cancer cell surface carbohydrates. All these detection strategies are based on the antibody and/or aptamer bonded on the conducting polymer-nanomaterials composite layer. The biosensors probe was characterized using XPS, SEM, QCM, and electrochemical methods. The experimental parameters affecting biosensor performance were optimized and the detection limit was evaluated. The developed methods effectively differentiate between normal, cancer cells, and drug resistant cancer cell in serum and blood samples.

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장소: 부산BEXCO

발표코드: **ELEC-3**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김종원

Surface Modification of Carbon-Based Materials with Dendrimer-Encapsulated Nanoparticles for Electrochemical Applications

김주훈

경희대 화학과

The surface modification of carbon-based materials with dendrimer-encapsulated nanoparticles (DENs) is described. There are two surface decoration methods involved in this study: electrochemical decoration of glassy carbon surfaces and covalent decoration of chemically converted graphene (CCG) surfaces. First, amine-terminated polyamidoamine (PAMAM) dendrimers were immobilized on glassy carbon electrodes (GCEs) via electrooxidative coupling of the terminal amine groups of dendrimers. The immobilization approach was applied to assemble DENs on GCEs, and further extended to construct bifunctional nanostructures, which conjugated biochemical and electrocatalytic activities, on GCEs. Second, we reported a universal method for preparing nanoparticle-decorated CCG composites, on which size-monodisperse nanoparticles were uniformly distributed with preservation of their original size, via covalent immobilization of DENs. The method allowed universal attachment of multiple nanoparticles with distinctively different sizes and compositions on the same CCG sheet with good control over particle sizes in the range of 1 to 2 nm. The electrochemical applications of the resulting DEN-CCG nanocomposites were also discussed.Referencesa) Kim, J. M.; Kim, J.; Kim, J.* Chem. Commun., 2012, 48, 9233-9235.b) Ju, H.; Koo, C. M.; Kim, J.* Chem. Commun., 2011, 47, 12322-12324. c) Kim, T. H.; Choi, H. S.; Go, B. R.; Kim, J.* Electrochem. Commun., 2010, 12, 788-791.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC-4**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 16:05, 좌장: 김주훈

Ultrasensitive electrochemical aptasensors using ferrocene-modified silica nanoparticles

신재호 구현우 이정봉 차근식 남학현

광운대 화학과

Immunosensors recently based on aptamers as a new molecular recognition element have received great attention. In comparison with antibodies, the aptamers (oligonucleic acid or peptide molecules) directly bind to a wider range of target molecules, and are more stable to thermal degradation, easier to obtain, and readily adaptable to the modification. To improve performance of aptamer-based sensors, it is particularly important to develop label-free detection methods. Several strategies to achieve label-free immunoassays have been demonstrated by using fluorescence, electrochemistry, quartz crystal microbalance (QCM), and surface plasmon resonance (SPR) spectroscopy. Herein we report on a new approach to design an electrochemical aptamer sensor based on label-free detection of various target molecules by utilizing ferrocene (Fc)-modified silica nanoparticles. The aptamers immobilized on gold electrodes lead to changes in the interfacial electron transfer properties of electrochemically active probes (e.g., Fc). Indeed, the surface coverage with target proteins specifically bound to aptamers prohibits the access of electroactive probes to the electrode surface. To amplify such blocking effects associated with target molecules-aptamer complex formation, Fc-modified silica nanoparticles were employed as a scaffold to design macromolecular electroactive probes. The Fc-modified silica nanoparticles were synthesized by carbodiimide coupling chemistry between ferrocenecarboxylic acid and amines functionalized on the silica surface. The effects of core particle size (7 and 14 nm), surface net charge of Fc-modified silica nanoparticles used to monitor signal changes on sensor performance (e.g., sensitivity and detection limit) are discussed. Furthermore, we investigate the feasibility of applying the concept to develop the aptasensors to detect cardiovascular disease markers, i.e., thrombin, B-type natriuretic peptide (BNP), and troponin I (TnI).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC-5**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 김주훈

Electrochemical-Chemical-Chemical Redox Cycling for Ultrasensitive Immunosensors

양해식

부산대 화학과

We reports electrochemical-chemical-chemical (ECC) and chemical-chemicla (CC) redox cycling, for use in ultrasensitive biosensor applications. A triple chemical amplification approach using an enzymatic reaction, CC redox cycling, and ECC redox cycling is applied toward electrochemical immunosensors of cardiac troponin I. An enzymatic reaction, in which alkaline phosphatase converts 4-aminophenyl phosphate to 4-aminophenol (AP), triggers CC redox cycling in the presence of an oxidant and a reductant, and electrochemical signals are measured with ECC redox cycling after an incubation period of time. To obtain high, selective, and reproducible redox cycling without using redox enzymes, two redox cycling reactions should be fast, but an unwanted reaction between the oxidant and reductant should be very slow. Because species that undergo outer-sphere reactions (OSR-philic species) react slowly with species that undergo inner-sphere reactions (ISR-philic species), highly OSR-philic Ru(NH3)63+ and highly ISR-philic tris(2-carboxyethyl)phosphine (TCEP) are chosen as the oxidant and reductant, respectively. The OSR- and ISR-philic QI/AP couple allows fast redox reactions with both the OSR-philic Ru(NH3)63+ and the ISR-philic TCEP. Highly OSR-philic indium?tin oxide (ITO) electrodes minimize unwanted electrochemical reactions with highly ISR-philic species. Although the formal potential of the Ru(NH3)63+/Ru(NH3)62+ couple is lower than that of the QI/AP couple, the endergonic reaction between Ru(NH3)63+ and AP is driven by the highly exergonic reaction between TCEP and QI (via a coupled reaction mechanism). The detection limit of an immunosensor for troponin I in serum, calculated from the anodic charges in chronocoulometry, is ca. 10 fg/mL.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC-6**

발표분야: Recent Trends in Electrochemical Sensors

발표종류: 심포지엄, 발표일시: 목 16:55, 좌장: 김주훈

Nanomaterial-Based Electrochemical Sensors for Detecting Biomolecules

이영미

이화여대 화학나노과학과

Interest in nanomaterials has been greatly increased due to their unique physicochemical properties. The nanostructured materials generally show highly enhanced electrocatalytic activity induced by the increased surface area and peculiar nanoscale morphology, and therefore have the versatile applicability in electrocatalysis. In this presentation, we demonstrate the electrocatalytic activity of nanostructured metals and conductive metal oxides for electrochemical detection of biomolecules. A variety of nanomaterials in different nanostructures such as nanoparticle, nanowire, and nanorod are synthesized using gold, palladium, platinum, iridium dioxide, and ruthenium dioxide. The electrocatalytic activities of the prepared nanomaterials are characterized for the electrochemical redox reactions of the following biological analytes: glucose, dihydronicotinamide adenine dinucleotide (NADH), hydrogen peroxide (H_2O_2), oxygen (O_2), proton (pH), etc.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-1**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이진우

New Electrode Materials for Li & Na Ion Batteries: Nanostucture, Crystal structure and Reaction Mechanism

이규태

울산과학기술대 친환경에너지공학부

근래에 들어 환경 오염 등의 문제를 개선하기 위하여 전기자동차 및 스마트 그리드 등의 개발에 대한 많은 관심이 집중되고 있다. 현재 리튬 이차 전지의 연구는 기존 에너지 밀도의 한계를 극복할 수 있는 새로운 소재나 시스템을 개발하고자 하는 노력이 진행 중이다. 예를 들어 이론 용량이 기존 상용화된 탄소 음극 소재보다 월등한 실리콘 소재의 개발이나 기존 시스템과 다른 Li-Sulfur 혹은 Li-air 전지에 대한 관심이 증대되고 있다. 뿐만 아니라 리튬 자원의 경제적 경쟁성 문제를 극복하고자 Na ion batteries 에 대한 연구도 최근 들어 활발하게 진행되고 있다고 할 수 있다. 따라서 본 발표에서는 1) 리튬 이차 전지의 고밀도 음극 소재인 실리콘 소재의 치명적 부피변화 문제의 극복 방안에 관해 논하고, 2) 차세대 전지인 Na ion batteries 의 새로운 전극 소재의 합성과 이의 구조적 분석 및 반응 메커니즘에 대해 다룰 것이다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-2**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 이진우

나노구조 재료를 통한 전지의 성능 향상

조국영 최재용 김미리[1]

공주대 신소재공학부 [1]공주대 신소재공학과

현재 산업기술의 발달로 지구온난화와 화석연료 고갈, 원유가격의 급등으로 인한 에너지와 환경문제가 심각해지고 있으며, 최근 친환경에 대한 인식이 크게 부각되면서 이를 동시에 해결하기 위한 신재생에너지 개발 연구가 분주하게 이루어지고 있다. 신재생에너지의 분야로써 많은 관심과 각광을 받고 있는 리튬 이차 전지와 태양 전지 등의 대체에너지원을 예로 들 수 있다. 리튬 이차 전지는 고에너지밀도 특성에 의해 모바일기기의 전원뿐만 아니라 최근에는 전기자동차의 전원으로도 활용되고 있으나, 낮은 용량 및 안정성 등의 문제가 대두되고 있다. 또한, 태양 전지는 에너지원으로 무한정의 태양광을 사용하나 낮은 효율 등의 문제로 이를 해결하려는 연구들이 진행되고 있다. 우리는 새로운 나노구조의 소재를 이용하여 대체에너지원들의 문제들을 해결하고 성능을 향상시킬 뿐만 아니라 소형화, 경량화 및 유연성으로 flexible electronic device 에도 적용이 가능하다. 본 연구에서는 나노구조의 flexible silicon anode 를 제조하여 높은 용량, 효율과 동시에 flexible 특성을 지니는 리튬 이차 전지와 1D photonic crystal 을 통해 light-harvesting efficiency 를 향상시켜 효율을 증가시키는 태양 전지에 관해서 보고하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-3**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

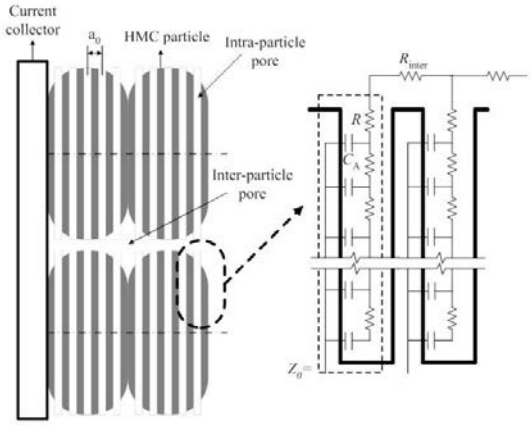
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이진우

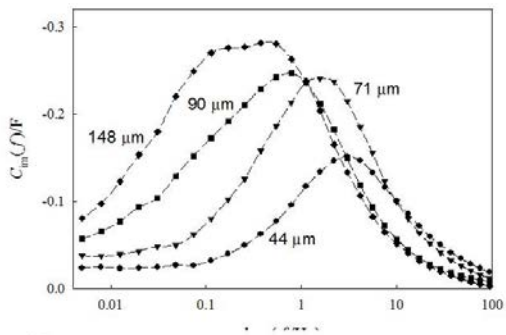
Characterization of supercapacitor performance using transient analysis based on transmission line model

윤성훈

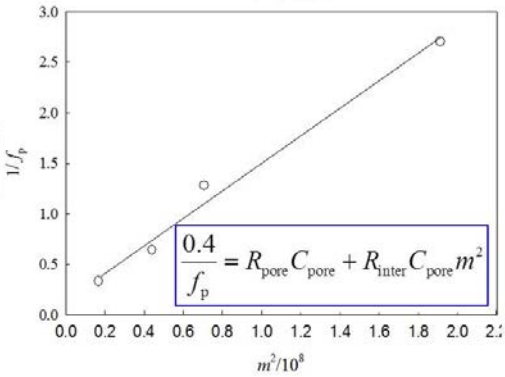
한국화학연구원 그린화학연구본부

Recently, supercapacitors have been intensively investigated as high power application due to its intrinsically fast charging-discharging and extremely high cycle life. Typically, supercapacitors employ the composite electrode system containing porous materials, which gives rise to complicate electrolytes (ions) transport phenomena within intra- and inter-particle pores during charging process. Clarification of electrolyte transport is highly important because it is dominant resistive process during charge storage and can strongly influence supercapacitor performance. In our study, the transport of electrolyte within supercapacitor electrodes was investigated using electrochemical transient methods such as chronoamperometry (CA), chronopotentiometry (CP), electrochemical impedance spectroscopy (EIS) and imaginary capacitance analysis (ICA). In order to describe ionic transportation within pores, 1-D and 2-D transmission line models (TLM) were employed and compared each other. Especially, 2-D transmission line model was utilized for ICA method since this approach requires very complex mathematical consideration. By approaching empirical analysis the obtained complicate equation, simple and useful equations were acquired. After establishment of descriptive models and useful equations, various porous carbon materials were developed using novel template method and applied to verify the obtained equations. From this analysis using porous carbons, the relationship between pore structures (size, length and connectivity) and electrolyte transport was investigated.





$$\frac{C(f)}{C_0} = \frac{1}{j2\pi\tau_1 f}\frac{1}{\sqrt{\rho}}\sqrt{\frac{\sqrt{j2\pi\tau_1 f}}{\coth\left(\sqrt{j2\pi\tau_1 f}\right)}}\tanh\left(\sqrt{\rho}\sqrt{\frac{\sqrt{j2\pi\tau_1 f}}{\coth\left(\sqrt{j2\pi\tau_1 f}\right)}}\right)$$



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-4**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 윤성훈

Nanostructured Polymer Electrolytes for All-Solid-State Lithium Batteries.

박문정

포항공과대 화학과

There are rising demands for developing more efficient energy materials to stem the depletion of fossil fuels, which have prompted significant research efforts on lithium ion batteries (LIBs). To date, LIBs are being widely developed to power small electronics, however, their utilization to medium-large sized electric power resources such as vehicle and stationary energy storage systems still appears distant. These technologies increasingly rely upon polymer electrolyte membranes (PEMs) that transport ions from the anode to the cathode to balance the flow of electrons in an external circuit, and therefore play a central role in determining the efficiency of the devices; as ion transport is a kinetic bottleneck compared to electrical conductivity, enormous efforts have been devoted to improving the transport properties of PEMs. In present study, we carried out an in-depth analysis of the morphology effects on transport properties of PEMs. By combining various anode active materials with our PEMs, we were able to evaluate the battery performance in the solid state. For example, with the use of Germanium nanoparticles (GeNPs) as anode active materials, it has been revealed that the GeNPs anode can deliver high reversible charge capacities of 1600 mAh/g with Coulombic efficiency over 90% at 1C rate up to 50 cycles, which is very close to the theoretical value of Ge. The system also shows rate capability during repeated cycles at 1C, 2C, 5C, and 10C rates.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-5**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 윤성훈

High-Perfomance Li ion Battery Electrodes Using Novel Ordered Mesoporous Materials Synthesized by Templates

이진우

포항공과대 화학공학과

For high performance supercapacitor and Li-ion battery electrodes, various mesoporous metal oxide materials have been synthesized by employing lab-synthesized block copolymers as a structure-directing agent or ordered mesoporous silica materials as hard templates. An ordered mesoporous WO3-X material with high electrical conductivity was employed for use as a supercapacitor electrode in 2.0 M H2SO4. The electrode made of mesoporous WO3-X exhibited a high rate capability and an excellent capacitance (366 ?Fcm-2, 639 Fcm-3), which were attributed to the large ordered mesopores, high electrical conductivity, and high material density. Fe3O4 nanocrystals confined in mesocellular carbon foam (MSU-F-C) are synthesized by 'Host-Guest' approach and tested as anode for lithium-ion batteries (LIBs). 13-27 nm magnetite Fe3O4 nanocrystals are formed inside ~30 nm pores of mesocellular carbon matrix. Fe3O4/MSU-F-C (45 wt% Fe3O4) exhibited 1007 mA h g-1 of first charge (Li de-insertion) capacity at 0.1 A g-1 and 111% of capacity retention at 150th cycle, and retains 37% capacity at 7 A g-1 (~7 C rate). For the first time, we synthesized mesostructured LTO/carbon composite (Lithium titanate/carbon) with large (> 15 nm) and uniform pores for high performance LIB anodes via a block copolymer assembly. The electrochemical characterization of this material will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR-6**

발표분야: Recent Trends in Nanostructured Materials for Energy Storage

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 윤성훈

Flexible Supercapacitors Based on Functionalized Graphenes

박호석

경희대 화학공학과

The chemical functionalization of graphenes is of prime importance in terms of expanding applicative fields and obtaining high performances of devices. Recently, we demonstrated the solution processable nanohybridization of graphenes by functional materials such as ionic liquids, polyelectrolytes, block copolymers, and biomaterials for electrochemical applications into fuel cells, supercapacitors, and biosensor devices. Herein, we report the preparation of all solid-state flexible supercapacitors (SCs) through the easy assembly of functionalized reduced graphene oxide (f-RGO) thin films (as electrode) and solvent-cast Nafion electrolyte membranes (as electrolyte and separator). In particular, the f-RGO-based SCs (f-RGO-SCs) showed a 2-fold higher specific capacitance (118.5 F/g at 1 A/g) and rate capability (90% retention at 30 A/g) compared to those of all-solid-state graphene SCs (62.3 F/g at 1A/g and 48% retention at 30 A/g). As proven by the 4-fold faster relaxation of the f-RGO-SCs than that of the RGO-SCs and more capacitive behavior of the former at the low-frequency region, these results were attributed to the facilitated ionic transport at the electrical double layer by means of the interfacial engineering of RGO by Nafion. Moreover, the superiority of all-solid-state flexible f-RGO-SCs was demonstrated by the good performance durability under the 1000 cycles of charging and discharging due to the mechanical integrity as a consequence of the interconnected networking structures. Therefore, this research provides new insight into the rational design and fabrication of all-solid-state flexible energy storage devices as well as the fundamental understanding of ion and charge transport at the interface.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS1-1**

발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry

발표종류: 심포지엄, 발표일시: 목 09:15, 좌장: 한상우

Boride materials with unexpected catalytic, thermoelectric and mechanical properties

Barbara Albert

Technische Universität Darmstadt

Metal borides are hard and refractory and they may exhibit properties that make them interesting materials. Chromium and manganese tetraborides for example were compared in literature to hypothetical tetragonal diamond. Compounds with ?-boron structure exhibit promising Seebeck coefficients, and nanoscale nickel and cobalt borides show catalytic activity. Solid state syntheses, crystal structures and characterization methods are highly divers [1] and allow for a broader discussion of the huge potential solid state chemistry presents to materials research. [1] B. Albert, H. Hillebrecht, Angew. Chem. Int. Ed. 48 (2009) 8640-8668

한국화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS1-2**

발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry

발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 한상우

Stepped Surfaces at the Nanoscale: High-Index-Faceted Nanocrystals

한상우

KAIST 화학과

Precise-tuning of exposed facets on the surface of metal nanocrystals (NCs) by manipulating NC shape has provoked increasing research interest, because the inherent characteristics of NCs ranging from catalytic function to plasmonic properties highly depend on their surface atomic arrangement. In recent years, the synthesis of high-index-faceted NCs has attracted a great deal of attention. High-index facets consist of surface atoms with relatively lower coordination numbers than those of low-index facets due to the presence of high-density atomic steps and kinks on them. As such, high-index-faceted NCs have shown greatly enhanced performance for specific catalytic reactions over NCs bound by low-index facets. Efficient surface-enhanced Raman scattering (SERS) activities of high-index-faceted NCs have also been reported. The pronounced SERS efficiencies were attributed to the presence of large numbers of well-defined tips and edges in high-index-faceted NCs, which can serve as hot spots for large E-field enhancement and thus give strong SERS signals. Herein, the synthesis of high-index-faceted mono- and bi-metallic NCs with unprecedented morphologies and their unique catalytic and optical properties are reported.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **KCS1-3**
발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry
발표종류: 심포지엄, 발표일시: 목 10:15, 좌장: 한상우

A Concept for Rational Materials Synthesis

Martin Jansen

Max-Planck-Institut für Festkörperforschung

Virtually during any technical innovation new, or at least modified, materials are employed. Thus, the availability of new and ever better performing materials is a crucial requirement for competitiveness at the global technological race, and there is a particular strong demand for efficiency in materials research, in general. The original task of chemistry within that interdisciplinary enterprise is to synthesize and characterize new solid compounds with promising properties. Most regrettably, a directed and purposeful synthesis of a solid of given composition, structure or even properties is not viable, even nowadays, and the approaches most widely applied are explorative in nature. We present a concept that points the way towards rational planning of syntheses in solid state chemistry. The foundation of our approach is the representation of the whole material world, i.e. the known and not-yet-known compounds, on an energy landscape, which implies information about the free energies of these compounds. From this follows at once that all chemical compounds capable of existence (both thermodynamically stable and metastable ones) are already present in virtuo on this landscape.Up to now, materials capable of existence are discovered in the course of an experimental exploration of the energy landscape; however, an a priori identification of a synthesis goal requires an exploration using theoretical methods. In contrast to those computational approaches currently employed for structure determination for fixed composition and already known unit cell, our aims clash with such restrictions, and full global optimizations have to be performed on the landscape. Feasibility of the approach, including experimental validations, have been demonstrated.Martin Jansen: A Concept for Synthesis Planning in Solid State Chemistry, Angew. Chem. Int. Ed. 41 (2002) 3746-66M. Jansen, K. Doll, J. C. Schön: Addressing chemical diversity by employing the energy landscape concept, Acta Cryst. A66 (2010) 518-534

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS1-4**

발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry

발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 한상우

Recent Research Activities on Thermoelectric Materials : Phonon Controlled Nano-engineering

김성진

이화여대 화학과

I will review recent research activities on phonon controlled thermoelectric materials and show recent results of our research. As an example of phonon controllable nano-engineering strategy, metal nanoparticles can be embedded by intercalation in a layered material. We report the effect of Cu intercalation on the thermoelectric properties of Bi_2Te_3 in the series compounds of $Cu_xBi_2Te_3$ ($0 \leq x \leq 0.1$). Such metal nanoparticles acted as electron donors, changing the native p-type character of Bi_2Te_3 to n-type. They also acted as phonon scatters, reducing thermal conductivity. $Cu_{0.07}Bi_2Te_3$ has high electrical conductivity of 681 S/cm and Seebeck coefficient of -236 μV/K with low thermal conductivity of 1.0 W/mK, thus enhancing the figure of merit, ZT, to 1.15 at approximately 300 K. This value is a 20% improvement over the peak ZT (0.9) of the current best-known value of n-type Bi_2Te_3. Such improvement arose from the formation of the Cu nanoparticles within the Bi_2Te_3 layers. Also, we will show a novel single step approach to fabricate nanoscaled heterophase interface in bulk thermoelectric materials through the bottom-up strategy and investigate their thermoelectric properties. This approach shows a simple synthetic route to construct energy filtering interfaces, thereby enhancing TE properties in bulk materials. The synthesized organic DDT and inorganic SnS_4^{4-} capped Bi_2Te_3 nanoparticles were compacted into nanostructured bulk samples by spark plasma sintering. The densification behavior, microstructure, and phase formation of sintered samples were characterized.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS1-5**

발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry

발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 한상우

Lithium solid electrolytes - Key components for next-generation batteries

Juergen Janek

Justus-Liebig-Universitaet Giessen

The demand for better and improved electrochemical energy storage systems (batter-ies) leads to steadily advancing requirements for the performance of battery materials. In particular, the quest for batteries with higher energy capacity causes the need for high-voltage stable electrolytes (for cells with high cell voltage) or mechanically imper-meable membranes (for e.g. Li/air or Li/sulfur batteries) with high lithium ion conductivity. Solid electrolytes with sufficient chemical stability, high ionic and very low electronic conductivity may thus become key components of future battery systems. One particu-lar class of lithium solid electrolytes, i.e. lithium-based garnet phases, recently attracts major interest due to their unique combination of chemical and electrochemical properties [1]. In this lecture the current state of knowledge is summarized and own work on garnet-type phases, including polycrystalline phases, thin films and single crystals is reported.[1] Structure and dynamics of the fast lithium ion conductor “Li7La3Zr2O12”, H. Busch-mann, J. D?lle, S. Berendts, A. Kuhn, P. Bottke, M. Wilkening, P. Heitjans, A. Seny-shyn, H. Ehrenberg, A. Lottnyk, V. Duppel, L. Kienle, and J. Janek, Phys. Chem. Chem. Phys. 13 (43) (2011) 19378-19392.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS1-6**

발표분야: KCS-GDCh-Angewandte joint symposium - Solid State Chemistry

발표종류: 심포지엄, 발표일시: 목 11:45, 좌장: 한상우

Nanostructured materials of designed architecture for catalytic challenges

유룡

KAIST 화학과

Nanostructured materials such as nanoparticles and nanoporous frameworks are the central subject to many important issues currently confronted by human beings including future energy problems, environmental pollution and healthcare. This lecture demonstrates that we are in a stage to synthesize simple functional nanostructured materials such as hierarchical zeolites, mesoporous silicas and nanoporous carbons in a rational way using structure-directing agent molecules. In principle, it is possible to inscribe functionalities as a blueprint inside structure-directing molecules so that they can generate complex levels of nanoarchitecture in a rationally designed manner. Furthermore, it is important to explore chemical reactions and associated mechanisms taking place in the nanoscale environments provided by these nanomaterials. Future researches in this direction are expected to address the longstanding challenges of green chemistry and reusable energy for the sustainability of human life.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS2-1**

발표분야: 미래의 IT를 위한 솔루션, 동우화인켐과 함께

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김상태

동우화인켐(주) 회사소개 및 채용 안내

박일성

동우화인켐

TBA

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS2-2**

발표분야: 미래의 IT를 위한 솔루션, 동우화인켐과 함께

발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 김상태

LCD 기술의 현재와 미래

송장근

성균관대 전자전기공학부

현재 장비분야를 포함한 평판디스플레이 시장의 90% 이상을 차지하는 LCD 는 두터운 후보기술군을 바탕으로 시장변화에 빠른 대응력, amorphous Si TFT 와 좋은 조합, 소재 및 부품산업의 발전 등을 기반으로 급속히 성장하여 왔다. 하지만, 최근 전통적 디스플레이 시장의 포화와 이에 따른 공급과잉으로 또 다른 변화가 필요한 시점이다. 본 강연에서는 기존 LCD 기술의 개요 및 주요 issue 들 그리고, LCD 핵심 부품 및 소재 분야, 특히 편광판과 보상필름 및 표면처리관련 기술들을 요약하고, 미래 기술로 주목 받는 AMOLED 기술과의 경쟁에서 LCD 의 전력적 위치가 어떠한지 고찰한다. 또한, LCD 패널회사에서 고민하는 가까운 미래기술전략과 학계에서 연구되고 있는 장기 미래 기술관련 하여 정리한다.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **KCS2-3**
발표분야: 미래의 IT를 위한 솔루션, 동우화인켐과 함께
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 김상태

IT 응용을 위한 흑연성 탄소소재 나노조립 및 도핑기술

김상욱

KAIST 신소재공학과

탄소나노튜브와 그래핀등의 흑연성 탄소나노소재는 우수한 전기전도도와 기계적 물성, 넓은 비표면적, 기계적 유연성등 우수한 물성을 지닌 첨단소재로서 많은 관심을 모으고 있다. 그러나 이들 탄소나노소재를 다양한 분야에 응용하기 위해 필요한 분자단위의 나노구조제어에 대한 연구는 아직까지 초기 단계에 머물고 있다. 본 발표에서는 IT 소재로 응용될 수 있는 3 차원 탄소나노소재 분자단위 조립기술의 기본원리와 이를 통해 지금까지 본 연구진이 개발해온 다양한 구조의 3 차원 탄소나노소재들을 소개하고자 한다 [1]. 용매 분산을 통해 손쉽게 구현할 수 있는 다양한 그래핀/탄소나노튜브 나노구조들은 저비용, 대량생산에 유리한 소재들이다. 나노촉매로부터 탄소나노물질들을 성장시키는 기술은 탄소물질의 형태 및 특성을 제어하고 다양한 형태의 거시적 배열을 구현하기위해 매우 중요한 기술이다. 또한 위에 언급한 기술들의 융합을 통해 유연한 그래핀 기판 위에 수직성장된 탄소나노튜브 어레이와 같은 이상적인 형태의 맞춤형구조 구현이 가능하다. 앞으로 이러한 맞춤형 탄소나노구조체들의 화학적 물성제어를 통해 복합소재, 메모리, 디스플레이, 에너지 저장 분야 등 IT 기술 분야에서 광범위하게 응용될 수 있을 것으로 기대된다. [2-5]

참고문헌[1]S. H. Lee, D. H. Lee, W. J. Lee, S. O. Kim* Adv. Funct. Mater. 21, 1338 (2011).
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[3]J. M. Lee, J. S. Park, S. H. Lee, H. Kim, S. Yoo,* S. O. Kim* Adv. Mater. 23, 629 (2011).
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[5]J. M. Yun, K. N. Kim, J. Y. Kim, D. O. Shin, W. J. Lee, S. H. Lee, M. Lieberman, S. O. Kim* Angew. Chem. Int. Ed. 124, 936 (2012).

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **KCS2-4**
발표분야: 미래의 IT를 위한 솔루션, 동우화인켐과 함께
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 김상태

플레시블 AMOLED 개발 현황 및 기술적 이슈

박상희

한국전자통신연구원

차세대 디스플레이로 주목받던 플렉시블 AMOLED 가 벌써 스마트폰에 탑재되어 제품으로 나오는 정도로 기술개발이 빠르게 진행되고 있다. 이는 고온공정을 가능하게 하는 플라스틱 기판 소재의 확보를 통해 이루어졌으나 그럼에도 불구하고 태블릿 PC 및 그외의 제품으로 개발되기까지 아직 소재, 공정, 소자, 그리고 시스템에서 해결해야 할 많은 문제점을 안고 있다. 본 발표에서는 플렉시블 AMOLED 의 개발 현황과 다양한 제품으로 개발하기 위해 해결해야 할 기술적 이슈에 대해 살펴보기로 한다. 특히 플렉시블 AMOLED 제품화에 필수적인 passivation 기술, 그리고 화학자 관점에서 들여다 봐야 할 재료적인 이슈에 대해 살펴본다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS2-5**

발표분야: 미래의 IT를 위한 솔루션, 동우화인켐과 함께

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 김상태

OLED 및 OFET 용 신개념 혁신 소재

박수영

서울대 재료공학부

이 강연에서는 고성능 OLED 와 OFET 에 응용될 새로운 개념과 성능의 분자 물질 군에 대해 소개하고자 한다. 구체적으로는 백색 발광이 가능한 다중발색 형광체, 인광체의 발색 조절을 위한 분자설계 방법, TADF 를 이용한 OLED, n-형 OFET 소재 및 구조 제어 등에 대한 최근의 동향 특히 발표자 그룹의 연구결과를 소개한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS3-1**

발표분야: Introduction of Intellectual Property for Researchers in the field of Chemistry

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이영민

연구자를 위한 지식재산 지원 제도 소개

윤내한

특허청 산업재산인력과

교재참조.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS3-2**

발표분야: Introduction of Intellectual Property for Researchers in the field of Chemistry

발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 이영민

연구자를 위한 특허제도 소개

이진홍

특허청 화학소재심사과

교재참조.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS3-3**

발표분야: Introduction of Intellectual Property for Researchers in the field of Chemistry

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 이영민

IP-R&D소개 및 CIGS 박막형 Solar Cell 사례

나용호

R&D 특허센터 IP 전략사업팀

교재참조.

대 한 화 학 회 · THE KOREAN CHEMICAL SOCIETY ·

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS3-4**

발표분야: Introduction of Intellectual Property for Researchers in the field of Chemistry

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 이영민

유.무기 복합 소재를 이용한 단열 및 흡음재 분야의 특허동향 분석

고기영

한국특허정보원 특허정보진흥센터 IP전략지원파트

교재참조.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS4-1**

발표분야: 연구지원정책, 연구윤리 및 후속 BK21 포럼

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이덕형

연구지원정책

이근재

교육과학기술부 기초연구정책관

TBA

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **KCS4-2**

발표분야: 연구지원정책, 연구윤리 및 후속 BK21 포럼

발표종류: 심포지엄, 발표일시: 금 11:20, 좌장: 이덕형

연구윤리소개: 연구부정행위와 관련규정 중심으로

이원용

연세대 화학과

2000 년대에 접어들면서 우리나라의 대학들이 연구중심기관으로 변모하기 시작하여 대학의 연구가 매우 활성화 되었다. 지난 2010 년 우리나라의 국가 R&D 투자 규모는 43 조 8548 억원으로 이중 정부에서 투자한 연구비는 13 조 6827 억에 이르며 이중 약 40%는 정부출연(연)에 25% 정도는 대학에 지원되었다. 이러한 연구비 투입으로 인하여 우수한 연구성과가 다수 얻어졌는데 그중 SCI 논문은 3 만 8651 편이 게재되어 세계 11 위를 차지하였다. 한편으론 논문 발표 등 연구실적이 대학 및 연구기관의 경쟁력 평가의 척도로 작용하게 되어 많은 연구자들이 기관의 강화된 업적 평가에 많은 부담을 갖게 되었고 이에 따라 연구부정행위가 서서히 증가되고 있는 추세에 있다. 연구부정행위는 연구개발과제의 제안, 연구개발의 수행, 연구개발결과의 보고 및 발표 등에서 행하여진 위조·변조·표절·부당한 저자 표시 행위 등을 말한다. 본 발표에서는 최근에 언론에 보도된 사례를 중심으로 연구부정행위에 대해 소개하고 이러한 부정행위와 관련된 정부의 규정에 대해 자세히 소개할 예정이다. 이와 더불어 실제로 연구부정행위가 발생되었을 때 공식적으로 처리되는 절차에 대해 소개 할 예정이다. 마지막으로 연구부정행위 예방을 위한 여러 가지 방안에 대해 소개할 예정이다.

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장소: 부산BEXCO

발표코드: **INOR.O-1**

발표분야: General Oral Presentation

발표종류: 분과기념강연, 발표일시: 금 10:00, 좌장: 이인수

Syntheses and Applications of Plasmonic Nanogap Structures

남좌민

서울대 화학부

Synthesizing and controlling plasmonic nanostructures such as Au and Ag nanoparticles (AuNPs and AgNPs) with high precision and high yield are of paramount importance in optics, nanoscience and materials science. It is particularly important to generate and control ~1-nm plasmonic gap because plasmonic gaps of ~1 nm or less can generate exponentially stronger plasmonic coupling signals than >1-nm plasmonic gap. Among many examples of the use of plasmonic nanogap, surface-enhanced Raman scattering(SERS)-based signal amplification and bio-detection methods using SERS-active plasmonic nanoparticles (NPs) have been drawing significant interest, and it has been known that SERS effect is intense when Raman dyes are located within

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장소: 부산BEXCO

발표코드: **INOR.O-2**

발표분야: General Oral Presentation

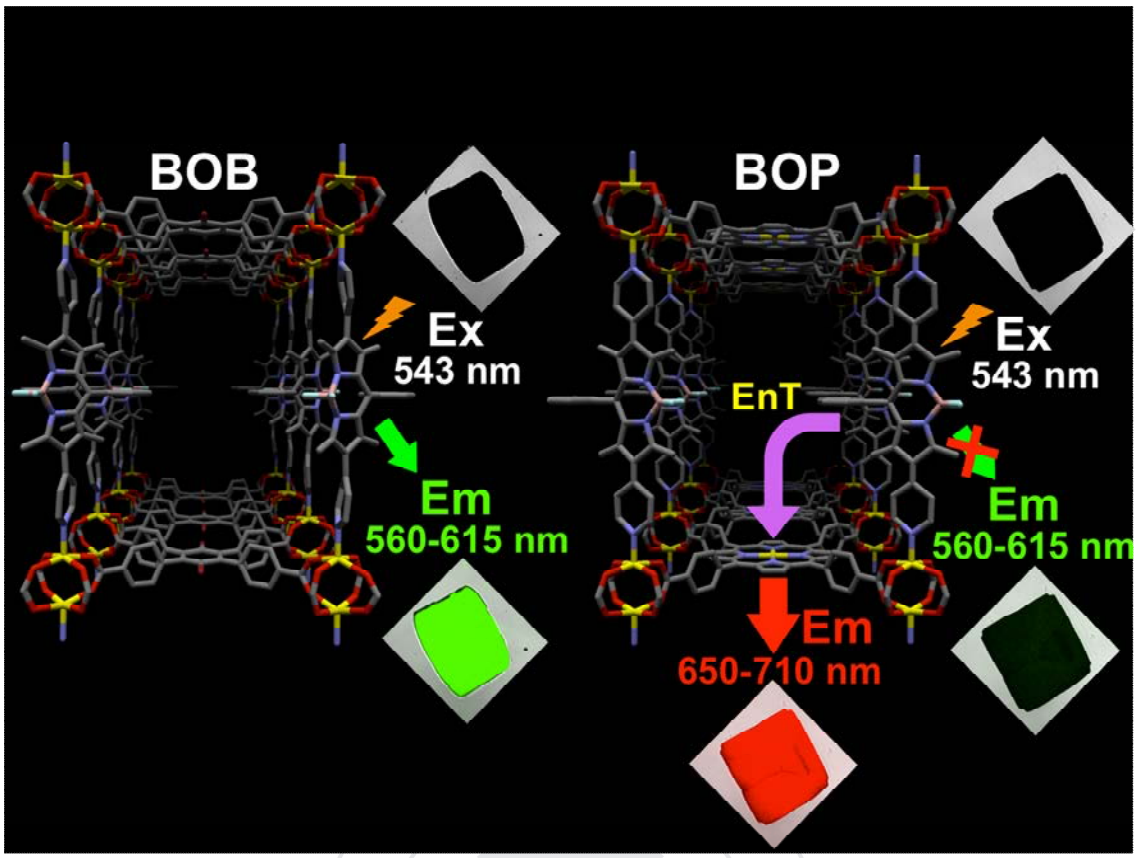
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 김종식

Light-Harvesting Metal-Organic Frameworks (MOFs): Efficient Strut-to-Strut Energy Transfer in Bodipy and Porphyrin based MOFs

이창연

인천대 에너지 화학공학과

A pillared-paddlewheel type metal-organic framework material featuring bodipy- and porphyrin-based struts, and capable of harvesting light across the entire visible spectrum, has been synthesized. Efficient ? essentially quantitative ? strut-to-strut energy transfer (antenna behavior) was observed for the well-organized donor-acceptor assembly consituting the ordered MOF structure.



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장소: 부산BEXCO

발표코드: **INOR.O-3**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 김종식

Programmable Soft Lithography: Solvent-Assisted Nanoscale Embossing (SANE)

이민형

경희대 응용화학과

This presentatioin reports an all-moldable nanopatterning process that can fabricate large-area nanoscale arrays with tunable feature sizes and pattern pitches. Solvent-assisted nanoscale embossing (SANE) could decrease the spacing of patterns down to 50% compared to the original mold master by heating thermoplastic substrates. Also, SANE could reduce the sizes of patterns down to 45% compared to the master by controlled swelling amount of molds with different solvents. SANE thechniques also have an advantage for the plasmonic researchers, becasue these methods can sequentially control plasmonic resonances of nanoparticles by continuously changing the pitches of metallic nanoparticles.

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발표코드: **INOR.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김종식

Direct Evidences of Hydrogen Spillover in Nano-hybrid System, Pt-MwCNT-MOF5

최용남 이희주 최상범[1] 김자헌[1] 조인화 강승기

한국원자력연구원 중성자과학연구부 [1]숭실대 화학과

Hydrogen can be stored on/in materials via physisorption or chemisorption processes. The requirements for a realistic on-board application are high usuable capacity, low cost, fast charging/discharging, reliable reproducibility, acceptible temperature/pressure and so on. Neither of the two storage mechanisms satisfies the whole requirements. Hydrogen storage by spillover process can be regarded as a combination or fusion of physisorption and chemisorption. Some of molecular hydrogens adsorbded on a nano-porous material can be dissociated into hydrogen atoms by catalyst. Those atoms are migrated through some nano-paths to the hydrogen acceptors which are the final destinations of the hydrogen atoms and chemically bind with them. Though there have been a lot of experimental reports on the existence of spillover process, it is hard to find a direct and/or a clear experimental evidence. And many researchers have failed to reproduce the results. From a carefully excuted in-situ neutron scattering experiment, a clear evidence of the spillover process was obtained in a nano-hybrid system, a composite of Pt nano particle decorated MWCNT and MOF5. The hydrogen acceptor was identified by a series of XPS measurement. Experimental details and a theoretical explanation of the spillover process will be discussed.

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장소: 부산BEXCO
발표코드: **INOR.O-5**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 이민형

Azaphenalene-based Ligands and Their Coordination Networks

Yakiyama Yumi 구진영 **Masaki Kawano**

포항공과대 첨단재료과학부

Proper ligand design is important to realize specific coordination networks which can show interesting properties. 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. In such networks, intriguing dynamic motion, electronic properties and catalytic reaction can be realized by electronic interactions or outer stimuli. Here, we will show our recent work on the azaphenalene-based coordination networks with focusing ligand design, structural characterization, and physical properties. Azaphenalene systems which have multi-interactive sites are the nitrogen analogues of redox-active phenalene compounds. Such features inspired us to apply azaphenalene as the main skeleton for multi-interactive as well as redox-active ligand design. First we focused on the hexaazaphenalene (HAP) in terms of multi-interactivity to synthesize TPHAP having with three pyridine moieties in gram scale. Coordination networks composed of TPHAP and various metal ions showed dynamic properties such as kinetic crystal formation followed by surface mediated structure transformation and encapsulation of various guest molecules. On the basis of the above results, we designed redox active ligands using diazaphenalene (DAP) which shows unique redox properties. A tripyridyl diazaphenalene ligand (TPDAP) can be prepared from commercially available reagents in a few steps. In sharp contrast to TPHAP, TPDAP is redox active because of a much lower HOMO-LUMO energy gap than that of TPHAP.

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장소: 부산BEXCO

발표코드: **INOR.O-6**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 이민형

Proton Conductivity in Metal-organic Framework Materials

정낙천

대구경북과학기술원(DGIST) 신물질과학

Metal-organic frameworks (MOFs) are an intriguing class of crystalline materials that can be readily assembled by combining metal ions (components of nodes) and multi-topic organic ligands (structural linkers) via coordination chemistry, typically under solvothermal reaction conditions. Often characterized by large internal surface areas and extended nanoscale porosity, MOFs are being examined as candidate materials for applications in chemical separations, gas storage, heterogeneous catalysis, sensing, ion exchange, and drug delivery. Recently, another potential property of MOFs, electrical conductivity - and, in particular, proton conductivity - has begun receiving attention. The attention comes, in part, from fundamental scientific interest in ionic conductivity in new environments; in part, from a desire to use conductivity as a real-time reporter on sorption of molecular guests. Here, we present a new approach to engender proton conductivity in MOF materials.

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장소: 부산BEXCO

발표코드: **INOR.O-7**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:15, 좌장: 이민형

New class of porous crystals obtained by the insertion of the second ligand during the construction of metal-organic frameworks

박태홍

한국원자력연구원 원자력화학연구부

Although the the assembly of single organic linking units with metal ions or metal clusters has been successful in building a variety of metal-organic frameworks (MOFs) with high surface areas, intriguing pore networks, and functionalities sufficient to diverse applications, coordination copolymerization using two or multiple ligands indeed leads to properties unprecedented with single linker MOFs. First, the coordination copolymerization of two isomorphic linkers has demonstrated the linear control of functionality within pores. We display here that an exclusive phase selection of a minority linker over the other can improve the properties of resulting MOFs in a nonlinear manner. Second, the MOF construction using two topologically distinct linkers has provided enormous surface areas with novel crystal structures. In such a case, the mole ratio of two ligands should be within a narrow range based on stoichiometry to obtain pure materials; if this is not the case, typically the structure of the resulting MOF is determined by the linker present in highest concentration. Although the minority linker can coordinate to some extent, the high reversibility during crystallization repairs such defect sites in a reaction solution. However, we propose that if the driving force for crystal growth of the majority linker is sufficient, the minority ligand can be incorporated within the framework, leading to defects with dangling ligands. Here we show that this approach produce a new material with a powder X-ray diffraction pattern nearly identical to that of the MOF derived from the dominant linker and displaying comparable gas sorption behavior. This new material possesses a significant number of defect sites that functionalize the pores and show unprecedented reactivity.

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장소: 부산BEXCO

발표코드: **INOR.O-8**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 이민형

Importance of interdimer spin exchange interaction in magnetic property of $Cs_3V_2Cl_9$: Density function theory study

이창훈 심지훈 강진희[1] Myung-Hwan Whangbo[1]

포항공과대 화학과 [1]North Carolina State University

Firstly, the crystal structure of $Cs_3V_2Cl_9$ was determined by Wessel and Ijdo [1]. The $Cs_3V_2Cl_9$ compounds crystallize in the hexagonal space group P63/mmc with cell parameters of a = 7.240 and c = 17.95 Å. It contains two isolated face shared dimer $V_2Cl_9^{3-}$ per unit cell which are aligned along the crystal c direction. The symmetry of a face shared $V_2Cl_9^{3-}$ unit is D3h and the single ion, VCl_6^{3-} octahedra, has C3v symmetry. In this study, we evaluated spin exchange interaction of $Cs_3V_2Cl_9$ by performing relative energy-mapping analysis based on density functional calculations to reveal magnetic structure of $Cs_3V_2Cl_9$ and the spin exchange interaction and magnetic properties were analyzed in terms of orbital interaction. As a consequence, the intradimer spin exchange interaction is the strongest one, but the interdimer spin exchange interaction along the crystal c direction (see fig1) play an important role to take place antiferromagnetic ordering at low temperature region. (1) G.J, .Wessel and D.I.W. Ijdo, Acta Cryst. 10, 446 (1957).

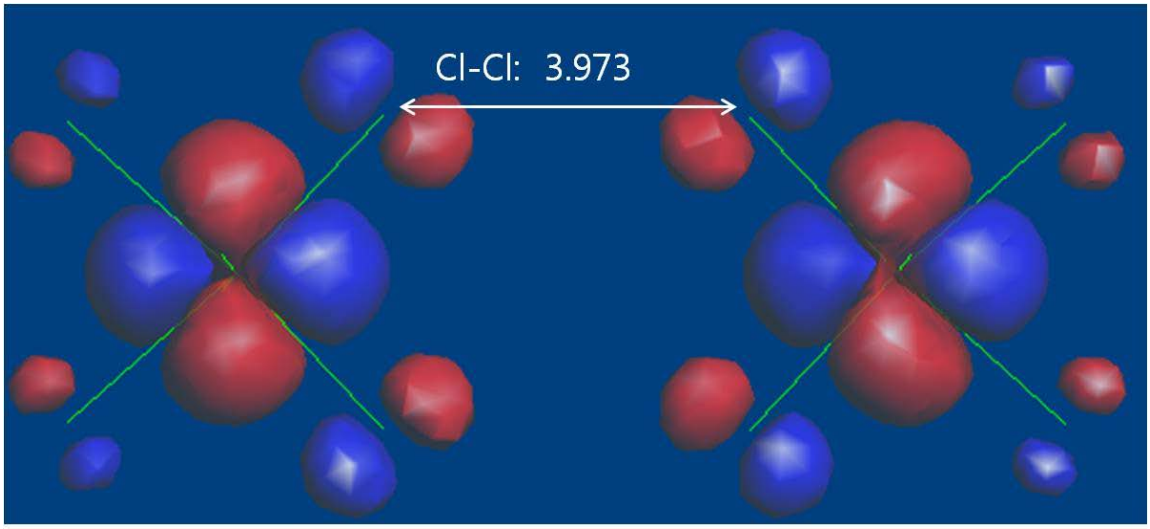

Figure 1. orbital interaction in J_3 Spin dimer

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장소: 부산BEXCO

발표코드: **PHYS1.O-1**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김준수

Folding/Unfolding Dynamics of Cytochrome *c*

Jungkweon Choi Tetsuro Majima

SANKEN, Osaka University

Since the protein structure is intimately related with the function of a protein, understanding the conformational change of a protein occurring in physiological condition is of critical importance. Especially, the protein folding process occurring in the biological system has been innumerably investigated to understand its structure and function as well as more complex biological phenomena such as the interaction between biomolecules and assembly of complex structures. Here, we have investigated the denaturant-induced conformational dynamics of yeast iso-1-cytochrome *c* (Cyt*c*) and the electron-transfer-induced folding dynamics of Cytc using pulse radiolysis. The unfolding process of Alexa 488-labelled Cyt*c* (Cyt*c*-A488) observed in the single-molecule and bulk phases can be explained well in terms of a three-state model. By quantitative analysis of fluorescence correlation spectroscopy (FCS) data, we were able to observe a relaxation time of ~1.5 μs corresponding to segmental motion and fast folding dynamics of 55 μs in the unfolded state of Cyt*c*. The results presented here support that a combination of single-molecule and ensemble-averaged spectroscopy is necessary to provide convincing and comprehensive assignments of protein kinetics. On the other hand, we show that at the presence of the high concentration of guanidine HCl (GdHCl), the reduction of the oxidized Cyt*c* takes place in a few microsecond time scales by the electron transfer from the guanidine radical that is formed by the fast reaction of the hydrated electron with GdHCl. Folding kinetics of Cyt*c* initiated by the electron injection span a wide time range and highly heterogeneous. The folding process of Cyt*c* is discussed based on these observations.

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장소: 부산BEXCO

발표코드: **PHYS1.O-2**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 김준수

Effect of Strong Electric Fields on the Vibrational Frequency and H-Bond of Acetone

강헌

서울대 화학부

고진공 용기 안에서 금속 표면 위에 얼음 박막을 증착하고 그 위에 이온을 뿌려서 ~10 nm 두께의 축전기를 제작하였다. 뿌려준 이온의 양을 조절하여 대전량을 변화시킴으로써, 얼음 박막 내부의 전기장의 세기를 10^9 V/m 까지 얻었다. 반사 흡광 적외선 분광법(Reflection Absorption IR Spectroscopy)을 사용하여 얼음 층에 갇힌 아세톤 분자의 C-O 진동 주파수가 강한 전기장 하에 변화하는 vibrational Stark shift 를 관찰하였다. 또한, C-O 진동수의 변화는 아세톤과 주변 물 분자와의 수소 결합 형태가 변화됨을 나타낸다.

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장소: 부산BEXCO

발표코드: **PHYS1.O-3**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 김준수

A Monte Carlo Simulation Study on Epoxy/CNT Nanofibers as Stretchable Electronics

조현우 성봉준

서강대 화학과

Stretchable electronics are a new class of materials that have promising applications in displays, wearable devices and energy storages. However, there have been few systematic studies on how mechanical elongation would influence the electrical conductivity and the molecular structure of materials. We elucidate the effect of mechanical elongation on the electric conductivity of epoxy/CNT nanofibers using Monte Carlo (MC) simulations and percolation theory. Using a coarse-grained model, we obtain equilibrium configurations of epoxy/CNT nanofibers. Then, we trace the change of electric conductivity during the elongation of the nanofiber. The electric conductivity decreases as Epoxy/CNT nanofibers are elongated. A decrease in the electrical conductivity is attributed to our observations that the effective volume fraction of CNTs in nanofibers decreases during the elongation process.

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장소: 부산BEXCO

발표코드: **PHYS1.O-4**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김준수

Coherent Nuclear Wave Packets of Salicylaldehyde azine and P.Y. 101 Induced by Proton Transfer Reaction in Excited State

이승노 주태하

포항공과대 화학과

Proton transfer is one of the most important elementary reactions in chemistry and biology found ubiquitously. The reaction dynamics and relevant potential energy surfaces (PES) have been the subject of extensive investigation. Excited state intramolecular proton transfer (ESIPT)1 has been studied as a model system of the proton transfer. An ESIPT reaction usually occurs barrierlessly within 100 fs, which can act as an impulsive excitation of the vibration to generate coherent nuclear wave packets in the product PES as shown in figure 1.2 Salicylaldehyde azine (SAA) and pigment yellow 101 (P.Y. 101) may show such phenomenon because of the ultrafast ESIPT reaction (figure 2). We investigated the ESIPT dynamics of SAA and P.Y. 101 by highly time-resolved fluorescence (TRF). Stationary emission spectra are dominated by the product keto emission with large Stokes shifts of 11000 and 6200 cm^{-1} for SAA and P.Y. 101, respectively,3 implying ultrafast ESIPT. TRFs of both molecules show ultrafast decay in the enol emission region; 23 and 30 fs for SAA and P.Y. 101, respectively. Corresponding rises were also observed at the keto emission region, verifying ultrafast ESIPT reaction. The ultrafast ESIPT reaction coherently excites some vibrational modes, which manifest themselves in the TRF; a coherent nuclear wave packet modulates the center frequency of the fluorescence spectrum in time to result in an oscillation of the TRF signal observed at a single frequency. The oscillatory components in the TRFs were analyzed by Fourier transform and linear prediction singular value decomposition.4 SAA has 130, 230 and 320 cm-1 components and P.Y. 101 has 40, 120, 150, 270 and 350 cm^{-1} components. Theoretical calculations by the normal-mode-projection method with ab-initio calculation are in good agreement with the experiment for both molecules, and result in a detailed picture of the molecular reaction dynamics of the ESIPT reaction.

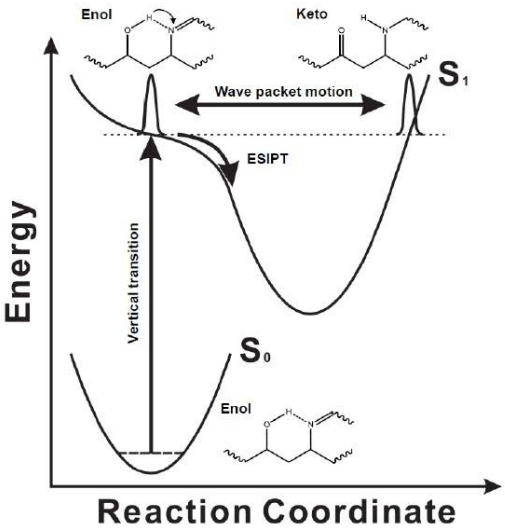

Figure 1. Reaction scheme of ESIPT and coherent nuclear wavepacket motion

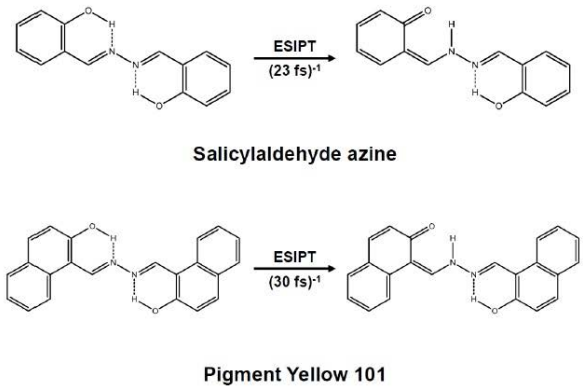

Figure 2. Molecular structure and rate of ESIPT of salicylaldehyde azine and pigment yellow 101

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장소: 부산BEXCO

발표코드: **PHYS1.O-5**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 성봉준

Drying Transition of Water Confined between Hydrophobic Pillars

김효정 장준경[1]

부산대 나노융합기술학과 [1]부산대 나노소재공학과

The phase behavior of the water confined between hydrophobic pillars was studied by using theory and simulation. Based on the thermodynamic approach, we expected the critical spacing between pillars which gives a Wenzel (WZ) to Cassie-Baxter (CB) transition of droplet. Our theory, agreeing with both simulation and experiment, predicts that sufficiently large circular pillars cannot maintain a CB state even if the pillars are in contact with each other.

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장소: 부산BEXCO

발표코드: **PHYS1.O-6**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 성봉준

Resonance Raman Spectroscopy of Dye Molecules Sandwiched between Two Single Layered Graphene

신동하

서울대 자연대 화학부

Raman scattering measurements of a few dye molecules confined in between two single layered graphene were conducted. Compared with recently reported Graphene-Enhanced Raman Spectroscopy (GERS) in which Raman scattering intensity of dye molecules adsorbed on graphene is quite enhanced, it was interestingly observed in this work that by covering with another single layered graphene sheet onto the substrate that has been used in GERS, the Raman scattering intensity is not always enhanced by adsorbed graphene but rather shows molecular resonance and excitation wavelength dependency. The Raman signal variation is assumed to follow the red-shift of the molecular spectral resonance induced by adsorption of graphene layer onto the molecules.

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장소: 부산BEXCO

발표코드: **PHYS1.O-7**

발표분야: General Oral Presentation (I)

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 성봉준

Development of Multi-mode (MALDI-SIMS) Mass Chemical Microscopic Molecular Imaging System

윤소희 오주연 문정희[1] 이태걸 문대원

한국표준과학연구원 나노바이오융합연구단 [1]한국생명공학연구원 단백체의학연구센터

Mass spectrometric imaging (MSI) has been emerged as a key method to get the spatial information about biomolecules from complex surfaces. Two popular ionization methods, matrix-assisted laser desorption ionization (MALDI) and secondary ion mass spectrometry (SIMS), are commonly used in MSI for analyzing high mass molecules such as peptides and proteins and low mass molecules such as metabolites and lipids, etc. respectively. We designed and constructed a MALDI-SIMS multi-mode molecular diagnostic microscope with high through-put and high content screening capability for mass imaging analysis.For achieving a micrometer spatial resolution and a high mass resolution, a microscopic ion optics lens system was designed and constructed. The instrument consists an ion source for MALDI/SIMS, a first time-of-flight (TOF) to time-separate the prompt ions generated by MALDI/SIMS, and two type of detectors, the IONPIX and delay line detectors for linear and reflectron TOF analysis. To enhance molecular secondary ion yields for large molecules, a pulsed Ar gas cluster ion gun was designed and constructed. The mass resolution was better than 3,000 and it was able to analyze the mass range up to 70 kDa in a MALDI experiment. To resolve the multi-hit problem in MALDI imaging, the IONPIX detector was adapted and tested. A microscopic image spectrum of a peptide sample under a mask of microarray-type was achieved with spatial resolution as 10 μm and with field of view as 500 x 500 μm^2. In the test of GCIB, widths of pulsed Ar cluster ion beam were measured at the sample plate. After two chopping, width of the ion beam was about 3 μs and the bunched ion beam was achieved up to 300 ns. More detailed results will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-1**

발표분야: General Oral Presentation (II)

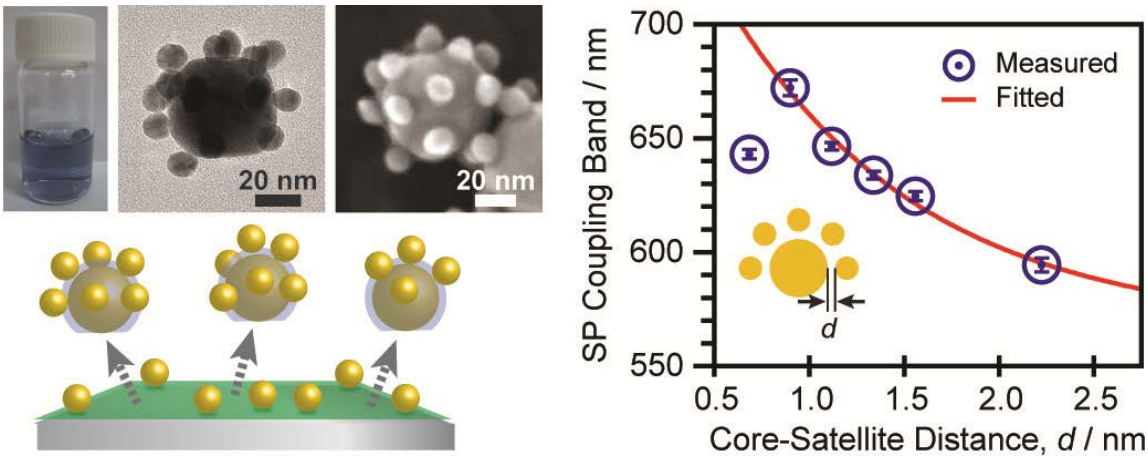
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 윤진환

Controlled Assembly and Plasmonic Properties of Asymmetric Core-Satellite Nanoassemblies

윤준희 임종휘 윤상운

단국대 화학과

The assembly of noble metal nanoparticles offers an appealing means to control and enhance the plasmonic properties of nanostructures. However, making nanoassemblies with easily modifiable gap distances with high efficiency has been challenging. Here, we report a novel strategy to assemble gold nanoparticles (AuNPs) into Janus-type asymmetric core-satellite nanostructures. Markedly different desorption efficiency between large and small AuNPs in ethanol allows us to prepare the asymmetric core-satellite nanoassemblies in a dispersed colloidal state with near 100% purity. The resulting nanoassemblies have well-defined structures in which a core AuNP (51 nm) is covered by an average of 13 ± 3 satellite AuNPs (13 nm) with a part of the core surfaces left unoccupied. Strong surface plasmon coupling is observed from these nanoassemblies as a result of the close proximity between the core and the satellites, which appears significantly redshifted from the surface plasmon resonance frequencies of the constituting nanoparticles. The dependence of the surface plasmon coupling on the gap distance less than 3 nm is systematically investigated by varying the length of the alkanedithiol linkers. The asymmetric core-satellite nanoassemblies also serve as an excellent surface-enhanced Raman scattering (SERS) substrate with an enhancement factor of ~10^6. Finally, we demonstrate that the presented assembly method is extendible to the preparation of compositionally heterogeneous core-satellite nanoassemblies. [*ACS Nano* 2012, *6*, 7199]



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-2**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 윤진환

Polyamorphism of Water inside Protein Crystals

김채운

Cornell University, CHESS

Protein crystals typically consist of 40 - 60 % water. The internal water forms solvent channels (2 - 4 nm in diameter) inside the crystals. We have studied the phase behavior of water inside protein crystals using a novel crystal freezing method: high-pressure cryocooling. Using X-ray diffraction, we demonstrated that the high-density amorphous (HDA) ice induced inside the high-pressure cryocooled protein crystal undergoes a phase transition to low-density amorphous (LDA) ice as the crystal is warmed from 80 to 170 K. We found that the intermediate states in the temperature range from 80 to 170 K can be reconstructed as a linear combination of HDA and LDA ice, suggesting a first-order transition. We also found evidence for a liquid state of water during the ice transition by monitoring the protein crystallographic data, suggesting a possible glass transition of HDA ice. Recently, we discovered that protein undergoes a dynamical transition as low as 110K during the water phase transition. These results provide new insights into the anomalous behavior of supercooled water and open a host of unanswered questions.References[1] Chae Un Kim, Mark W. Tate and Sol M. Gruner (2011), Protein dynamical transition at 110 K, Proc. Natl. Acad. Sci. USA 108, 20897-20901.[2] Chae Un Kim, Buz Barstow, Mark W. Tate and Sol M. Gruner (2009), Evidence for liquid water during the high-density to low-density amorphous ice transition, Proc. Natl. Acad. Sci. USA 106, 4596-4600.[3] Chae Un Kim, Yi-Fan Chen, Mark W. Tate and Sol M. Gruner (2008), Pressure induced high-density amorphous ice in protein crystals, J. Appl. Cryst. 41, 1-7.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-3**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 윤진환

Efficient N-doping of grapheme films by APPE(Aminophenyl Propargyl Ether)

전학림

서울대 화학과

Surface doping might be attractive method to modulate electrical properties of 2D materials. Especially for graphene, doping might be easy method to change Fermi energy level. Here, we found APPE (aminophenyl propargyl ether) as new n-type dopant for graphene. The characteristics of APPE doped graphene FET are studied using Raman spectroscopy as well as transport measurement. The statistical intensity ratio of 2D/G between pristine graphene and APPE doped graphene FET is reduced upto 40% in Raman spectroscopy, indicating pristine graphene is doped. To measure n-doping effect, we conducted transport experiment. The amount of change of Dirac point to negative was 133V. Two characteristics of APPE doped graphene FET didn't follow reported tendencies. First, unlike reported n-doped graphene, G peak of APPE doped graphene FET was upshifted. In addition to this, electron mobility of APPE doped graphene FET was nearly constant. While the structure of APPE has amine group as electron donating group, it also has acethyl group, acting as electron withdrawing group. This might result in unexpected G peak tendency in Raman spectroscopy and constant electron behaviors in transport measurement. These results assumed based on Hammett equation, which explains empirical substituent effect. As a result, sheet resistance of APPE doped graphene reduced to 70%, which might have its potential for future electronic application. Also acetylene group of APPE might introduce click chemisty into present results.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-4**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 윤진환

Optical Separation of Mechanical Strain from Charge Doping in Graphene

류순민

경희대 응용화학과

Graphene, due to its superior stretchability, exhibits rich structural deformation behaviors and its strain-engineering has proven useful in modifying its electronic and magnetic properties. Despite the strain-sensitivity of the Raman G and 2D modes, the optical characterization of the native strain in graphene on silica substrates has been hampered by excess charges interfering with both modes. Here we show that the effects of strain and charges can be optically separated from each other by correlation analysis of the two modes, enabling simple quantification of both. Graphene with in-plane strain randomly occurring between -0.2% and 0.4% undergoes modest compression (-0.3%) and significant hole doping upon thermal treatments. This study suggests that substrate-mediated mechanical strain is a ubiquitous phenomenon in two-dimensional materials. The proposed analysis will be of great use in characterizing graphene-based materials and devices.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-5**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 류순민

Molecular Dynamics Simulation of Phonon conductivity of High *ZT* thermoelectric In_4Se_{3-x}

지효석 이창훈 심지훈

포항공과대 화학과

In_4Se_{3-x} is an n-type thermoelectric material which was reported to have a high *ZT* of 1.48 at 705 K. The electronic properties (electrical conductivity and Seebeck coefficient) were well described by band theory and Boltzmann transport equation. However, thermal conductivity is not described well because the lattice part of thermal conductivity is dominant in thermal conductivity of In_4Se_3. In this study, we develop interatomic potentials and perform equilibrium molecular dynamics (MD) simulation to investigate lattice thermal conductivity of In_4Se_{3-x}. The result shows anisotropic change by applying Se vacancy. For In_4Se_3 (x = 0), obtained thermal conductivity is larger than experimental result (In_4Se_{3-x}, x = 0.22) in b-c plane while a-b plane thermal conductivity is well matched. And for $In_4Se_{2.5}$ (x = 0.50), the thermal conductivity on b-c plane is in a good agreement with experimental result. We confirm that the Se vacancy only affect c-directional thermal conductivity by phonon dispersion and structural point of view. Decomposition result also shows that the Se vacancy supresses the long-range phonon in the c-direction much. So we conclude the Se vacancy has an important role in describing anisotropic thermal conductivity of In_4Se_{3-x} compound.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-6**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 류순민

Identifying Stacking Orders of Graphene Synthesized by Chemical Vapor Deposition

배수강

성균관대 나노소재기반휴먼인터페이스 융합연구센터

The graphene films were synthesized using a chemical vapor deposition (CVD) method on Cu foils. The graphene grown on commerciaaly available Cu foils with 0.1 ~ 0.2 % impurities inevitably forms multilayer island, and sometimes, it is possible to grow bilayers by controlling the growth conditions. Here, we demonstrate that number of graphene layers as well as their stacking orders can be identified by electrostatic force microscopy (EFM), scanning Kevin probe microscopy (SKPM), and Raman spectroscopy. Using SKPM, we also confirm that the work-functions of randomly stacked graphene bi-layers are lower than those of A-B stacked bi-layers. We also investigated the bi-layer graphene which covers grain boundaries of Cu, and the different stacking orders was found from the graphene grown on the different grains of Cu.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-7**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 류순민

Nanostructure characterization of graphene films formed by using chemical vapour deposition

조성표 배수강[1] 홍병희

서울대 화학부 [1]성균관대 성균나노과학기술원

Transmission electron microscopy (TEM) and Scanning TEM (STEM) have recently seen a dramatic improvement in instrumentation with the emergence of hardware aberration correction. However, imperfections in the preparation of TEM samples often become the limiting factor of the information to be obtained. For example, Nano-materials, as well as biological molecules are typically prepared across support films for imaging by the electron beam. Graphene has renewed interest in crystalline TEM supports, because it provides supports of single atom thickness, extreme physical stability, periodic structure, and excellent electrical and thermal properties. Recently, we developed and reported a technique for growing the high crystalline quality and the lagre-scale graphene films using chemical vapour deposition (CVD). These results can expect application as effective crystalline TEM supports. In the present study, first we have synthesized graphene films with very good crystal quality. Their domain sizes were more than a few hundred nano-meters. Also, we have evaluated their detailed nanostructure characteristics by using High Resolution TEM and EELS (Electron Energy-Loss Spectroscopy) spectrum.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS2.O-8**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 류순민

Time dependent dynamics of graphene electrons and new design of graphene FET without an energy gap

김형준

KAIST EEWS 대학원

Graphene is a room temperature ballistic electron conductor and also a very good thermalconductor. Thus it has been regarded as an ideal material for post-silicon electronic applications.A major complication is that the relativistic massless electrons in pristine graphene exhibitunimpeded Klein tunneling penetration through gate potential barriers. Thus previous efforts torealize a field-effect transistor for logic applications, have assumed that introduction of a bandgap in graphene is a prerequisite. Unfortunately extrinsic treatments designed to open a bandgap seriously degrade device quality, yielding very low mobility and uncontrolled on-off currentratios. To solve this dilemma and control the dynamics of graphene electrons, we developed a finite-difference time-domain simulation method for the dynamics of graphene electrons, named as a GraFDTD. By using GraFDTD, we investigated the temporal behavior of graphene electrons, and propose a noble gating mechanism by engineering the gate geometry, which can lead a hundred-fold enhancement in on/off ratio. This suggests that intrinsic graphene can be used in designing logic devices without serious alteration of the conventional field-effect transistor architecture, and a new variable for the optimization of the graphene-based device ? geometry of the gate electrode.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-1**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김주훈

Conformational Study of Intrinsically Disordered Proteins Using Ion Mobility Mass Spectrometry

이신정 김준곤

포항공과대 화학과

Proteins which lack defined structures under physiological conditions are categorized as intrinsically disordered proteins (IDPs). Although conformational transitions of IDPs are known to be associated with various disorders such as amyloidosis, diabetes, and neurodegeneration, the conventional methods to probe protein structures (e.g. X-ray crystallography and NMR spectroscopy) provide only limited features for studying IDPs. Relevance between protein conformations and specific charge states of protein ions in the gas phase has been investigated in the conformation analysis using electrospray ionization mass spectrometry. Additionally, hydrogen/deuterium exchange or ion mobility experiments have been contributed to expand the application of mass spectrometry as a tool for structural investigation.With assistance of molecular chaperones, we generate several conformations from IDPs and probe structural changes upon solution to gas phase transition using mass spectrometer combined with travelling wave ion mobility spectrometry. In this presentation, the application of ion mobility mass spectrometry for the conformational analysis of IDPs will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-2**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 김주훈

Electrokinetic Concentration on Microfluidic Chip for Small Molecule Immunoassay

한동훈 김주훈[1] 정택동

서울대 화학부 [1]경희대 화학과

We have devised a unique method to enhance the sensitivity of competitive immunoassay using electrokinetic concentration near a pair of highly charge-selective polymer [poly-2-acrylamido-2-methyl-1-propanesulfonic acid (pAMPSA)] plugs on a microfluidic chip. The fluorescent indicators on magnetic microparticles are displaced by unlabeled target molecules in the sample and then electrokinetically preconcentrated in a single spot on the microfluidic chip to be detected by laser-induced fluorescence, leading to the sensitive assessment of the unlabeled small target molecules. As a proof-of-concept, the competitive displacement assay of unlabeled 1 nM biotin was accomplished with *ca*. 2000-fold enrichment within 3 min by employing this novel strategy. The proposed immunoassay system showed good selectivity for biotin against a 100-fold higher concentration of a biotin analogue, biocytin, 2-iminobiotin and desthiobiotin.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-3**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 김주훈

Detection of protein biomarker using Surface-enhanced Raman scattering (SERS) combined with Field Flow Fractionation (FFF)

신가영 김광수[1] 윤지혜 이승호[2] 정회일

한양대 화학과 [1]삼성전기(주) 중앙연구소 / FP Lab [2]한남대 화학과

Disease diagnosis by detecting a specific protein biomarker has been extensively studied recently. Since the concentration of protein biomarker in biological samples is extremely low in many cases, highly sensitive tagging methods such as surface-enhanced Raman scattering (SERS) are usually applied. Although sensitive analytical detection is possible using SERS, the resulting reproducibility is insufficient to adopt for real clinical analysis. The degraded reproducibility of SRES is mainly due to many factors such as unexpected particle aggregation and inhomogeneous distribution of hot-spots. Moreover, in immunoassay performed on the SERS-active substrate such as Au surface, uncontrollable non-specific binding of SERS probes on the substrate is always problematic. Therefore, new analytical strategy that can dramatically improve the reproducibility of SERS measurement is critically in demand. The feasibility study for detection of Anthrax biomarker, protective antigen (PA), by combining SERS and field flow fractionation (FFF) will be presented. The key concept is to perform all SERS measurements in a solution phase to remove the possibility of non-specific bindings, which always occur in solid substrate based SERS measurement. The mixture of bound SERS probes with PA, unbound probes, and PA could be separated in a micro-channel with proper external perturbation. During separation, laser radiation was continuously illuminated on the separation column, and SERS-based fractogram was acquired to determine the concentration of PA.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-4**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 김주훈

GC-MS based steroid signatures reveal physiological changes in hormonal dependent diseases

문주연 문명희[1] 정봉철[2] 최만호

KIST 미래융합기술연구본부 [1]연세대 화학과 [2]KIST

Steroid hormones regulate endocrine systems and their abnormal metabolism lead to hormonal imbalance, which is responsible for the development of endocrine diseases. The comprehensive quantification of steroid hormones in biological specimens is therefore needed to physiological changes in steroid metabolism. The GC?MS based steroid profiling techniques have been validated and generated by hierarchical-clustering analysis (HCA) to allow “steroid signatures” The optimized profiling techniques could be successfully applied into the assessment of drug efficacy in a CYP3A4 inducer rifampicin and understanding physiological effects on femur geometry from postmenopausal osteoporosis as well as prostate diseases. The devised non-invasive profiling techniques showed predictable CYP enzyme activities and better understanding of the pathogenesis of endocrine-related disorders where highly sensitive quantification is required.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-5**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 11:05, 좌장: 김주훈

Quantitative proteomics: Multiple reaction monitoring for targeted proteomics

김준석 양은경[1]

KIST 테라그노시스연구단 [1]KIST 의과학연구센터

The development of multiple reaction monitoring (MRM) with triple quadrupole (QQQ) MS system brought a new analytical area as an attractive biomarker discovery tool. The advantages of MRM are various. MRM strengthens genomics-driven findings as well as MS-based proteomics such as shotgun-MS approach, by targeting and quantifying interesting analytes. Although massive genomic data continue to flood into diagnostic laboratories, absolute quantitation in proteome level is inevitable since the expression level of a protein in a biological sample is critical in disease. Nano-LC interfaced MRM enables multiplexed and low abundant targets to be simultaneously quantified. It is very important since various targets play a critical role in a disease. Also, MRM creates rapid, selective, sensitive and cost-effective bioanalytical strategy. The scheduling algorithms in recent QQQ instruments facilitate over 1000 targets to be scanned in pre-defined time zone in a single run. This feature is comparable to ELISA that needs more than a day to analyze 96 target proteins. Moreover, the analyzing process in MRM does not require any antibody for most experiments since it needs only the transitions of the proteotypic peptides of targets. In this presentation, the technical applications of MRM will be introduced with quantification of clinical samples.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-6**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 김준곤

Top-down analysis of intact lipoproteins by on-line coupling of chip-type asymmetrical flow field-flow fractionation and electrospray ionization-Tandem mass spectrometry

김기훈 문명희

연세대 화학과

Chip-type thin asymmetrical flow field-flow fractionation (AF4) channel was developed for on-line analysis of proteome and lipoproteins by top-down mass spectrometry strategy. The new channel provides convenient assembly by stacking flat metal plates and frits. The optimization and evaluation process were performed about size sorting and molecular weight determination of protein standards with full scan and CID spectra. By utilizing chip-type AF4, high density lipoprotein (HDL) and low density lipoprotein (LDL) are separated by hydrodynamic diameters in an aqueous solution with the simultaneous desalting at micro flow rate regime. It was found that on-line desalting by AF4 enhances ionization of macromolecular species and tandem MS analysis during electrospray ionization when it was compared to the direct infusion of lipoproteins to MS. Evaluation of top-down lipidomic analysis is made with the efficiency test of the in-source fragmentation during cAF4-ESI-MS on the dissociation of lipoprotein particles into individual lipid molecules. It was also performed that the comparison of relative ratio of phosphatidylcholines (PCs) in human plasma between coronary artery disease(CAD) patients and healthy controls.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-7**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 김준곤

Ion Mobility and photoexcitation techniques for biomolecule analysis

이선영

한국원자력연구원 원자력화학연구부

Ion mobility spectrometry (IMS) is a powerful analytical technique for the separation of gas phase ions. IMS coupled with mass spectrometry (MS) can be utilized to separate and characterize individual components within a complex mixture that may not be resolved by MS alone. The first part of the talk describes a new IMS method that constructs ion mobility distributions of precursor ions by extracting drift time distributions of selected fragment ions. Photodissociation of the mobility-selected ions generates unique product ions that are useful for distinguishing individual components from the mixture. The following studies involve a novel approach to produce new molecular species in the gas phase. Photoexcitation (157 nm) of long-lived, charge-bound dimer complexes appears to be a general phenomenon, resulting in the loss of water and the formation of covalent bonds between many types of molecules. Several examples are described, including: the linear coupling of amino acid chains that produce octapeptides from tetrapeptide complexes; inter-molecular cross-linking of amino acid side chains; and glycosidic bond formation between disaccharides.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-8**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 김준곤

Determination of Kinetic and Thermodynamic Parameters for Electrochemical Reactions by New Fourier Transform Electrochemical Impedance Spectroscopy.

고영훈 박수문[1]

울산과학기술대 친환경에너지공학부 [1]울산과학기술대 에너지공학부

Studies on electrode-electrolyte interfaces are very important in electrochemistry as they provide much information on how the electrode and the electrolyte communicate electronically. However, the information on the interface cannot be fully resolved using conventional electrochemical data such as *i-E*, *i-t*, and/or *E-t* curves. These methods provide only currents and/or potentials resulting from both faradaic and non-faradaic components convoluted together. For that reason, electrochemical impedance spectroscopy (EIS) is a useful method in measuring how efficiently an electrochemical reaction takes place at the electrode/electrolyte interface. We report hereby the staircase cyclic voltammetric-Fourier transform EIS (SCV-FTEIS) method, in which both SCV and FTEIS experiments are combined using a series of incrementing and/or decrementing small potential step signals to acquire impedance data in a wide frequency range throughout the whole voltage range scanned. With the SCV-FTEIS experiments, kinetic and thermodynamic parameters are obtained for electrochemical reactions. By analyzing raw impedance data thus obtained, we determine all kinetic parameters including exchange rate constants (k^0) and electron transfer coefficients (α), exchange currents (i^0), diffusion coefficients (D) as well as thermodynamic parameters such as half-wave potentials ($E_{1/2}$) and the number of electrons transferred. An example will be given to demonstrate how these parameters are actually obtained.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-9**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 12:25, 좌장: 김준곤

Electrochemical analysis of fluorine substituted olivine materials for Li rechargeable battery

신병철 이영일

울산대 화학과

There has been considerable interest in olivine structure as a cathode active material for Li rechargeable battery due to its strong phosphate-oxygen covalent bond, environmental friendly benefit, and excellent stability. The fluorine substituted $LiFe_{0.4}Mn_{0.6}PO_4$ composites have been synthesized by solid state reaction using planetary mill method without carbon coating. The XRD and XPS results of composite indicate fluorine anions have been completely substituted to PO_4 sites without structural modification. Electrochemical analysis has been performed with various C-rates, and initial discharge capacity of 150 mAh/g at 0.1 C rate for $LiFe_{0.4}Mn_{0.6}(PO_4)_{0.99}F_{0.03}$ has obtained.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-10**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 12:40, 좌장: 김준곤

Single Molecule Analysis for UV-induced DNA Damage

이진용

서강대 화학과

We report single molecule based analysis of single strand breaks (SSBs) on lambda phage DNA molecule. UV exposed lambda phage DNA produce a cyclobutane pyrimidine dimer (CPDs) lesion. Then repair of CPDs can be started with the base excision repair (BER) pathway, utilizing pyrimidine dimer glycosylase (PDGs) and Polymerase I. In the BER process we additionally utilize alexa-fluor labeled dNTPs for visualize repaired location, then we can make radiation induced SSBs lesion map by nicktranslation on the lambda DNA molecule. Single molecule observations map locations of DNA radiation-mediated SSBs revealing sequence-dependent DNA damage that was induced by short wavelength ultraviolet irradiation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.O-11**

발표분야: Diversity of Analytical Chemistry

발표종류: 구두발표, 발표일시: 금 12:55, 좌장: 김준곤

Liquid-liquid-liquid extraction in digital microfluidics

최기환 Aaron R. Wheeler

University of Toronto, Canada

We report the coupling of liquid-liquid-liquid extraction (LLLE) and digital microfluidics (DMF). LLLE is the technique of sample enrichment and purification technique using an organic membrane sandwiched between two aqueous solutions. In this work, the organic membrane was formed in a DMF device by actuating organic solvent to the a hydrophobic pillar structure. This structure stabilized the membrane position during the extraction process. Then sSample solution and acceptor solution droplets were actuated to opposite sides of the membrane. Analytes having neutralized form in the sample solution were partitioned into the organic membrane. Conversely, ionized solutes did cannot penetrate the membrane. The partitioned analytes were back-extracted and ionized into the acceptor solution to prevent repartitioning to membrane. The effects of pHs of aqueous the acceptor and donor solutions and extraction time were investigated and fluorescein was successfully extracted from the biologic fluid droplets within 60 min.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-1**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 조은진

Synthesis and Applications of Two-Photon Fluorescent Graphene Qauntum Dots for Bioimaging

정철

서울대 화학과

현재 '꿈의 신소재'라 불리우는 그래핀에 관한 연구가 활발하게 진행되고 있으며, 전기적 특성 외에도 바이오 쪽으로도 많은 연구가 이루어 지고 있는 실정이다. 그 중에서도 제로 밴드갭을 갖는 그래핀이 화학적 혹은 물리적인 방법으로 박리 및 쪼개지면서 생성되는 그래핀 옥사이드와 그래핀 퀀텀닷의 경우 형광을 띠고 있으며 기능화를 통해서 형광의 세기 증가 시키거나 색깔을 바꿀 수 있다. 선행연구에 의해 그래핀 옥사이드의 경우 이광자 흡수 성질이 있음을 알게 되었고 본 연구실에서 만들어진 그래핀 퀀텀닷 역시 이광자 흡수 성질이 있음을 알게 되었다. 따라서 기존의 유기물이 아닌 그래핀 퀀텀닷으로 새로운 이광자 형광 물질을 개발하고 이를 바이오 영상에 응용하여 생체 영상 물질분야에 새로운 장을 열고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-2**

발표분야: Oral Presentation for Young Organic Chemists

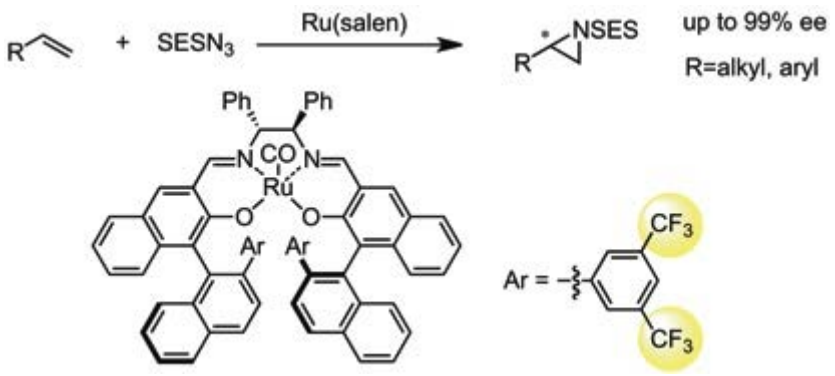
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 조은진

Asymmetric Olefin Aziridination Using a Newly Designed Ru(CO)(salen) Complex as the Catalyst

Chungsik Kim Tatsuya Uchida Tsutomu Katsuki

International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

Ru(II)(salen) complexes have been recognized as efficient catalysts for asymmetric formation of aziridines with diverse nitrene sources. Based on our previous investigations,[1-3] we developed a robust and catalytically highly active Ru(CO)(salen) complex 1 carrying 3,5-di(trifluoromethyl)phenyl group at C2” and achieved enantioselective aziridination employing not only conjugated but also isolated olefins with 2-(trimethylsilyl)ethanesulfonyl azide (SESN3). The trifluoromethyl substituent is considered to enhance the reactivity of N-sulfonyl nitrenoid intermediate through n-?* interaction between the lone pair electrons on the N-sulfonyl oxygen atom and the anti-bonding orbital of C-F bond. The reactions of conjugated olefins need only 0.5-1 mol % catalyst under mild condition and afforded excellent yields with excellent enantioselectivity (90-99% ee). The reactions of non-conjugated olefins also provided the desired aziridines in moderate to excellent yields (45-91 %) and good to excellent enantioselectivity (80-99 % ee). Besides, the SES protecting group can be easily deprotected under mild conditions.[1] Kawabata, H.; Omura, K.; Uchida, T.; Katsuki, T. Chem. Asian. J. 2007, 2, 248.[2] Kawabata, H.; Omura, K.; Katsuki, T. Tetrahedron Letters. 2006, 47, 1571. [3] Omura, K.; Uchida, T.; Irie, R.; Katsuki, T. Chem. Comm. 2004, 2060.



대한화학회
THE KOREAN CHEMICAL SOCIETY

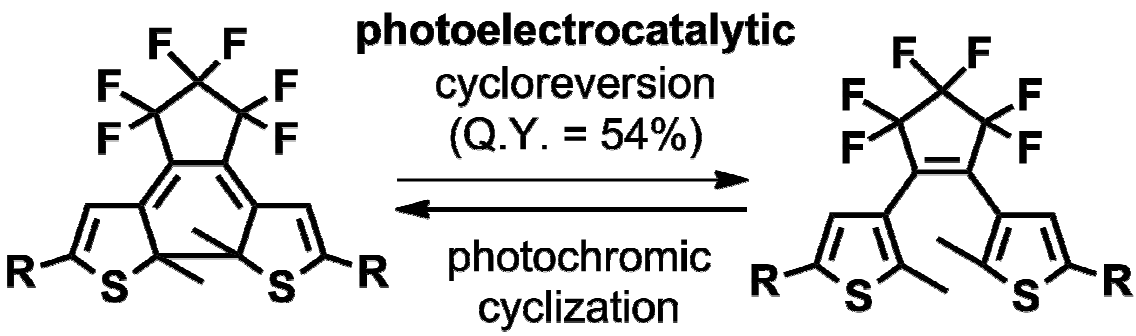
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.O-3**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 조은진

Electrochromism in Photochromic Dithienylethene Compounds

유영민 남원우[1]

KIST 의공학연구소 [1]이화여대 화학과

Photochromic *cis*-1,2-dithienylethene compounds (DTEs) are ideal candidates for application in photo-driven molecular switch because they feature great advantages with respect to fatigue resistance, thermal stability, and photosensitivity. Utility of DTEs has, however, been limited by low cycloreversion (ring-opening) quantum yields. We have developed a novel photoelectrocatalytic strategy that allowed us to achieve one order enhancement in the cycloreversion quantum yield. Photoirradiation of 9?mesityl?10?methylacridinium ion acting as a photoredox catalyst evoked catalytic cycloreversion of the DTE compounds. The kinetic processes of the reaction intermediates involved in the photoelectrochemical ring opening of DTEs have been observed for the first time, where the electronic nature of the DTEs is the key factor that governs the rate-determining step. Mechanistic studies further revealed the important steps determining the quantum yields in the course of the photoelectrocatalytic cycloreversion. As a useful demonstration, the dual chromic property, photochromism and electrochromism, has been implemented to a single molecular fluorescence memory.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-4**

발표분야: Oral Presentation for Young Organic Chemists

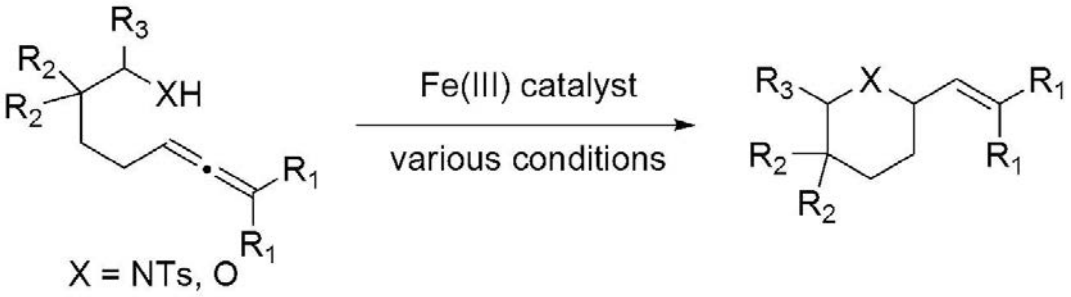
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 조은진

New Type of Reactions with Fe(III) Catalyst: Hydroalkoxylation and Hydroamination of Allenes

정민석 강은주[1]

경희대 응용화학과 [1]경희대 화학과

The use of transition metals as catalysts to induce new C-C, C-O, or C-N bond formation continues to grow exponentially for efficient and atom-economic organic transformations. It is worthy to investigate the cheaper and more easily available eco-friendly catalyst as unsaturated C-C bond activators toward nucleophilic attack. In our research aiming to develop green catalytic reactions, the nucleophilic cyclization reactions of allenes were catalyzed by Fe(III) to afford the corresponding heterocycle compound. Fe(III) catalysts were applied in the reactions of allenyl amides or allenyl alcohols and cyclized compounds containing O or N heteroatom were produced with moderate to good yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-5**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 조은진

Unique Donor-Acceptor-Donor Triad Incorporating Dicyanodistyrylbenzene and Carbazole Units : New Scaffold for Solid-State Fluorescent Smart Materials

권민상 박수영

서울대 재료공학부

The artificial molecular systems which are comprised of electron donor (D)?acceptor (A) connected by spacers with different nature, i.e. supramolecular DA systems, have been intensively investigated to understand the fundamental characteristics of charge-transfer (CT) interactions, photo-induced electron transfer (eT), and energy transfer (ET) reactions and to develop novel material systems for solar energy conversion or molecular optoelectronics. In particular, the studies on stimulus-response behaviors of fluorescent supramolecular DA systems represent an important topic due to their potential utilities for fluorescent chemosensors, molecular switches, molecular logic gates, and molecular computation.In this regard, de Silva and co-workers have developed a smart supramolecular DA platform, i.e. chemical-responsive donor?spacer?fluorescent acceptor, which respond to external stimulus with detectable changes of their fluorescence properties in fluid solutions, and thoroughly investigated its derivatives.While remarkable advances were made in fluid solutions, the studies on stimulus-responsive fluorescent DA systems in the solid state have been limited by fundamental reasons, i.e. (i) the strong quenching effect of common organic luminophores in the solid state, and (ii) uncontrollable photo-induced eT in molecular assemblies, despite great potential in practical applications such as portable sensors, security papers, optoelectronic devices, and data storage devices.In this presentation,we present a new approach to solve these unexplored issues.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.O-6**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 조은진

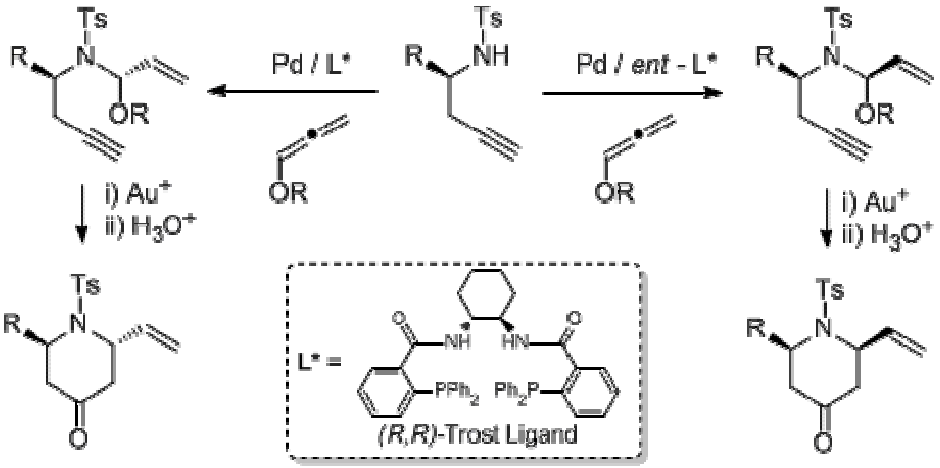
Synthesis of stereodefined *N,O*-acetals and applications

김해진 이영호

포항공과대 화학과

Developing a new reaction affording various azacyclic compounds with reactive functional groups is considered as one of the most important topics in organic synthesis. In particular, *N,O*-acetals have been conceived as a precursor for the iminium ion-mediated C-C bond formation.[1] In most cases, however, the stereochemical information of the *N,O*-acetal is easily destroyed due to the instability of the *N,O*-acetal, which limits further utilization in synthesis. Herein, we wish to represent our recent advances in synthesis of chemically labile *N,O*-acetals and their synthetic application.[2] The synthesis of labile *N,O*-acetals was accomplished by highly efficient and chemoselective Pd-catalyzed asymmetric hydroamination of alkoxyallene. In addition, we combined the stereodefined *N,O*-acetal with Au(I)-catalyzed cycloisomerization to afford *cis*- and *trans*-2,6-disubstituted piperidines.[3] Furthermore, applications of the *N,O*-acetals as diversity-generating and stereocontrol element will be also discussed. We expect our recent novel methodology of the asymmetric synthesis and utilization of stereodefined*N,O*-acetal opens the access to various azacyclic natural compounds and natural-product-like compounds.

[1] For a review on the use of *N,O*-acetals, see: Warriner, S. Category 4: *Compounds with Two Carbon-Heteroatom Bonds in Science of Synthesis: Houben-Weyl Methods of Molecular Transformations*; Georg Thieme Verlag: Stuttguart; 2007; Vol 30, p 7.
[2] Kim, H.; Rhee, Y. H. *J. Am. Chem. Soc*. 2012, *134*, 4011
[3] Kim, C.; Bae, H. J.; Lee, J. H.; Jeong, W.; Kim, H.; Sampath, V.; Rhee, Y. H. *J. Am. Chem. Soc*. 2009, *131*, 14660.



High stereroselectivity, Excellent yield
Retention of stereochemisty

대한화학회
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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-7**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 조은진

Efficient Hydrosilyloxylation Driving Tandem Aldol and Mannich Reactions Catalyzed by Gold

강동진 이필호

강원대 화학과

The chemoselective formation of an enolate from alkyne in the presence of a carbonyl and imine group was realized, which constructed a variety of structural motifs under exceedingly mild reaction conditions in a tandem process. Reaction driving tandem hydrosilyloxylation/aldol reactions was achieved through the formation of enol silyl ethers catalytically generated in situ from readily available alkynes. These reactions were expanded to obtain β-amino enol silyl ethers in good yields via the tandem hydrosilyloxylation/isomerization/Mannich reaction.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-8**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 조은진

The growth of high quality graphene using the optimal ratio of hydrogen and methane gases

황순휘 홍병희[1]

성균관대 나노과학기술학과 [1]서울대 화학부

We investigated the effect of growth conditions on the optical and electrical properties of graphene films grown by chemical vapor deposition on Cu foil. We show that the ratio of hydrogen and methane gases is critical condition for graphene grown by low pressure chemical vapor deposition (CVD) that affects the surface morphology and electrical properties of graphene. The surface morphology of graphene was analyzed by Scanning Electron Microscope (SEM) and Optical Microscope (OM). The electrical and optical properties of graphene were characterized by 4-point probe system and UV-vis-NIR. The optimized graphene exhibits a maximum mobility of 4500 cm2/Vs.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.O-9**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 조은진

헛개나무 열매로부터 화합물의 분리 및 화학구조 규명Isolation and Structure determination of compounds from *Hovenia dulcis* Fruits

서진아 고은희 정하숙[1]

덕성여대 화학과 [1]덕성여대 식품영양학과

헛개나무(*Hovenia dulcis* Thumb)는 갈매나무과의 교목으로 지구자 나무라고도 불리며, 열매는 알코올 분해능과 간 해독작용이 있어, 주독제거 및 과음 시 부작용으로 나타나는 황달, 지방간, 간경화증 등의 간 기능 보호에 효능이 우수한 것으로 보고되고 있다. 본 연구는 예로부터 기능성 식·의약 소재로 널리 이용되고 있는 헛개나무의 부가가치 증진을 목적으로, 피로회복 효능이 우수한 헛개나무 열매의 열수추출물을 실험에 사용하였다. 열매의 열수추출물을 산 가수분해 후 ethyl acetate 분획물로부터 2 종의 단일 화합물을 분리하였고, 원시료를 ethyl alcohol 로 추출한 후 *n*-hexnae, chloroform, ethyl acetate 및 *n*-butyl alcohol 로 분획한 후, 효능이 우수한 용매분획물로부터 3 종의 단일 화합물을 분리하였다. 분리한 순수 화합물을 1D-NMR(^{1}H-NMR, ^{13}C-NMR) 및 2D-NMR(DEPT, COSY, HMQC, HMBC)의 spectral data 를 이용하여 화학구조를 규명하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.O-1**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 양해식

Enhanced Performance of a Glucose Microbiofuel Cell using Conductive Polymer Composites

노희복 심윤보

부산대 화학과

The 2,2′:5′,2″-terthiophene-3′-(p-benzoic acid) (TTBA) and 2,2′:5′,2″-terthiophene-3′-ylhydrazine (TTHyd) were synthesized and self-assembled on gold nanoparticles (AuNPs). Self-assembled TTBA-AuNPs was electropolymerized on a microfluidic chip wall surface for immobilization of enzyme catalysts (glucose oxidase (GOx) or horseradish peroxidase (HRP)) through covalent bond formation, which allowed for direct electron transfer processes of the enzymes. Self-assembled TTHyd-AuNPs was electropolymerized on a microchip wall surface as a nonenzymatic catalyst for a microbiofuel cell. The microbiofuel cell composed of the anode (GOx/polyTTBA-AuNPs) and cathode (HRP/polyTTBA-AuNPs and polyTTHyd-AuNPs) were assembled and examined for cell performance. The microbiofuel cell operated in the solution containing glucose and anode-produced H2O2 generated an open-circuit voltage of approximately 435.0 mV, while the maximum electrical power density extracted from the cell was 53.1 ?W/cm2.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.O-2**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 09:42, 좌장: 양해식

Fabrication of Poly (thionine)-Gold Nanocomposite Modified Indium Tin Oxide Electrode for DNA Hybridization Detection

Md.Mahbubur Rahman

건국대 신기술융합학과

We developed a DNA hybridization sensor by poly (thionine) [PTH]-gold nanoparticles (GNPs) composite on indium tin oxide (ITO). GNPs with a spherical shape and the average particle size of ca.100 nm were directly electrodeposited on ITO surface. Then, PTH was electrochemically deposited on GNPs/ITO electrode. The average particle size of the GNPs increases up to ca. 180 nm upon PTH deposition with the absorption maximum of PTH at 650 nm and confirmed the PTH/GNPs composite formation. Pendant amine group (-NH2) of the PTH was utilized for covalent grafting of ss-DNA by phosphoramidate bond formation. The hybridization with different DNA segments on PTH/GNPs/ITO electrode induced the change of the oxidation signal of PTH with the maximum sensitivity of 51.10x10-2 uAcm-2pM-1 for complementary target DNA in a very wide dynamic range of 1 uM-1 pM.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.O-3**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 09:54, 좌장: 양해식

Electrochemical Characterization of Water-Soluble Au_{25} Nanoclusters Protected with (3-Mercaptopropyl)sulfonate and their Application.

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연세대 화학과 [1]Nano Materials Laboratory in India

In recent years, the synthesis and characterization of thiolate-protected Au_{25} clusters have drawn broad research interests because of their unique electrochemical and optical properties as well as their distinguished stabilities. In this presentation, we present the synthesis and electrochemical characterization of a new water-soluble Au_{25} cluster protected with (3-mercaptopropyl)sulfonate (MPS-Au_{25}), and their application for glucose biosensor is included. The MPS-Au25 exhibits the similar UV-vis absorption profile and electrochemical feature as we have reported before. The electrochemical characterization was carried out by transferring them into organic solvent using a phase transfer agent. The detailed voltammetric investigation of the phase-transferred Au_{25} in dichloromethane has revealed that the HOMO-LUMO gap varies from 1.39 to 1.66 V with solvent polarity. The origin of the solvent dependence is explained by the electrostatic field effect and through-bond inductive effect of the sulfonate anion on the HOMO and LUMO levels. In addition, the application of MPS-Au_{25} for glucose biosensor will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.O-4**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 10:06, 좌장: 양해식

Electrochemical Study of Proton-Coupled Electron Transfer Reactions of Calcium Ion-Calix[4]arene Monoquinone Complex in Aqueous Media

김양래 정택동

서울대 화학부

Proton-coupled electron transfer reactions of water-soluble calix[4]arene-triacid-monoquinone (CTAQ) and its Ca^{2+} complex (CaCTAQ) in a buffered aqueous solution were investigated by voltammetry and spectroelectrochemistry data of quinone moiety. CaCTAQ undergoes two successive one-electron reduction steps in a buffered basic solution, sensitively varying with the stability of the semiquinone radical of CaCTAQ. Based on this behavior, the disproportionation equilibrium constant was calculated and the comproportionation reaction was demonstrated to be responsible for the semiquinone radical of CaCTAQ at neutral pH. In the presence of Ca^{2+} ions less than one-equivalent of CTAQ, homogeneous electron exchange occurs. Ca^{2+} ions can significantly modify the proton-coupled electron transfer reactions of CTAQ such as disproportionation, comproportionation, and homogeneous electron exchange, leading to unusual electrocatalytic phenomenon.

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장소: 부산BEXCO

발표코드: **ELEC.O-5**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 10:18, 좌장: 양해식

Three dimensional alloy nanodendrite structure and its analytical application

Tran Ngoc Huan 김샛별 정희일

한양대 화학과

The 3D Au-Ag nanodendrite structure was constructed on a platinum surface through the electrodeposition of Au and Ag simultaneously under the presence of hydrogen bubbles generated from the same surface. Iodide was used as a co-regent for the formation of dendrite structure. The SERS intensity of Au-Ag nanodendrite was much enhanced comparing with only Au nanodendrite. The SERS signal was increased linearly with the presence of Ag in alloy from 0 to 6%. At higher percentage of Ag, the dendrite structure was gradually disappeared, so the SERS signal was also decreased. The enhancement of SERS intensity could be explained by the presence of some pinholes in the bimetal of alloy structure, it acts as hot spots for electromagnetic field enhancement. In addition, the galvanic replacement reaction has been also demonstrated for synthesizing of Ag-Pt alloy nanodendrite structure. Cyclic voltammetry was used to investigate the electrochemical properties of Ag-Pt alloy in electrochemical performance. The result showed that Ag-Pt alloy nanodendrite presented high catalytic activity in electro-oxidation reduction as well as oxygen reduction reaction in alkaline solution.

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발표코드: **ELEC.O-6**

발표분야: Oral Presentation of Young Electrochemists

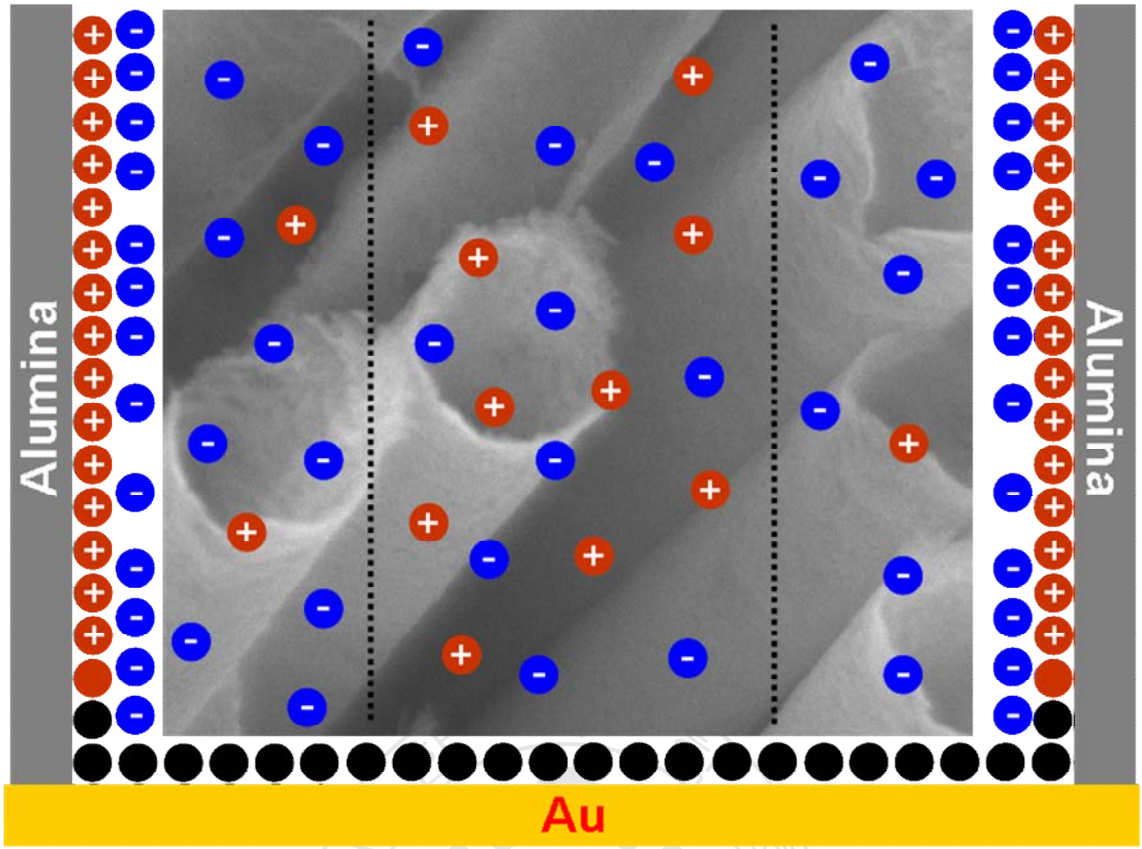
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 양해식

Direct Formation of Thin-Walled Palladium Nanotubes in Nanochannels under an Electrical Potential

LIULICHUN

성균관대 화학

An extremely simple methodology for highly efficient formation of vertical Palladium (Pd) nanotubes array is introduced. The hydroxyl-terminated surface of nanochannel in an alumina membrane is useful to form interfacial double layer by specifically adsorbing hydrogen ions (H^+) from an acidic solution and leaving counter ions predominant in the diffuse layer. Locally enriched H^+ ions produce higher content of adsorbed hydrogen on electrochemically reduced metallic Pd surface under the action of an appropriate electric potential. Higher Pd growth rate at peripheral positions than elsewhere in a nanochannel is due to the dual reductions of Pd(II) compound through hydrogen and electric potential. The disparity of growth rates in combination with diffusion-controlled growth efficiently give rise to nanotubes with a diameter as low as 6 nm. This thin-walled and vertically aligned Pd nanotube structure would be potentially significant in maximum mass usage in catalysis, sensing and energy storage.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.O-7**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 10:52, 좌장: 장병용

Molecular Ion Transport in Mesoporous Zirconia Thin Films with Three-Dimensional Pore Structures

고영선 권영욱

성균관대 화학과

We prepared mesoporous zirconia thin films (MZTFs) with highly ordered and three-dimensionally organized pore structures by employing an evaporation induced self-assembly method. The 3D pore structures allow the films to serve as nanofluidic systems for molecular ion transport through mesopores. The transport experiments were conducted and investigated through cyclic voltammetry with $Fe(CN)_6^{3-}$/$Fe(CN)_6^{4-}$ redox probe ions. The molecular ion transport in the confined pores was affected by not only the surface charge of the film but also specific adsorption of redox ions. Unlike the typical behavior on electrochemical analyses of specific adsorption, our result showed a different tendency for the ratio of voltammetric peak currents. It will be discussed on this talk in terms of the structural difference in systems and the difference in charge strengths of the oxidized and reduced species. This discussion demonstrates that the molecular ion transport in the MZTFs exhibits discriminative properties compared with a nonporous electrode surface, which is expected to provide useful information in understanding or designing sensors based on nanofluidic systems.

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발표코드: **ELEC.O-8**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 11:04, 좌장: 장병용

Impacts of Oxygen Content and Interfacial Reactions on Cycling Performance of SiOx Anodes in Rechargeable Lithium Batteries

Nguyen Cao Cuong 송승완

충남대 정밀응용화학과

Silicon (Si)-based anode materials have been received particular attention for use as anode for next generation of rechargeable lithium batteries because of superior high theoretical capacity of Si (3579 mAhg-1 for Li15Si4) at room temperature compared with 372 mAhg?1 of graphite that is currently used in commercial batteries. Rapid capacity fade due to severe volume change during alloying/dealloying however obstructs their use in commercial batteries. Silicon monoxide (SiO) and sub-oxide (SiOx) anodes have been intensively investigated since they provide improved cyclability despite reduced specific capacity. The reaction of SiOx with lithium ion is known to form Li2O and lithium silicates, which behaves as the buffer for volume change. However, the interfacial reaction of SiOx anodes with electrolyte and the SEI layer formation, and its impact on cycling performance have not been studied throughout. We report here the impacts of oxygen content and interfacial reaction on cycling performance of SiOx (x = 0.4 -1.3) anodes in the commercial electrolyte, through thin film studies of SiOx electrodes prepared by pulsed laser deposition (PLD).

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장소: 부산BEXCO

발표코드: **ELEC.O-9**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 11:16, 좌장: 장병용

Li storage performance of ordered mesoporous carbon as an anode material in Li ion battery

김민식 박진솔[1] 양대수 최혁수[1] Chaudhari Sudeshna A[2] 유종성

고려대 신소재화학과 [1]고려대 소재화학과 [2]고려대 세종캠퍼스 소재화학과

Rod-shaped ordered mesoporous carbons (OMCs) with different channel lengths, prepared by replication method using the corresponding size-tunable SBA-15 silicas with rodlike morphology as templates, are explored as anode material for Li-ion battery. All the as-synthesized OMCs have exhibited much higher Li storage capacity and better cyclability along with comparable rate capability as compared with commercial graphite. Particularly, the OMC with the shortest length has demonstrated the highest reversible discharge capacity of 1012 mAh.g-1 at 100 mA.g-1 and better cyclability with 86.6 % retention of initial capacity. Although the coulombic efficiencies of all the OMCs are relatively low at the beginning, they improve promptly and after 10 cycles reach the level comparable to natural graphite. Based on their specific capacity, coulombic efficiency and rate capability, the OMC-3 outperforms considerably its carbon peers with longer length. This behavior is mainly attributed to the higher specific surface area, which provides more active sites for Li adsorption and storage, and the larger mesopore volume with the larger mesopore size, facilitating fast Li species diffusion and electrolyte transport.

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장소: 부산BEXCO

발표코드: **ELEC.O-10**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 11:28, 좌장: 장병용

Novel functionalized graphene sheets as metal-free cathode electrocatalysts for enhanced oxygen reduction

Mohammad Shamsuddin 전승원

전남대 화학과

Tridodecylmethylammonium chloride (TDMAC) functionalized reduced graphene oxide (TDMAC-RGO) has synthesized by a simple physicochemical process. The resultant functionalized graphene imparts electrocatalytic activity as metal- free catalysts for the oxygen reduction reaction (ORR) in fuel cells (FCs), with long-term operational stability, and tolerance to methanol and ethanol via a four-electron pathway in alkaline FCs. The ORR activities have systematically investigated by cyclic voltammetry (CV) and rotating ring disk electrode (RRDE) techniques. The results show that the TDMAC-RGO demonstrates excellent catalytic activity for oxygen reduction. Raman and X-ray photoelectron spectroscopic (XPS) measurements indicate charge transfer from the graphene sheets to the TDMAC via intermolecular charge-transfer. TDMAC-RGO catalysts are low-cost, free of metal and costly polymers, and are an efficient approach to FC applications.

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장소: 부산BEXCO

발표코드: **ELEC.O-11**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 11:40, 좌장: 장병용

Ag/Ag_2O 전극시스템을 이용한 전기삼투펌프의 안정성 및 성능 향상

Enhua Zhu 신운섭[1]

서강대 바이오융합기술 [1]서강대 화학과

본 연구진은 백금 전극 대신 Ag/Ag_2O 전극시스템을 이용하여 가스 발생이 없이 낮은 전압에서도 구동이 가능한 전기삼투펌프를 구현한 바 있다.[1] 이 펌프에서는 anode 에서의 Ag 의 Ag_2O 로의 산화반응에 따른 H^+의 생성과 cathode 에서의 Ag_2O 의 Ag 로의 환원에 따른 H^+ 소모를 근간으로 일정 전압 하에서 유체가 안정적으로 이동한다. 이 과정 중 부반응으로 생기는 Ag^+ 이온은 멤브레인에 침전되기도 하고 cathode 쪽까지 이동하여 Ag 로 환원되기도 하는데 이는 펌프의 성능과 안정성을 떨어뜨릴 수 있다. 본 연구에서 Ag/Ag_2O 전극을 Nafion 으로 코팅함으로 Ag^+의 용액으로의 유출속도를 떨어뜨려 훨씬 안정한 펌프를 구현하였다.[2] 2 mm 두께, 8 mm 지름의 펌프는 1.0 V 에서 20 μL/min 의 안정한 유속을 보이며 유속은 가한 전압에 비례하여 커지는데 0~2.0 V 의 전압을 가했을 때 0~40 μL/min 의 유속의 규현이 가능했다. 2.3 C 의 전하량을 가진 Ag/Ag_2O 전극으로 총 3~4 mL 의 유체 전달이 가능했다. Pulsed operation 으로 0.1 μL/min 의 속도로 미량 주입도 가능하였다. 이 펌프를 이용하여 약물주입기 prototype 을 구성하였다.[3]

References

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3. W. Shin, S.J. Shin, J.M. Lee, R.K. Nagarale, A. Heller, Drug Delivery Transl. Res. 2011

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장소: 부산BEXCO

발표코드: **ELEC.O-12**

발표분야: Oral Presentation of Young Electrochemists

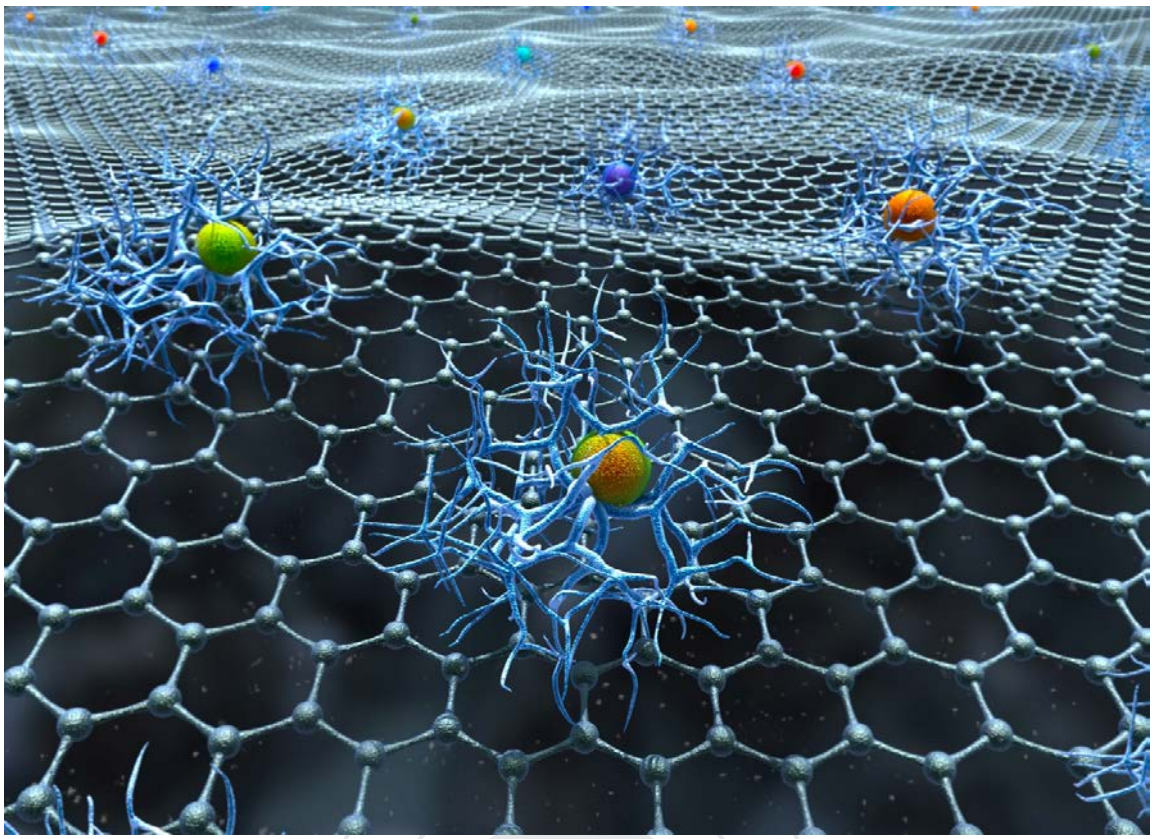
발표종류: 구두발표, 발표일시: 목 11:52, 좌장: 장병용

Synthesis of Dendrimer-Encapsulated Nanoparticle/Chemically Converted Graphene Nanocomposites and Their Electrochemical Applications

김준명 김주훈

경희대 화학과

In this study, we described a method for preparing nanoparticle-decorated chemically converted graphene (CCG) nanocomposites, on which size-monodisperse nanoparticles (with dia. of less than 2 nm) were uniformly distributed with preservation of their original size, via covalent immobilization of dendrimer-encapsulated nanoparticles (DENs). The resulting DEN/CCG nanocomposites were characterized by transmission electron microscopy (TEM), UV-vis spectroscopy, atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and electrochemical measurements. This approach allowed universal assembly of multiple nanoparticles with different sizes and compositions on a single CCG surface with good control over particles sizes in the range of 1 to 2 nm. We also explored the possibility to use the DEN-decorated CCG nanocomposites as electrocatalysts for electrochemical reduction of O_2.



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발표코드: **ELEC.O-13**

발표분야: Oral Presentation of Young Electrochemists

발표종류: 구두발표, 발표일시: 목 12:04, 좌장: 장병용

Improved oxygen reduction of carbon nanomaterials by covalently anchoring with CoTAPP via diazonium salt reactions

김슬기 전승원

전남대 화학과

In the presentwork,we used diazonium salt reactions to improve the production of covalent bonding between cobalt[tetrakis(*o*-aminophenyl)porphyrin] (CoTAPP), having an o-aminophenyl and sp^2 carbon, and three different carbon nanomaterials (CNMs; graphene, single-walled carbon nanotubes (SWCNT), and multi-walled carbon nanotubes (MWCNT)) in order to increase the effectiveness of cobalt porphyrin electrocatalysts. The surface morphologies of anchored CoTAPP on CNMs were evaluated using Field emission scanning electron microscopic (FE-SEM), Atomic force microscope (AFM), and Raman microscope. Also, we examined electrocatalytic activities using electrochemical impedance spectroscopy (EIS). The electrocatalytic activity of the anchored CoTAPP on CNMs for oxygen reduction reactions (ORR) have been investigated by rotating ring-disk electrode (RRDE) techniques in 0.5 M H_2SO_4 aqueous solution. The electrocatalytic reduction of O_2 on glassy carbon electrodes (GCEs) modified with these CoTAPP anchored CNMs established a pathway of four-electron transfer reductions to H_2O. Among the CoTAPP anchored CNMs, anchored graphene with CoTAPP showed the best electrocatalytic effect and the most efficient electrocatalytic performance for oxygen reduction reaction (ORR) without any precious metals.

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발표코드: **EDEC.O-1**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 목 14:30, 좌장: 유미현

'우리 주위의 화합물' 학습과정에 따른 중학생들의 개념 생태 지위 변화 분석

김경미 최병순[1] 박국태[1]

장산중학교 [1]한국교원대 화학교육과

이 연구에서는 '우리 주위의 화합물' 단원의 학습과정에 따라 8 학년 학생들이 인식하는 개념 간의 관계 이해를 생태 지위적 접근을 통하여 개념의 다양성, 개념의 관련성 및 빈도율의 변화, 개념 간 근접성 요소에서 분석하였다. 이를 위하여 8 학년 학생 200 명을 대상으로 우리 주위의 화합물을 주요 개념별로 순물질, 혼합물, 이온결합, 공유결합, 화합물 영역으로 나누어 수업 전, 이온결합 수업 후, 공유결합 수업 후, 화합물 수업 후의 학습과정에 따라 개념의 관련성 및 빈도율을 조사하여 분석하였다. 연구 결과, 학습과정은 학습자의 선개념 및 현재 학습에 영향을 끼치며, 이온결합 및 공유결합 수업 후에는 그 영향이 더욱 뚜렷이 나타났다. 학습과정에 따라 학생들이 많이 인식하는 개념과 관련성이 높다고 생각하는 개념은 달랐으며, 공통적으로 학생들은 과학적 개념을 중요하다고 생각하지만 생활 속에서 쉽게 접할 수 있는 친숙한 사례들을 가장 많이 인식하고 있었다. 오개념은 학습과정에 따라 과학적 개념과 함께 학습자의 개념 생태내에서 서로 공존하면서 생태 지위를 차지하였다. 이러한 연구 결과로부터 학습과정 동안 학생들의 인지구조 속에 과학적 개념들과 경쟁하는 개념들의 종류와 그들의 생태 지위를 알 수 있었으며, 과학적 개념들의 생태 지위를 높여주고 강화할 학습 과정의 시점을 알 수 있었다. 이는 개념 간 근접성 인지도를 통하여 학생들이 유사성 높게 인식하는 개념들을 알고, 핵심이 되는 과학적 개념들을 중심으로 개념들이 근접할 수 있도록 지도함으로써 학생들의 개념 학습에 도움을 줄 수 있음을 시사한다.

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발표코드: **EDEC.O-2**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 목 14:55, 좌장: 유미현

한국과학영재학교 유기화학 수업모형: 팀별 문제 해결 중심의 발표 수업모형

오진호 천만석[1] 임길선

한국과학영재학교 화학생물학부 [1]한국과학영재학교 화학

KAIST 부설 한국과학영재학교는 학생의 관심과 재능에 맞춘 개인형 맞춤식 심화 및 속진 중심의 수학/과학 교육과정, 3 년에 걸친 체계적인 연구활동, 단체 및 봉사활동과, 국외위탁교육 프로그램을 중심으로 한 다양한 국제교류 프로그램을 제공하여 영재학교 학생들을 미래 글로벌 과학 리더로 교육시켜오고 있는 2003 년 개교한 최초 한국과학영재학교이다.화학교과에서는 화학분야에 관심과 재능이 있는 학생들이 필수교과목으로 “ 화학 및 실험 I, II ”, 선택교과목으로 대학에서 학점을 인정을 받을 수 있는 AP 교과목인 “ 일반화학 I ”, “ 일반화학 II ”, “ 일반화학실험 I ”, “ 일반화학실험 II ”과 대학수준의 심화교과목인 “ 유기화학 ”, “ 양자와분광학 ”, “ 분석화학 ”, “ 물리화학 ”, “화학결합론 ”, 과 “ 화학특강 ” 교과목을 선택하여 공부해 오고 있다.본 연구에서 2012 학년도 1 학기 “ 유기화학 ” 교과목에서 시행한 “ 팀별 문제 해결을 바탕으로 한 발표 중심의 수업” 을 한국과학영재학교의 유기화학 수업모형으로 발표한다.유기화학 수업에서 학생들은 스스로 팀을 구성하여 함께 문제를 해결하고, 학생들이 발표 수업을 통해 함께 문제에 대해 토론을 했다. 이 수업의 장점은 학생들이 모두 적극적으로 수업에 참여하여 발표 수업을 통해 함께 토론하면서 학업성취도를 높이는 효과를 보였다. 또한 학생들은 팀별 프로젝트 활동으로 학생들은 유기합성에 대한 연구계획서를 제출하여 자신이 목표한 물질을 합성하여 1H NMR, IR 스펙트럼을 통해 분석하여 그 연구결과를 발표하였다. 또한 학생들은 자신의 연구분야와 관련된 유기화학 내용을 정리하여 보고서로 제출함으로서 유기화학적인 지식을 배우도록 하였다.Key Words: 한국과학영재학교 유기화학 수업 모형, 팀별 문제 해결 중심의 발표 수업, 유기화학 프로젝트 활동

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탈북청소년을 위한 교육지원으로서 중학교 과학 표준(보충)교재의 개발 사례- '분자운동과 상태변화' 단원을 중심으로 -

윤희숙

강원대 과학교육학부

1990 년 중반 이후 북한의 어려운 경제상황과 체제에 대한 반발로 인해 탈북주민의 수가 급증하고 있으며, 2000 년대에 들어서면서는 가족단위의 입국이 많아지고 있다(통일백서, 2010). 이로 인해 탈북청소년(초중고 학생)의 수도 증가하고 있으며, 2012 년 4 월 현재 2200 여명의 청소년이 정규학교나 대안시설에서 교육을 받고 있는 것으로 보고되고 있다(강구섭, 2012). 그러나 이들 탈북청소년들은 대부분 북한의 경제난과 탈북과정에서 필연적으로 발생되는 상당 기간의 교육 공백기를 가지고 있을 뿐 아니라, 남북한의 교육과정과 교수-학습 방법의 차이, 학습능력과 동기 부진, 가정환경의 어려움 등으로 인하여 낮은 학업성취를 보이고 있다(최정호, 2011). 이러한 낮은 학업성취는 학교 부적응의 주된 원인 중 하나로 작용한다. 따라서 이들의 성공적인 학교적응과 학습 성취를 위한 교육지원이 절실한 상황이다. 한국교육개발원 탈북청소년교육지원센터에서는 탈북청소년의 학교 적응 및 교육지원의 일환으로, 2009 개정 교육과정에 맞추어 탈북청소년의 학습을 돕기 위한 표준(보충)교재의 개발 과제를 수행하고 있다. 본 연구는 이를 위한 작업으로, 중학교 과학 중 화학분야인 '분자 운동과 상태 변화' 단원의 효과적인 학습을 위한 표준(보충)교재를 개발하는 것을 목적으로 하였다. 이를 위해 첫째, 관련 선행연구를 참고하여 남북한 관련 교육과정을 분석하고, 남북한 용어를 비교하였다. 둘째, 탈북청소년의 정의적인 특성 및 북한의 교수학습 방식을 고려하여 교재의 틀을 마련하였다. 셋째, 학습내용에 적절한 교수학습 자료를 수집하고, 교재를 집필하였다. 북한 주민의 입국자 규모는 계속해서 증가하고 있다. 따라서 탈북 청소년을 위한 교육지원으로서 보충교재의

개발은 현재의 문제를 해결하기 위한 과제인 동시에 미래의 통일을 준비한다는 점에서 의의가 있을 것이다.

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고등학교 융합형 과학의 운영 실태와 융합형 과학을 수업한 교사들의 인식 조사

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이 연구의 목적은 2009 개정 교육과정에 따라 고등학교에 도입된 소위 융합형 과학의 운영 실태와 융합형 과학을 수업한 교사들의 인식을 알아보는 것이었다. 이를 위해 2011 학년도에 융합형 과학을 1 년간 수업한 전국 16 개 시도 인문계 및 실업계 과학교사 157 명(인문계 42 개교 127 명, 실업계 13 개교 30 명)을 대상으로 설문 조사를 실시하였다. 융합형 과학 운영 실태를 보면, 40%의 학교에서 융합형 과학을 5 명이상의 교사가 나누어 지도하였으며, 운영방식은 40%의 학교에서 1 명의 교사가 모든 단원을 수업하고, 49.1%의 학교에서는 전공별로 여러 교사가 나누어 수업하는 것으로 나타났다. 융합형 과학을 선택한 이유로 35%의 교사는 이전 교육과정과 같이 필수인줄 알았다고 응답하였으며, 7.6%가 과학 중점학교 등의 이유로 선택할 수 밖에 없었다고 응답하였다. 그러나 29.9%의 교사는 학생들의 과학적 소양 함양을 위해 선택하였다고 응답하여 교육의 목적에 맞춰 교과목을 선택하였음을 알 수 있다. 조사대상 중 96.4%의 학교에서 내년에도 과학을 선택하겠다고 응답하였고 주로 1 학년에서 선택하겠다(94.6%)고 하였다. 선택을 안하겠다고 응답한 학교는 첨단 과학 내용이 어렵거나 다른 교과목과의 시수 조정 등의 학교 사정을 이유로 들었다. 융합형 과학에 대한 인식을 조사한 결과, 융합형 과학이 기존의 과학과 가장 큰 차이점으로 59.2%의 교사는 주제 중심의 통합적 내용 구성을, 37.6%의 교사는 첨단 과학 내용의 포함을 선택하였다. 융합형 과학의 내용에 대한 인식을 분석한 결과, 융합형 과학은 학생들의 과학적 소양 함양을 위해 필요한 과목(36.9%)이며, 과학개념을 통합적으로 잘 구성(40.8%)하였고, 개념을 제시하는 과정에서 과학-기술-사회의 연관성이 잘 나타났다(42.6%)고 응답하였다. 또한, 융합형 과학 교과서가 교육과정 내용을 잘

반영하였다는 인식이 전반적으로 높게 나타났다. 그러나 41.4%의 교사가 첨단과학 내용을 설명하기 위해 도입된 용어나 개념의 수준이 높다고 응답하였는데, 이는 융합형 과학이 현장에 자리 잡기 위해 교육내용의 보완이 요구된다는 것을 시사한다. 융합형 과학을 지도할 때, 60.6%의 교사들은 과학적 소양 함양을 가장 중요하게 생각하고 있었으나 실제 평가에서 중점을 두는 것은 기본 개념과 개념들 간의 유기적이고 통합적인 이해인 것으로 나타났다. 이는 평가에 대한 교사들의 보다 명확한 인식과 함께 과학적 소양을 평가하는 방법에 대한 다양한 정보가 제공되어야 함을 시사한다고 말할 수 있다.

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주사기와 압력계를 이용한 물의 증기압 측정방법 연구 : 상온에서 80 ℃ 범위에 적용 A Method Measuring Vapor Pressure of Water Usiing Syringe and Pressur Guage from Room Temperature to 80 ℃

우현승 정대홍

서울대 화학교육과

고등학교 화학 II 에 처음 도입되는 액체의 증기압은 후기 형식적 조작기의 인지 수준에 해당하는 개념으로 대부분 구체적 조작기나 과도기 수준에 있는 고등학교 2 학년 자연계열 학생들에게 어려운 개념으로 인식되고 있다. 그러나, 이것은 '끓는점 오름', '어는점 내림', '삼투압' 등 '용액의 총괄성'을 이해하기 위한 선행 개념이기 때문에 정확한 이해가 필요하다. 안타깝게도 교사들은 학생들에게 증기압 개념을 정확하게 이해시키는데 어려움을 느끼고 있으며 그것은 대학수학능력시험에서 증기압을 포함한 용액의 총괄성 관련 단원 문항의 정답률이 가장 저조한 것으로도 반증된다. 이런 측면에서 볼 때 과학 교과의 장점인 실험활동을 통해 구체적 경험을 제공하여 개념 수준과 학생들의 인지 수준의 간극을 줄일 필요가 있다. 그러나 제 7 차 교육과정에 의한 고교 교육과정 중 이 영역에 해당하는 교과 내용을 분석해 보면 실험 재료의 위험성과 실험 적용의 한계 등을 이유로 대부분 자료해석이나 추리, 예상 등의 형태로만 제시되고 있을 뿐 실질적인 실험활동이 이루어지지 않는 것으로 나타났다. 이러한 한계를 극복하기 위해 본 연구에서는 학생들이 학교에서 안전하고 간단하게 물의 증기압을 측정할 수 있는 도구를 개발하고 이를 이용하여 상온에서 80℃까지의 온도 구간에서 물의 증기압을 측정하는 방법을 제안한다. 주사기와 범용 압력계만을 사용하여 기구를 휴대하기 편하고 단순하게 설계하고 현장에서 쉽게 접근할 수 있도록 측정방법을 현실화하는 것이 연구의 목적이다. 본 학회에서 장치의 신뢰도를

검증하고 보정하기 위해 시도했던 일련의 연구 과정과 정확도 높은 측정 결과를 보고하고, 이를 이용한 확장된 개념 탐구 모델을 소개하고자 한다.

대 한 화 학 회
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화학 교육의 영역 - 세계적 동향

도춘호

(전) 순천대

우리나라에서 화학 교육자와 화학자 그리고 시민들이 일반적으로 논의하는 화학 교육의 영역은 주로 교육적인 부분에 한정되는 것 같다. 화학 교육과 관련한 국제적 학술대회의 주제들과 발표 내용을 살펴보면 그 범위가 다양하고 우리나라에서 다루는 영역은 좁다는 것을 알게 된다. 국제적 학술발표회의 주제들을 살펴보고, 우리나라에서 적용하거나 우리나라의 화학 교육의 영역을 넓히는 방법을 논의하고자 한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

New Materials from Agricultural Products and Byproducts

LinShu Liu

Eastern Regional Research Center, Agricultural Research Service, U.S. Department of Agriculture

The use of edible agricultural products and byproducts to construct DDS for the oral controlled release of therapeutics has been successfully applied for clinical treatment of several diseases. A typical example is the encapsulation and the consequent delivery of P40, a probiotic bacterial-derived water soluble protein, to the colon site. The DDS from the complex of a polysaccharide and a protein used in this study was able to maintain the therapeutic activity of P40 that activated EGFR in colon epithelial cells, reduced intestinal epithelial apoptosis and disruption of barrier function in the colon epithelium, thereby preventing and treating DSS-induced intestinal injury and acute colitis. Three-dimensional scaffolds were prepared from selected groups of polysaccharides and proteins. In combination with an appropriate growth factor, the scaffolds can stimulate various skeletal tissue regenerations, depending on the composition, ratio of the components, and the tissue sites. The microenvironment created by matrix and growth factor guider cell differentiation and eventually, tissue regeneration.

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Structural Dynamics of Self-Assembling β-Sheet Peptide Nanostructures Decorated with Multivalent RNA-binding Peptides

한상헌 임용범[1]

*연세대 신소재공학과 [1]*연세대 신소재공학과*

Self-assembled peptide nanostructures (SPNs) hold great potential as promising biomaterials. Researches are in progress to devise SPNs that can mimic the diverse functions of natural proteins. β-sheet-mediated SPN formation has been the focus of extensive research both by the possibility to fabricate biomaterials and by the relation to amyloidogenic disease. In an “amyloidogenic disease perspective”, understanding the mechanism of protein aggregation is fundamental in devising therapeutics for this intractable disease. Understanding dynamic properties of system is important since the function of many important biomolecules comes from their dynamic properties. Electron paramagnetic resonance (EPR) spectroscopy is a useful technique for studying dynamic behavior of system. EPR has been used to probe structural dynamics of macromolecule and nanostructures. Site-directed spin labeling (SDSL) is used to monitor the behavior of a stable nitroxide radical. In this study, we combined SDSL with EPR spectroscopy to investigate structural and conformational dynamics of bioactive β-sheet SPN system. We synthesized block co-peptides spin labeled with 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) group at C-terminus or N-terminus. The block co-peptide consists of a bioactive segment and a self-assembling β-sheet segment. The bioactive segment is an RNA-binding peptide sequence derived from HIV-1 protein, which is known to form α-helical conformation upon RNA binding. The block co-peptide system was investigated by TEM, CD, IR, DLS, Zeta-potential and EPR. Information of structural and conformational dynamics of the system was obtained and this study gives important insight into the dynamics of the assembly system of β-sheet block co-peptide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-3**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polynorbornene Copolymers with Triarylamine and Styrene Side Groups: Synthesis and Crosslinking Behavior

이민형 박성훈

울산대 화학과

Vinyl addition copolymerization of norbornene monomers functionalized with N,N'-bis(naphthalene-1-yl)-N,N'-bis(phenyl)-benzidine (NB-NPB) and styrene (NB-SM) side groups has been investigated to produce polynorbornene copolymers with pendant NPB and SM groups by use of Pd(II) catalyst. The catalytic system efficiently produced soluble copolymers with high molecular weight. The copolymers contain free SM groups whose amount is in proportion to the NB-SM feed amount. When exposed to thermal annealing of the polymer film, almost complete crosslinking of polymer chains was observed, affording an insoluble film. Details of synthesis, characterization, and thermal crosslinking behavior of the copolymers will be presented.

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발표코드: **POLY.P-4**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoimprinting with photopolymerization using epoxy prepolymer synthesized by sol-gel reaction

이지원 신재섭

충북대 화학과

Nanoimprint lithography gets much attention as an alternative method which can be substituted for the optical lithography. A lot of kinds of polymeric materials and manufacturing methods were used to improve the nanoimprinting technique. In this study the prepolymers were synthesized by sol-gel reaction with methyltrimethoxysilane (MTMS), 3-glycidoxypropyl trimethoxysilane (GPTMS), phenyltrimethoxysilane (PTMS), and (3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octyl)trimethoxysilane (TFTMS). The nanoimprinting with the prepolymers was conducted with sulfonium salt as a photoinitiator, and the cationaic polymerization proceeded with UV light during the nanoimprint process to form the crosslinked epoxy polymer. The optimum formulation of epoxy resin was found to get the high aspect ratio structure by nanoimprint and the producing ability for the large area imprinting respectively. The content ratio of PTMS was significant to get the high aspect ratio structure. And the content ratio of MTMS was significant to conduct the large area imprinting. The content ratio of TFTMS was significant to conduct the demolding process but the increasing of the content ratio of TFTMS caused decreasing the physical property of the nanoimprint.

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장소: 부산BEXCO

발표코드: **POLY.P-5**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Homogeneous surface coating method by a mussel-inspired approach

송인택 이해신

KAIST 화학과

표면개질 (Surface modification) 은 물질표면에 기존과는 다른 성질을 부여하는 과정을 말한다. 한 물질 안에서 다양한 function 을 가지게 되는 hybrid 물질, multi-function 물질의 중요성이 대두되고 있는 요즘 표면개질 분야는 점점 중요시되고 있다. 이런 표면개질 분야에서 최근 polydopamine 을 사용한 표면개질 chemisty 가 각광 받고 있는데, 홍합 접착 물질로부터 모방되어 다양한 표면 코팅 (universal surface coating) 이 가능한 방법이다. 하지만 polydopamine coating 방법은 micro particle 을 이루며 coating 이 되기 때문에 표면의 morphology 를 그대로 유지시키기는 어렵다는 단점이 있다. 그래서 micro-, nanosize particle 을 개질 시키거나, 표면의 morphology 를 유지시키려면 더 even 한 코팅 방법이 필요하다. 본 연구에서는 그 단점을 극복하기 위에 sPEI-cat(polyethylene imine ? catechol (MW : 2000)) 을 사용하여 even 한 coating 방법을 개발하였고 다양한 표면 및 nanoparticle 에도 적용 가능함을 보였다. 더 나아가 표면위에서의 primary amine 기를 통한 application 이 가능함도 확인하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-6**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Functionalized Polyisocyanate Block copolymers via Thiol-ene Click Chemistry

채창근 이재석[1]

광주과학기술원 나노바이오재료전자공학과 [1]광주과학기술원 신소재공학과, PIMS

Synthesis of functionalized polyisocyanate block copolymers was approached through thiol-ene click chemistry as a post-polymerization modification. First, the polyisocyanate, which include the alkene group in the side-chain was prepared by anionic polymerization of allyl isocyanate (AIC) using sodium benzanilide (Na-BA) as an initiator and acetyl chloride as a terminator in tetrahydrofuran (THF) at -98 ℃ under high vacuum (10-6 Torr). The polymerization resulted in PAIC with predictable molecular weight and narrow molecular weight distribution. Furthermore, most of the allyl groups remained unreacted in a resulting polymer. Synthesis of PAIC block copolymer including poly(n-hexyl isocyanate) (PHIC) block was also carried out. Resulting PAIC-b-PHIC was used for thiol-ene click reaction with 2-mercaptoethanol and 2,2'-azobis(4-methoxy-2.4-dimethyl valeronitrile) (V-70) radical initiator. Functionality of the block copolymer was confirmed by NMR, SEC-MALLS and FT-IR analysis.

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장소: 부산BEXCO

발표코드: **POLY.P-7**

발표분야: 고분자화학

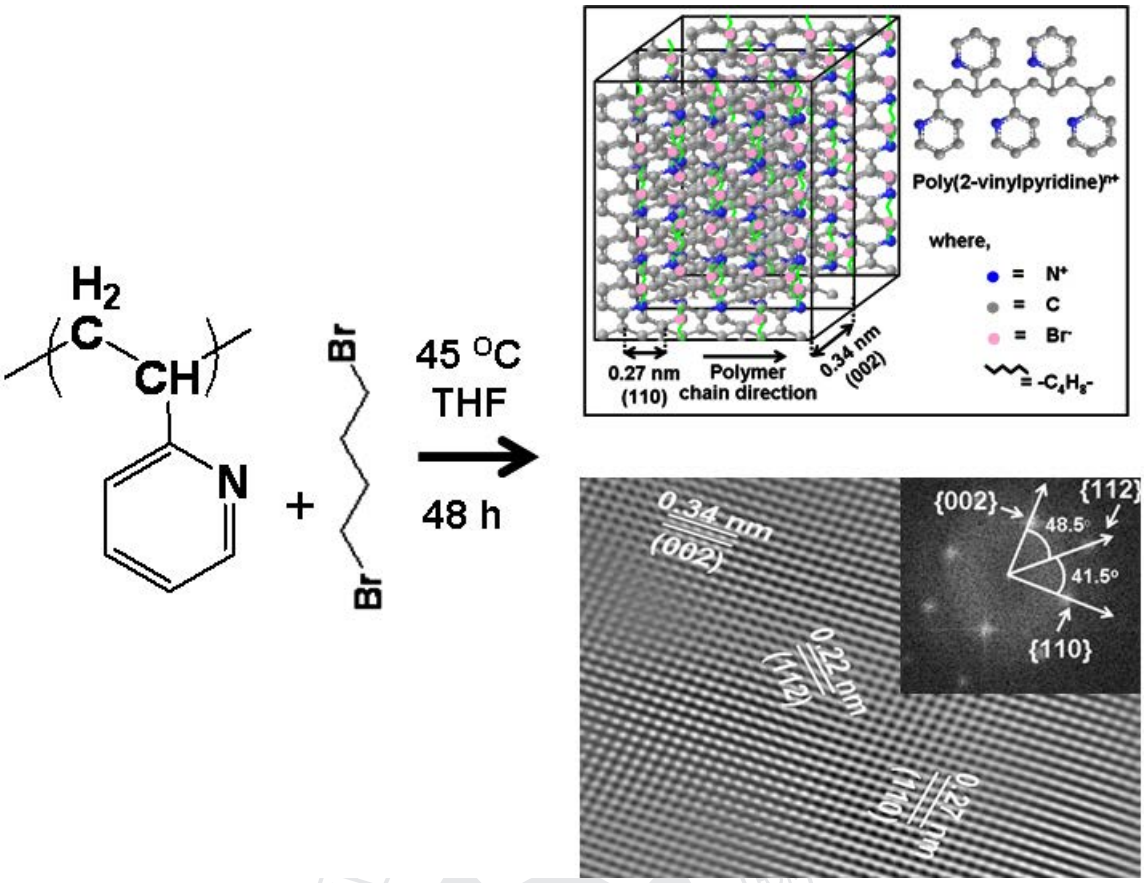
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile, Controlled Molecular Level Ordering of Poly(2-vinylpyridine) via Chemical cross-linking

채창근 이재석[1]

광주과학기술원 나노바이오재료전자공학과 [1]광주과학기술원 신소재공학과, PIMS

3-D molecular-level ordering is an important and challenging objective of current research in materials chemistry and physics. It can improve the efficiency of systems or generate entirely new types of systems containing functionalities that were previously unattainable. Self-assembly is emerging as an elegant and powerful approach to fabricating nano-structured materials. However, controlling the precise arrangement of molecules on the molecular scale is most demanding due to the difficulty in making such small structures. Molecular-level self recognition and organization during the chemical reaction of poly(2-vinylpyridine) (P2VP) with 1,4-dibromobutane influence the tacticity of P2VP, leading to the sub-nanometer level molecular ordering of pyridine moieties in the polymer chain. This long range hexagonal organization switches P2VP from an amorphous to a 3-D metallic polymer.



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-8**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Antimicrobial Activity by Multi-functionalized Graphene Oxide by Catechol Quaternized Poly (Ethylene Glycol) and Silver Nanoparticles

남정아 박성영

한국교통대 화공생물공학과

This paper stays to represent the development of water soluble reduced graphene oxide (rGO) showing antimicrobial activity following simultaneous reduction and functionalization of graphene oxide with grafted bio-inspired adhesive catechol and hydrophobic alkyl group (C12) to PEG. Catechol moiety 2-chloro-3',4'-dihydroxyacetophenone (CCDP) and C12 quaternized poly(ethylene glycol)-g-poly(dimethylaminoethyl methacrylate) [PEG-g-PDMA] has been constructed in such a way as it can act as a reducing agent for the reduction of graphene oxide and antimicrobial functionality. Also the catechol segment of polymer is proved to provide additional functionality of rGO as a reducing agent participating in reduction of AgNO3 allowing spontaneous Ag nanoparticles (Ag NPs) formation which further boosts the antimicrobial properties.

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장소: 부산BEXCO

발표코드: **POLY.P-9**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Spiropyran-conjugated Pluronic as Dual Responsive Colorimetric Detector

이강석 박성영

한국교통대 화공생물공학과

Novel spiropyran-conjugated Pluronic [polyethylene oxide (PEO)-b-polypropylene oxide (PPO)-b-polyethylene oxide (PEO)] micelles are developed as new colorimetric detector showing photo- or thermo-switchable behavior. Facile conjugation of spiropyran to Pluronic was confirmed by 1H NMR, UV-Visible and Fluorescence spectroscopy. A switchable photoluminescence is found depending on the irradiation with either UV or visible light, and temperature resulting from structural isomerization of spiropyran between spiropyran (SP) and merocyanine (MC) form. Cytotoxicity of the spiropyran-conjugated Pluronic (SP-PL) was evaluated following MTT assay while photo responsiveness of spiropyran within the micelles was determined by confocal laser scanning microscopy.

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장소: 부산BEXCO

발표코드: **POLY.P-10**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Beacon Aptamer-based ATP Detection

정지은 우한영[1]

부산대 대학원 인지메카트로닉스 공학과 [1]부산대 나노기술대학 나노정보소재공학과

Molecular beacon (MB) is a probe oligonucleotide, which is a hairpin shaped molecule labeled with a fluorophore and quencher at both termini. After the ATP (Adenosine 5'-triphosphate) aptamer sequence is introduced as the molecular recognition element, with cationic conjugated polyelectrolytes (CPEs), molecular beacon aptamer (MBA) undergoes a conformational change to either an open chain form (turn-on state; CPE-induced FRET signal) or a G-quadruplex (turn-off state; quenching) in the absence or presence of ATP. Thus, with clear turn-on/-off signal, highly sensitive and selective ATP detection is possible. Here we report the CPEs-based ATP detection with modification in the stem stability in MBA. Depending on binding strength in the MBA stem part, the equilibrium between the open-chain and hairpin structures of MBA can be adjusted, resulting in fine-tuning of sensor properties.

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장소: 부산BEXCO

발표코드: **POLY.P-11**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of thieno[3,4-c]pyrrole-4,6-dione based copolymers and their application for polymer solar cell

염승집 우한영

부산대 나노융합기술학과

Three alternating D-A type copolymers were synthesized through Suzuki polycondensation of the thieno[3,4-c]pyrrole-4,6-dione (TPD) acceptor unit with different thiophene derivatives (thiophene (P1), thieno[3,2-b]thiophene (P2), to bithiophene (P3)). A carbazole unit was introduced to ensure the solubility of copolymers. Different types of thiophene spacers influence not only optical, electrochemical properties but also morphological, photovoltaic properties. Absorption was red-shifted and HOMO energy level was up-shifted in the order of P1, P2 and P3. Fabricated polymer solar cell (PSC) with [6,6]-phenyl-C_{71}-butyric acid methyl ester ($PC_{71}BM$) as an acceptor, showed power conversion efficiency (PCE) up to ~3%. Their structure-property relationship will be discussed in detail.

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장소: 부산BEXCO

발표코드: **POLY.P-12**

발표분야: 고분자화학

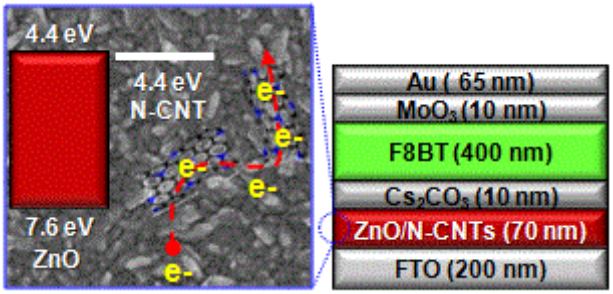
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Charge Transport in Polymer Light-Emitting Diodes Using ZnO/N-Doped Carbon Nanotube Nanocomposites

박지선 김상욱[1]

전자부품연구원 에너지나노소재연구센터 [1]KAIST 신소재공학과

We present the remarkable electro-conductivity enhancement of solution processable ZnO charge transport layers upon dispersing a tiny amount of chemically doped CNTs and the corresponding device performance improvement of light-emitting diodes. Among various undoped or doped CNTs, whose work function was systematically tuned by substitutional doping of electron deficient B or electron rich N, N-doped CNT showed a lowered work function well-matching with the conduction band of ZnO. Consequently, ZnO/N-CNT nanocomposites transport layer with 0.08 wt% N-CNT showed a five-fold enhancement of electron mobility, while maintaining the intrinsic bandgap energy levels, optical transparency and solution processability of pure ZnO. The inverted OLEDs employing ZnO/N-CNT nanocomposites electron transport layer could facilitate well-balanced electron/hole injection and, thus, more than two-fold enhancement of maximum luminance and efficiency.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-13**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of surface structures of blending homopolymer and diblock copolymer films by AFM

강민화 이지혜[1] 이연희[1]

과학기술연합대학원대 나노및바이오표면과학 [1]KIST 특성분석센터

Atomic Force Microscopy(AFM) is one of the useful instruments to measure nano structures of material surfaces. Surface pattern formation in blending homopolymer and diblock copolymer films was investigated as a function of film thickness and annealing time. In this study, surface structures of blending homopolymer[deuterated polystyrene(Mn 20,000), poly(methyl methacrylate)(Mn 18,000)] and diblock copolymer[Poly(deuterated styrene(d8)-b-methyl methacrylate)(Mn 19,500-18,100)] films were observed. The AFM result indicated that the thickness of the films and surface structures depended on temperature, concentration and solvent. In order to monitor the solvent effect of blending homopolymer and diblock copolymer, polymer solution of 10 mg/L was prepared by dissolving in THF, CHCl3 and toluene. Polymer films were annealed at 140℃ for 6 hours and for 48 hours in vacuum dry oven and then were compared with samples stored at room temperature to observe microphase separation.

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장소: 부산BEXCO

발표코드: **POLY.P-14**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photophysical Properties of a Blue Light-Emitting Hyperbranched Poly(fluorene)

김택준 안택

경성대 화학과

Various new conjugated polymers have been designed and synthesized, for efficient light emission or charge transfer. So far, the majority of work on conjugated polymers has been focused on linear one-dimensional polymers. Although a few of two-dimensional conjugated polymers, such as hyperbranched conjugated polymer have been reported to exhibit comparable charge transferring and processing properties to their linear counterparts, two-dimensional conjugated polymeric light-emitting materials have been less discussed in the literature. Here, we report the synthesis and light-emitting properties of hyperbranched polyfluorene (PF) through A2 and B3 type monomer. A synthesized hyperbranched PF showed pure blue emission as film state at 419 nm in photoluminescence (PL) measurement and was found to showing almost no excimer emission peak even the polymer film was annealed at 80 oC for 5 hours. Detailed synthetic routes and photophysical properties of new hyperbranched PF will be discussed.

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장소: 부산BEXCO
발표코드: **POLY.P-15**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

pH Induced High Modulus Coacervate Formation by Bio-inspired Catechol Chemistry

박성영

한국교통대 화공생물공학과

A novel bio-inspired hydrogel system based on complex coacervate formation of binary polymers: dopamine conjugated hyaluronic acid (HA-DN) and lactose modified chitosan (chitlac) has been prepared. HA was conjugated with dopamine by simple carbodiimide chemistry in the presence of N-(3-Dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride (EDC), yielding HA-catechol (HA-DN) with superior biocompatibility and degradability. Coacervation was achieved by both electrostatically driven inter-polymer chain interactions as well as Michael addition reaction of catechol molecules at alkaline pH, creating the structural complexity within the hydrogel system. A binary interpenetrating polymer system was followed due to its advantages for easy, quick and reproducible preparation. HA-DN was employed as an anionic polymer in our system. Rheological studies were carried out to evaluate the stability of the formed coacervate while zeta-potential and XPS data concluded that this interpenetrating binary hydrogels were physically more stable and robust due to the formation of inter-molecularly polyelectrolytes complex coacervation as well as covalent crosslinking formed via catechol cross-linking and cyclization. The developed bio-inspired coacervate hydrogels possessed the properties of aquamaterials with enhanced physical properties such as an excellent long-term physical stability that would become an attractive candidate for various biomedical and tissue engineering applications.

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장소: 부산BEXCO

발표코드: **POLY.P-16**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Refractive poly(phenylene thioether) Containing Triazine Unit

유남호

KIST 복합소재연구소

Highly refractive and transparent poly(phenylene thioether) containing a triazine unit has been developed. The polymer was prepared by a polycondensation procedure from 4,4'-thiobisbenzenethiol and 2-methylthio-1,3,5-triazine-4,6-dithiol, and showed high thermal stabilities such as relatively high glass transition temperature of 116 oC and the 5% weight loss temperature (T5%) of 367 ºC. The optical transmittance of the polymer at 400 nm is higher than 80%. The triazine unit with sulfur atoms provides the polymer with high refractive index of 1.7492 which is very high value.

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장소: 부산BEXCO

발표코드: **POLY.P-17**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Polymers based on Benzimidazole Segments for Polymer Solar Cells

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대구경북과학기술원 에너지시스템공학과 [1]대구경북과학기술원 에너지시스템공학전공

Polymer solar cells (PSCs) have attracted considerable attention due to their low manufacturing costs, flexibility and simple processability. However, it is necessary to develop new types of electron-donor polymers to achieve high power conversion efficiency (PCE). In this study, a series of polymer which were based on electron-deficient benzimidazole segments and electron-rich benzodithiophene segments for polymers solar cells were designed and synthesized. Typically, benzimidazole derivatives have high electron accepting and transporting properties. Moreover, the optoelectronic properties of the benzimidazole segments can be easily tuned by introducing various functional groups. The synthesized polymers containing benzimidazole segments exhibit low bandgaps and suitable HOMO and LUMO energy levels for photovoltaic applications. The optical and electrochemical properties of the synthesized polymers were characterized by UV/Vis spectroscopy and cyclic voltammetry measurements. The polymer solar cell devices with benzimidazole based polymers achieved high PCEs due to its enhanced light harvesting property and efficient interpenetrating network. This work will provide more opportunities for development of new materials for polymer solar cells which can achieve high PCEs.

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장소: 부산BEXCO

발표코드: **POLY.P-18**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymer solar cells based on N-(4-Octylphenyl)dithieno[3,2-b:2',3'-d]pyrrole Polymers

김상준 **V. Tamilavan** 현명호

부산대 화학과

N-(4-Octylphenyl)dithieno[3,2-b:2',3'-d]pyrrole (N-aryl DTP) based π-conjugated monomer unit was prepared and polymerized with thiophene-benzothiadiazole-thiophene (TBT) derivative to afford alternating copolymer DTPTBT. The optical study showed that the absorption band of the polymer DTPTBT was quite broad from 300 nm to 800 nm. In order to extend the absorption of the polymer DTPTBT, we incorporated 2,1,3-benzothiadiazole (B) and benzimidazole (BI) in polymer DTPTBT main chain by copolymerizing there different comonomers (N-aryl DTP, TBT and B or BI) at 2:1:1 ratio to afford random copolymers DTPTBTB and DTPTBTBI, respectively. The absorption bands of the polymers DTPTBTB and DTPTBTBI were found to extend up to 1000 nm and 1200 nm, respectively. The optical band gap of the polymers was calculated to be 1.62, 1.33, and 1.07eV, respectively, which is correlated well with the electrochemical band gap values calculated from CV analysis. The polymer solar cell device containing DTPTBT:PC60BM (1:3 wt %) as an active layer gave the best result with an open-circuit voltage (Voc) of 0.545 V, a short-circuit current (Jsc) of 8.91 mA/cm2, and a fill factor (FF) of 42.09 %, offering an overall power conversion efficiency (PCE) of 2.04 %.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-19**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of monodisperse poly (methacryloyl phosphatidyl choline) hydrogel microspheres in micro-capillary devices

박종희

한양대 응용화학과

This study introduces a flexible and straightforward method for generating monodisperse suspensions of hydrogel microspheres by using a microcapillary device-based microfluidic technique that enables tight control over the size and monodispersity of droplets as well as the interfacial property of monomer drop structures. We fabricates a new type of hydrogel microspheres mainly consisting of poly (methacryloyl phosphatidyl choline)(PMPC) because this polymer displays a highly enhanced biocompatibility due to the biological affinity of phosphatidyl choline moieties. We characterize not only how their surface affects the cell viability but also how encapsulated molecules behave through the internal structure of the hydrogel phase. The robustness and versatility of our microfluidic approach are expected to generate more complex hydrogel systems, thus creating new possibilities to engineer the key functions that are suitable for many advanced biological applications.

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장소: 부산BEXCO

발표코드: **POLY.P-20**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Study of Adsorption characteristics on Anionic Surface by the Modified Cationic Starch

김유미 김한영[1]

애경산업(주) 기반기술연구팀 [1]애경산업(주) 중앙연구소

The adsorption characteristics of cationic starches and starch-oligomers were investigated using the Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D). Adsorption amount of modified starches was higher than cationic surfactants such as C12~C16 trimethylammonium bromide, and, cationic starches did not showed the tendency of the degree of cationic substitution and molecular weight. On the other hand, the softness of adsorption layer was increased with the molecular weight of cationic starches in visco-elasity terms. In addition, the rigidity of adsorption layer of cationic surfactant in desorption step was decreased. but, cationic starches was increased.

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장소: 부산BEXCO

발표코드: **POLY.P-21**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-anticorrosion performance with a new triazole corrosion inhibitor

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한국화학연구원 그린화학연구단 [1]한국화학연구원 응용화학연구단 [2]한국화학연구원 계면화학 공정 연구팀

This study was investigated for self-anticorrosion efficiency after scratching. A corrosion inhibitor was encapsulated using polyurethane (PU) for a self-anticorrosion mechanism on metallic substrates, and was successfully fabricated via interfacial polymerization in an oil-in-water emulsion. Corrosion resistance mechanism on the microencapsulation system was successfully appreciated for a controlled specimen and four samples. Polyurethane microcapsules were filled with Az-C12, and its properties were observed for specific properties such as the yield, wall shell thickness, microcapsule size, capsule size distribution and core fraction. Microcapsule sizes were arranged between 27 and 276 ㎛, and the thickness was observed at around 20 ㎚-100 ㎛, at 1000-9000 rpm. Simultaneously the yield of microcapsules decreased with an increasing of the agitation rate from 27 to 75 %. Core fraction and microcapsules sizes significantly contributed to self-anticorrosion preventing system.

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발표코드: **POLY.P-22**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of biohybrid materials based on self-assembling peptides and gold nanoparticles

김보람 임용범[1]

*연세대 신소재공학과 [1]*연세대 신소재공학과*

Function of peptides can be improved when their secondary structures such as alpha-helix or beta-sheet are stabilized by the process of self-assembly. Peptides can be easily synthesized due to their shorter sequences when compared to proteins. Inorganic materials such as nanometer-scale gold nanoparticles have been used in various applications including biosensors, drug delivery devices, and biological contrast agents. Thiolated organic ligands can bind to the surfaces of gold nanoparticles, which can lead to the fabrication of nanoparticles. In this presentation, we used a tumor suppressor protein p53 as a model of the organic ligand. p53 activates transcription of genes that suppress proliferation of tumor cells. This function is closely related to the degree of p53 alpha-helix secondary structure stabilization. Here, we used the cyclized version of the p53-based block peptides that have multiple thiol groups. Circular Dichroism (CD) data proved that the cyclic peptide help stabilizing the alpha-helix secondary structure of p53 peptide. Moreover, it was shown that the color of colloidal gold sol changed by the aggregation of gold nanoparticles, which was shown to be dependent on the interaction between MDM2 and alpha-helix segment of cyclic peptide on hybrid nanoparticles. This hybrid nanoparticle has the advantages of selective recognition of cognate binding proteins. The functionalized biohybrid nanoparticles have great potential to become novel biomaterials that can control functions of intracellular proteins.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Suzuki and Ullmann Reactions in the Presence of New Crosslinked Polymer Particles

전보람 변인준 한양규

한양대 화학과

We synthesized new crosslinked polymer particles from new acrylamide based monomer in the presence of divinyl benzene by a suspension polymerization. The porous crosslinked polymer particle was used in the conventional aromatic coupling reactions known as suzuki and ullmann reactions: aryl halides (iodobenzene, bromobenzene, chlorobenzene and their derivatives) were reduced to the resulting coupling compounds using a palladium catalyst in water in the presence of the prepared polymer particles without any organic solvents at mild conditions. Unlike the conventional coupling reaction systems, the use of small amount of the crosslinked polymer particle enables the highly selective coupling reaction of aryl halides to biphenyl compounds due to its fixation and orientation effects.Keywords: aromatic coupling reaction, suzuki reaction, ullmann reaction, crosslinked porous polymer.

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장소: 부산BEXCO

발표코드: **POLY.P-24**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Process and evaluation of free radical grafting reaction with the acryl compounds contain quaternary ammonium salt in cellulose fibers

김태경

한국화학연구원 그린화학연구단 환경자원센터

The free radical grafting reaction of the acryl compounds contains quaternary ammonium salt with cellulose fibers was carried chemically using redox system. The effect of initiator concentration and monomer concentration on the grafting efficiency was studied. In this study, we used the selected free radical grafting process for increasing graft weight, antibiosis and other functionality. We evaluated the grafting rates by Diamond-ATR and tested physical properties of cellulose yarns. The focus of this study was to optimize the antibiosis finishing on cellulose fabrics with free radical grafting.The resulting cellulose fibers have different dyeing properties and antibiosis that makes them suitable for use in such cellulose products as paper towels, diapers, and sanitary products.

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장소: 부산BEXCO

발표코드: **POLY.P-25**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

PVDF-HFP와 amphiphilic polymer brush의 blend를 통한 protein-resistance 향상

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공주대 신소재공학과 [1]공주대 신소재공학부 고분자공학전공 [2]공주대 신소재공학부

Poly(vinylidene fluoride-co-hexafluoroproylene)(PVDF-HFP)는 높은 열적 안정성, 기계적 강도 및 내후성을 갖고 있어 고분자 전해질, 멤브레인에 응용된다. PVDF-HFP 멤브레인은 기계적 물성은 뛰어나지만 소수성으로 단백질 흡착 특성을 갖기 때문에 오염저항이 낮아 보완이 요구된다. 본 연구에서는 PVDF-HFP 와 상용성 있는 Poly(methyl methacrylate)(PMMA) 메인사슬에 친수성 poly(ethylene glycol)(PEG)가 브러쉬 사슬로 구성되어 있는 amphiphilic polymer brush 를 사용하였다. PVDF-HFP 와 amphiphilic polymer brush 의 blend 를 통해 친수성이 향상되어 물 흡수율 증가를 나타냈고, 단백질 흡착 능력을 저하시켰다.

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장소: 부산BEXCO

발표코드: **POLY.P-26**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Manipulation of Ipso Carbon Reactivity of Triphenylamine-Based AB Type Monomers

이진희 김상율

KAIST 화학과

The triphenylamine derivatives have been widely investigated and applied in various electro-optical materials. We synthesized AB type triphenylamine monomers for polymerization via nucleophilic aromatic substitution (S_NAr). Although the monomers have the electron-donating amine group at the para position of the fluorine-leaving group, the reactivity of monomers was successfully regulated by introducing electron-withdrawing groups (EWGs) into the triphenylamine. In addition, the photoluminescence (PL) of the monomers was efficiently tuned according to the strength of intramolecular charge transfer (ICT). Detailed synthetic method and properties of the monomers and polymers will be presented.

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장소: 부산BEXCO

발표코드: **POLY.P-27**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bio-based isosorbide를 이용한 polyester의 합성 및 특성 조사

김정진 공명선

단국대 나노바이오의과학과

Polyester (PEs)는 생체 적합성 고분자로써 생분해 능력이 탁월하고 분해 생성물이 인체에 독성을 띄지 않아 생체조직공학의 재료로 많은 관심을 받으며 널리 이용되고 있다. 특히 succinic acid (SA) 계 polyester 가 널리 이용되고 있으며 디올로서 ethylene glycol (EG)과 bio-base isosorbide (IS)의 비율에 따라 여러 가지 다양한 물성이 기대된다. 그러나 IS 는 2 차 알콜기를 가지기 때문에 SA 와의 반응성에 차이가 나기 때문에 본 연구에서는 SA 를 대신하여 succinic anhydride (SAn)를 이용하여 중합반응이 용이 하도록 하였으며 SAn 과 IS 및 SAn 과 EG 의 각각의 dimer 를 형성하고 이들 dimer 의 비율을 조절하여 여러 가지 조성을 가지는 PEs 를 합성하였다. GPC 를 이용한 분자량, DSC 와 TGA 를 이용한 열적 성질을 측정하였다. 기계적 성질을 보기위하여 인장강도를 측정하였다. PBS 및 NaOH 수용액을 이용한 생분해성 정도를 조사하여 생체 적합성을 확인 하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-28**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Isosorbide와 isomannide를 이용한 생분해성 polyurethane 합성과 물성비교

오소연 공명선

단국대 나노바이오의과학과

폴리우레탄은 polyol 과 diisocyanate 의 중축합 반응으로 합성하여 반복단위가 우레탄기로 결합되어 있는 중합체이다. 폴리우레탄은 체내에서 안정하고 혈액접합성이 우수하여 혈액과 직접 접촉하는 장기인 인공혈관, 인공심장 등에 주로 이용되고 약물 전달체, 피부 재생을 위한 scaffold 등의 의료 분야뿐만 아니라 비분해성 폴리머의 생분해성 부여 등 다양한 분야에 널리 응용되고 있다. 본 연구에서는 생체적합성 폴리우레탄을 합성하기 위하여 뛰어난 생분해성 거동을 보이는 poly(ε-caprolactone)과 hexamethylene diisocyanate (HDI)을 이용하고 hard segment 역할을 할 수 있는 diol 로서 입체 이성질체인 1,4:3,6-dianhydro-D-sorbitol(isosorbide) 과 1,4:3,6-dianhydro-D-manniol (isomannide)를 넣어 다양한 비율의 PU 를 합성하였다.각 성분의 조성 변화에 따른 물성 변화를 GPC, DSC, TGA, 용해도, 인장강도 등의 기계적 특성 및 열적 특성을 측정하여 특성 변화를 조사하였다.

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장소: 부산BEXCO

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Novel Click-crosslinked Micelle based on Poly(amino acid)s Derivatives for Controlled Drug Release

김소은 김종득[1]

KAIST(KAIST) 생명화학공학과 [1]KAIST 생명화학공학과

The aim for this study is to design a novel drug delivery carrier with high stability. Cu(I)-catalyzed Huisgen 1,3-dipolar cycloaddition of terminal alkynes with organoazides, a most famous click chemistry, is used in order to develop a click-crosslinked micelle for controlled drug release. Propargyl amine with alkynyl group and 11-Azido-3,6,9-trioxaundecane-1-amine with azide group are conjugated to poly(2-hydroxyethyl aspartamide) back bone grafted with octadecyl amine and mPEG-AM2000 (PHEA-g-C18-PEG). These two amphiphilic graft copolymers, PHEA-g-C18-PEG-AK and PHEA-g-C18-PEG-AZ, form spherical micelles in aqueous solution. By mixing them with copper(Ⅱ) catalyst and sodium ascorbate under N2 injection, it turns to a shell-crosslinked structure. Characterization of the click-crosslinked particle was fully investigated via H1NMR, FT-IR, DLS, and so on. This study could further be applied as an early detection of cancer, and become an advanced research of designing drug and gene delivery carriers.

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장소: 부산BEXCO

발표코드: **POLY.P-30**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Self-assembly of Photoresponsive Organogelators Containing Azobenzene and Diacetylene Groups

김지성 서명은 김상율

KAIST 화학과

Responsive organic materials to external stimulus have been of much interests due to their high potential in many applications. As one of responsive materials, low-molecular weight organogelators with specific functional groups show macroscopic changes induced by molecular level structural transition via self-assembly. We synthesized photoresponsive organogelators containing azobenzene and diacetylene groups which show reversible gel-sol transition and photo-induced polymerization. Various Structural modification was attempted to study the effect of photoresponsive units in gelation and gel-sol transition.

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장소: 부산BEXCO

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cationic amino acids modified poly(amidoamine) dendrimers for enhanced gene transfection efficiency and low cytotoxicity

유광식 배윤미 최준식

충남대 생화학과

Polymer-based gene delivery carrier systems has limitations on its cytotoxicity and poor transfection efficiency. To overcome these limitations, various methods have been developed and applied for reinforce their shortcomings. In this study, we developed cationic dendrimer system consisting of poly(amidoamine) (Cystamine core, Generation 3th) with amino acid modification on their peripheral end functional amine groups. Grafting histidine (His) and arginine (Arg) residues to the surface of dendrimer resulted in enhanced transfection efficiency and low cytotoxicity. Synthesized cPAM G3-His-Arg was analyzed its physicochemical properties using various methods such as ^{1}H-NMR, gel electrophoresis, acid-base titration and dynamic light scattering. To evaluate the possibility of cysPAM G3-His-Arg as a non-viral gene delivery vector, luciferase assay, MTT assay and confocal microscopy study were conducted.

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장소: 부산BEXCO

발표코드: **POLY.P-32**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

고 굴절률 투명 나노 입자를 이용한 composite 형성과 실리콘 기반 LED 봉지재 합성

맹일호 PIAO LONGHAI 김진권

공주대 화학과

현재 고출력 white LED 와 높은 효율의 필요성이 증대되고 있다. LED 봉지재는 외부로부터 LED 칩을 보호하고 전기적으로 절연시켜주며 빛을 투과시켜 외부로 빛을 방출시키는 기능을 수행한다. 연구 결과에 따르면 굴절률이 증가함에 따라 광 추출 효율이 증가하는 것으로 알려져 있다. 본 연구에서는 silicone 기반 가교제를 합성하여 epoxy group 이 있는 resin 과 반응 시켜 봉지재를 합성 하였으며 고 굴절 투명 나노입자를 surface modification 을 통해 composite 을 만들어 투과율과 굴절률의 변화를 연구하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-33**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The surface modification of Ag nanowire using PVP-b-PEG diblock copolymers

ZHAOHESONG 김상호 **PIAO LONGHAI**

공주대 화학과

Different chain length of poly(vinyl pyrrolidone)-b-poly(ethylene glycol) diblock copolymers were synthesized through the reversible addition-fragmentation transfer-mediated(RAFT) polymerization. Monodisperse silver nanowires with little nanoparticals were synthesized through a simple one-step method by reducing $AgNO_3$ with ethylene glycol in the presence of PVP-b-PEG diblock copolymer without seed forming procedure. The diameter of silver nanowires can be controlled by changing the molar ratio of $AgNO_3$ and PVP-b-PEG diblock copolymers from 100nm to 700nm with the average length of 17μm. Importantly, these nanowires can disperse in not only polar solvent such as ethanol but also non-polar solvent like toluene and THF. This may be attributed to the PEG block tails on the surface of silver nanowires.

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장소: 부산BEXCO

발표코드: **POLY.P-34**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrical Characterization of Well-defined Ambipolar Polymer-Based Nonvolatile Memory Device

유용균

광주과학기술원(GIST) 신소재공학부

To improve the non-uniform dispersion and prevent aggregation caused by mixing or doping, we synthesized new ambipolar polymers of poly(9-(4-vinylphenyl)carbazole)-b-poly(2-vinylpyridine) (PVPCz-b-P2VP) and poly(2-(N-carbazolyl)ethyl methacrylate) end-capped with fullerene(PCzMA-C60) consisting of electron donors as carbazole(PVPCz, PCzMA) and electron acceptors as pyridine and fullerene(P2VP, C60) by anionic polymerization in this study (Figure 1a, 1d). Electrical behaviors(metallic, bistable switching, and insu?lating) of PVPCz-b-P2VP were determined by various morphologies (from spherical to lamellar) derived from different donor-acceptor ratios of PVPCz and P2VP. Especially, the devices showing a lamellar structure exhibited non-volatile memory performance(Figure 1b and c). Moreover, new ambipolar polymer on high loaded C60(PCzMA-C60) allows non-volatile memory to get excellent reliability, stable endurance, and long retention time(Figure 1e). We will discuss relation between donor-acceptor ratios and electronic properties for nonvolatile memory

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-35**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Well-Defined Ambipolar Block Copolymers Containing Monophosphorescent Dye

유용균

광주과학기술원(GIST) 신소재공학부

Well-defined ambipolar block copolymers containing carbazole, oxadiazole moieties, and only one homoleptic iridium(III) complex between the carbazole and oxadiazole blocks were successfully synthesized by sequential living anionic polymerization with controlled molecular weights (Mw), a narrow molecular weight distribution (Mw/Mn < 1.15), and a high conversion yield (98?100%). The optimum conditions for the successful controlled synthesis of an oxadiazole-containing the homopolymer of poly(2-phenyl- 5-(6-vinylpyridin-3-yl)-1,3,4 oxadiazole) have been established by controlling the nucleophilicity strength of the carbanion. In addition, the location and concentration of the homoleptic iridium(III) complex were controlled by linking it to 1,1-diphenylethylene, which exhibits monoaddition characteristics in the main chain of the block copolymer.

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장소: 부산BEXCO

발표코드: **POLY.P-36**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermoresponsive Fluorinated Polyacrylamides with Low Cytotoxicity.

김경빈

울산대 화학과

We demonstrate that the thermosensitivity of fluorinated polyacrylamides can be easily controlled by changing the number of fluorine atoms in terminal alkyl group of N-ethyl moiety (Scheme 1a). Mono-fluorine substituted poly[N-(2-fluoroethyl)acrylamide] (P1F) is water-soluble while tri-fluorine substituted poly[N-(2,2,2-trifluoroethyl)acrylamide] (P3F) is water-insoluble. Interestingly, di-fluorine substituted poly[N-(2,2-difluoroethyl)acrylamide] (P2F) exhibits a LCST in water around 26~28 oC, which is comparable to that of poly(N-isopropylacrylamide) (PNIPAM). Interestingly, from the view of chemical structure, -CH2CHF2 group of P2F and ?CH(CH3)2 group of PNIPAM have similar hydrophobicity, judging from the similar LCST of two polymers. The gradual replacement of hydrogen atom by fluorine atom in terminal alkyl group led to substantial increase in hydrophobicity. The wide range of LCST values was covered by random copolymers prepared by the combination of three monomers.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-37**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In situ thermogelling polypeptide for human adipose-derived stem cell 3D culture

연보라 계은정[1] 최정윤

이화여대 바이오융합과학과 [1]이화여대 화학나노과학과

We are reporting the use of reverse thermal gelling polypeptides which are the diblock mPEG-L-PA copolymers as promising platforms for the 3D culture of human adipose-derived stem cell. In order to show a similar reverse themal gelling behaviour, the molecular weight of the PEG was fixed at 5000 Daltons, while that of L-PA was varied 600 Daltons, 1200 Daltons, and 2500 Daltons. Polymers were synthesized by ring-opening polymerization, and were characterized by 1H-NMR, GPC, FTIR, CD and TEM. Thermal properties were investigated by Rheometer. To see the feasibilities of hydrogels, cell proliferation and viability of human adipose-derived stem cell in polymer aqueous solution were investigated. In our system, mPEG-L-PA hydrogel induced selective differentiation of human adipose-derived stem cell

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-38**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photovoltaic Properties of Polymers Containing 1,2,4-Oxadiazole as an Electron Acceptor Moiety in Their Main Chain

RajalingamAgneeswari V. Tamilavan 현명호

부산대 화학과

Pyrrole-based electron rich (N-aryl DTP) and 1,2,4-oxadiazole-based electron deficient (TBOBT) units were prepared and copolymerized by using stille polymerization. The resulting alternating copolymer P1 was found to show their absorption band from 300 nm to 530 nm. To extend the absorption of polymer P1, we incorporated other electron deficient units such as thiophene-benzothiadiazole-thiophene (TBT) derivative and benzothiadiazole (B) in polymer P1 main chain by copolymerizing there different comonomers (N-aryl DTP, TBOBT and TBT or B) at 2:1:1 ratio. The resulting random copolymer P2 and P3 showed their absorption band up to 600 nm and 800 nm, respectively. The electron deficient monomers TBOBT and B were also copolymerized with thiophene derivative with aim of knowing the potential of N-aryl DTP unit to afford polymer P4. The absorption band of the polymer P4 was found to be covers the region from 300 nm to 600 nm. All the synthesized polymers were used as electron donating material in polymer solar cell application. The maximum energy conversion efficiency was achieved for polymer P3 to be 1.33 % with a Jsc of 4.95 mA/cm2, a Voc of 0.68 V and a FF of 40 %, measured using AM 1.5 G solar simulator at 100 mW/cm2 light illumination.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-39**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of β-Cyclodextrin-graft-Polyvinylpyrrolidone Copolymer via Xanthate-Mediated RAFT Polymerization

강건위 **PIAO LONGHAI**

공주대 화학과

The β-cyclodextrin (β-CD) derivative with an average degree of substitution of 4 (4Br-β-CD) was synthesized by treating β-CD with 4 equivalents of 2-bromo-propionyl bromide. It was then reacted with potassium ethyl xanthate to produce β-cyclodextrin xanthate derivativeas the chain transfer agent (CTA) in reversible addition-fragmentationchain transfer polymerization (RAFT). The graft copolymers β-CD-graft-PVP (polyvinylpyrrolidone) with different chain length were prepared. The structures of 4Br-β-CD, CTA and copolymers were characterized with 1H NMR spectra, and their molecular weight distribution of the copolymers were measured by GPC.

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장소: 부산BEXCO

발표코드: **POLY.P-40**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of inorganic nanoparticles chemically grafted with zwitterionic biopolymers

김영선 안소연[1]

한양대 화학공학과 [1]한양대 응용화학과

We introduce a robust method for synthesis of inorganic nanoparticles chemically grafted with a zwitterionic poly(2-methacryroyloxyethylphosphorylcholine) biopolymer. The essence of our synthetic approach is to chemically tag double bonds onto the inorganic nanoparticles and then to control the polymerization loci during the initiation stage, which leads to favorable nucleation and growth of growing polymer chains on the surface of the inorganic nanoparticles. Use of this synthesis protocol allows us to obtain inorganic hybrid nanoparticles with a polymer shell of which thickness ranges even in a few nanometers. Basically, in this study, we have tried to demonstrate that surface chemistry of our hybrid nanoparticles is indeed important and plays a role in regulating particle-to-particle interactions in suspension, thus providing a useful means to improve suspension stability of inorganic nanoparticles in complex formulations. (Y. Kim and S. An equally contributed to this work)

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-41**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of a New Conjugated Polymer Containing Thiophene Ring and Fluorine

황선우 김중일 장원 박정호[1] 김홍선 김인태 이상우

광운대 화학과 [1]광운대 화학과/고분자연구실

A new conjugated polymer containing thiophene and Fluorine is successfully synthesized by electrochemical reaction. The new polymer has good solubility in organic solvent such as Chlorobenzene. The new polymer was characterized by ^{1}H NMR, ^{13}C NMR, GPC and TGA. Electochemical and optical properties of the polymer are measured by UV-vis spectroscopy, PL spectroscopy and cyclovoltammetry. This polymer shows photoluminescence properties as blue color. The new polymer will be used for organic light emitting device.

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-42**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Characterization, and properties of a new conducting polymer containing pyrrole derivatives.

박은랑 채영준 이영남 김인태

광운대 화학과

Substitution of various functional groups on pyrrole is suggested as a method to modify and to improve the electrical properties and optical properties of pyrrole. A resulting new polymer is soluble in organic solvent such as THF, $CHCl_3$ and DMF. The polymer was characterized by ^{1}H NMR, ^{13}C NMR and FT-IR. The UV-vis spectroscopy absorption of the new polymer shows at about 268nm, 337nm and 366nm in $CHCl_3$ solution. Photoluminescence of the new polymer in $CHCl_3$ shows at about 530nm. The polymer will be applied to LED as emitting material.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-43**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Characterization and Properties of ConjugatedPolymers Containing Thiophene Derivative for Polymer Solar Cells

김중일

광운대 화학과

Conjugated polymers containing thiophene derivative are successfully synthesized by Stille'scoupling reaction. The new polymers have good solubility in organic solvents such as $CHCl_3$, and Chlorobenzene. The new polymers are characterized by ^{1}H NMR, ^{13}C NMR, GPC and TGA. Electochemical and optical properties of the polymers are measured by UV-vis spectroscopy, PL spectroscopy and cyclovoltammetry. The new polymers will be used for polymer solar cell device.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-44**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of catalyst to the molecular weight control in polyethylene isophthalate synthesis

차미선

호남석유화학(주) 연구 4팀

폴리에틸렌 이소프탈레이트를 제조하는 과정에서 에스테르화 반응 단계에 촉매를 투입해 분자량 증진이 가능한 폴리에틸렌 이소프탈레이트 연구를 수행하였다. 에스테르화 반응시 촉매없이 진행되는 기존 반응에서 금속촉매 투입 시 이소프탈레이트에서 비스(2-하이드록시에틸)이소프탈레이트가 형성되는 반응을 촉진시켜 주는 역할을 하는 것으로 예측된다. 또한 산 촉매를 이용해 고분자 내 존재하는 불순물의 양을 감소시키고 분자량을 증가시키는 효과가 예측된다. 이렇게 제조된 폴리에틸렌 이소프탈레이트의 물성 및 performance 에 대해 분석하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-45**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Porous Polyimide Composites Containing Metal Oxide Particles

이지목 정현민

금오공과대 응용화학과

나노다공성 폴리이미드는 폴리이미드 고유의 열적, 기계적 안정성과 우수한 내화학성을 가지고 있고, 다양한 촉매 활성을 갖는 금속 산화물 입자들과 혼성되어 사용할 때 신규의 우수한 특성들을 기대할 수 있다. 본 연구에서는 금속 전구체와 반응할 수 있는 기능기를 도입한 soluble 폴리이미드를 합성하고, '가역적 교차결합 및 침전'을 이용한 나노 다공구조 형태를 구현하였고, 금속 산화물 입자들을 균일하게 포함한 다공성 폴리이미드-촉매 복합체를 제조하였다. Ti, ruthenium 혹은 copper 산화물이 복합화된 복합체를 제조하고 구조적 특징을 FE-SEM 과 TGA 로 분석하였다. 또한 촉매 지지체 및 촉매 복합체로서의 성능을 모델 화합물의 광촉매적 분해작용 특성을 p25, lump, film 에 따라 성능을 확인하였으며, 본 연구의 폴리이미드의 특성을 이용하여 만든 film 형태의 촉매에서 기존의 p25 에는 미치지 못하지만 lump 형태보다 더 뛰어난 특성을 가진 촉매를 만들 수 있었다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-46**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and Synthesis of N-Heterocyclic Carbene-Containing Conjugated Polymers

박지영

성균관대 화학과

N-Heterocyclic carbenes (NHCs) easily form complexes with various metals and have been widely used as a ligand for various organic catalysis. Due to their excellent stability and strong metal-binding ability, NHCs have made their way to materials chemistry, such as electrochromic devices. We envision that NHC can control conductivity or electrochemical activity of conjugated polymers (CPs) by affecting the pathway of electron transfer through the coordinated metals. We synthesized NHC-containing CPs by electrochemical polymerization from metal-coordinated NHC building blocks. We investigated photo and electrochemical properties of NHC-containing CPs by cyclic voltammetry, fluorescence and spectroelectrochemistry.

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장소: 부산BEXCO

발표코드: **POLY.P-47**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conductive Polymer/Graphene Oxide Nanocomposites for Supercapacitors

이은지

성균관대 화학과

Supercapacitors have been highlighted as the next generation energy storage devices 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 graphene oxide (GO) and novel quinone polymers containing 3,4-ethylenedioxythiophene (EDOT). GO and new quinone polymer nanocomposites were prepared from one-step coelectrodeposition. During the process of electrochemical polymerization, the anionic GO acted as a weak electrolyte and was entrapped in the conductive polymer nanocomposites. We investigated electrochemical properties, cycling performance and capacitance of GO/quinone polymer nanocomposite, and also compared with those of PEDOT.

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장소: 부산BEXCO

발표코드: **POLY.P-48**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and Synthesis of Donor/Acceptor Copolymers for Highly Efficient Organic Photovoltaics

양기석

성균관대 화학과

Control of bandgap and molecular energy levels improves photovoltaic properties of conjugated polymers. Copolymerizing with different units is a general way to adjust structures of the polymers. Herein, we designed and synthesized six conjugated polymers through copolymerizing three electron-accepting monomers (thienothiophene, fluoro-thienothiophene, imidazolium chloride) and two electron-donating monomers (benzodithiophene, naphthodithiophene). We show that the bandgap and molecular energy levels are effectively controlled by polymerizing with different units. We also characterized each polymer through UV-vis absorption spectroscopy, fluorometry and cyclic voltammetry.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-49**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Template-free Synthesis of Uniform-sized Hollow-structured Poly (vinylamine) (PVAm) Hydrogel Microparticles

shahinur acter 김영선[1]

한양대 응용화학과 [1]한양대 화학공학과

This study reports a vigorous and straightforward method for the synthesis of uniform-sized hollow-structured poly (vinylamine) (PVAm) hydrogel microparticles without using any template. This method combines the dispersion polymerization and consecution hydrolysis/crosslinking. We have found that the shell thickness is independent of the reaction parameters, which attributes to the fact that the hydrogel shell is readily formed by a diffusion-limited crosslinking reaction process. Our hydrogel shell microparticles showed cell internalization ability as well as optical responsiveness, which opens up a possibility to use them for selective encapsulation of drug molecules and their targeted releasing.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-50**

발표분야: 고분자화학

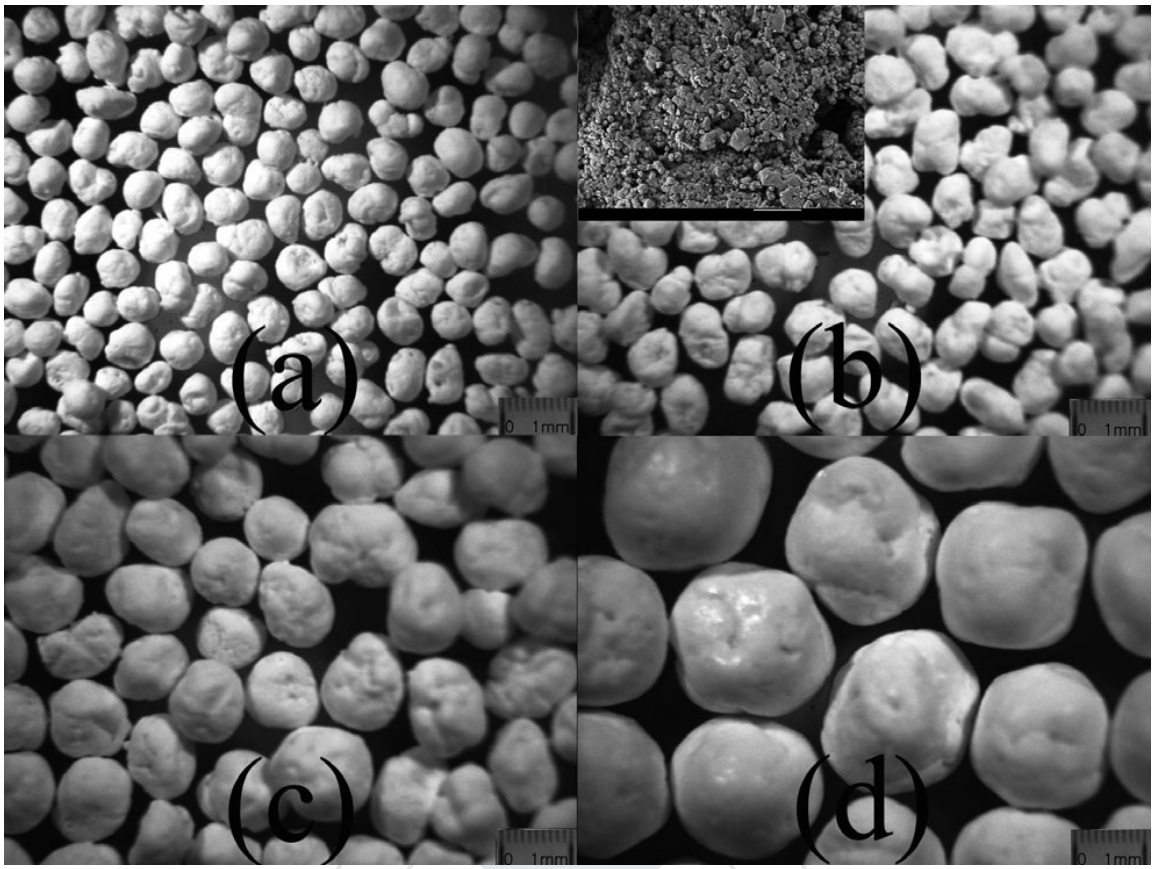
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly active catalyst for olefin/carbon monoxide (CO) copolymerization and morphology control of the polymer particles

박지혜 이분열

아주대 분자과학기술학과

Since the discovery of a highly active catalyst for olefin/carbon monoxide (CO) copolymerization by Shellsubsequent investigations have been made in both academic and industrial settings. Although Shell discontinued research in this area in 2001, Asian industrial development has continued, particularly in areas related to development of fiber applications. The copolymer is insoluble in common organic solvents and precipitates during copolymerization as irregular snow-white particles of low bulk density or as a lump, causing problems in the postreaction processes. Some of the polymer sticks to the reactor walls and agitator, creating a problem in large-scale synthesis called “reactor fouling”. To control the morphology of the polymer particles in the ethylene/CO copolymerization, a strategy is implemented inthis work that mimics the traditional suspension polymerization technique. Pressurizing with CO/ethylene gases on catalyst-containing 1-octanol droplets dispersed in water produces well-controlled polymer particles with bulk densities in the range of 0.20?0.30 g/mL. The catalyst should be harnessed with a lipophilic group on both the bisphosphine ligand framework and anion.



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일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **POLY.P-51**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Inkjet Printed CNT as Electrodes for Paper Digital Microfluidic Chips

고효진 권오선 신관우[1]

서강대 화학과 [1]서강대 화학과 및 바이오융합과정

Open digital microfluidic chips with a single plate, driven by electrowetting force on dielectrics (EWOD), were fabricated. An array of patterned electrodes was printed on a paper substrate in the inkjet printing method with carbon nanotube (CNT) ink. Patterning electrodes on planar substrates can never be achieved just in one-step for common photolithographic method which demands the successive multi-processes, such as spin coating, baking, expose and develop. These high cost procedures also need using hazardous chemicals and complicate equipments. Using an inkjet printer, the CNT solution has been easily printed out the designed patterning electrodes on paper only in one-step in sub-millimeter scale with good conductivity. The performances of CNT electrodes, when they are applied in electrowetting and in moving a liquid drop on a opened microfluidic chip, were highly comparable to that of the photoresist patterned electrodes. Based on these results we constructed the flexible opened chips on paper substrates for merging and moving the liquid drop samples.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-52**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Proton exchange membranes prepared by a sequential radiation grafting of styrene and TMSPM onto an ETFE film

이지홍 송주명 손준용 신준화

한국원자력연구원 첨단방사선연구소 공업환경연구부

ABSTRACT Several silane-crosslinked proton exchange membranes were prepared by a sequential radiation grafting of styrene and TMSPM onto an ETFE film, and subsequent chemical treatments. The polystyrene graft polymer was used to provide the proton conductivity after the introduction of sulfonic acid group and PTMSPM graft polymer was used to provide silane-crosslinked structure after the sol-gel processing. The water uptake and ion exchange capacity of the prepared membranes were measured. The prepared membranes were also characterized by FT-IR, TGA, and SEM-EDX.

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Structural investigation of polystyrene-grafted poly(ethylene-*alt*-tetrafluoroethylene) (ETFE) films

송주명 고범석 손준용 신준화

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Polystyrene-grafted poly(ethylene-*alt*-tetrafluoroethylrene) (ETFE) films were prepared by a simultaneous radiation grafting method and the crystalline structure of the grafted film were studied by DMA, DSC, XRD, and SAXS instruments. The dynamic mechanical study indicates that the ETFE phase and the PS phase are separated in the PS-grafted ETFE film. The DSC and XRD data show that the ETFE natural crystalline structure in the PS grafted ETFE films are not affected during the γ-ray simultaneous radiation grafting process. In the SAXS profiles of the PS-grafted ETFE films, the inter-crystalline distance of the ETFE films increases with increasing the degree of grafting. This result implies that the formation of PS graft polymer domains by the γ-ray simultaneous irradiation has a significant impact on the ETFE amorphous morphology of the resulting grafted ETFE film. Thus, it is suggested that the styrene monomer is mainly grafted on the ETFE amorphous regions during the γ-ray simultaneous radiation grafting process.

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Fabrication of Crosslinked SPEEK Membrane Containing Zirconium Phosphate

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Crosslinked SPEEK membranes containing zirconium phosphate were fabricated by radiation crosslinking followed by the introduction of zirconium phosphate. The zirconium phosphate particles were introduced into the crosslinked SPEEK membranes by the immersion of the membranes in zirconium dichloride oxide solution followed by the treatment with phosphoric acid. The morphology of the prepared membranes was investigated by SEM-EDX, SAXS, and ultra high resolution TEM. The results indicate that the zirconium phosphate particles were successfully embedded into the crosslinked SPEEK membranes.

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Preparation of Transparent Conductive Films with High Transparency and Low Sheet Resistance by Dispersed Single-Walled Carbon Nanotubes Using Poly[2-(dimethylamino) ethyl methacrylate]-co-Polystyrene

김현성 백현종 김봉수

부산대 고분자공학과

The single-walled carbon nanotubes (SWNTs) coatings on glass and plastic film have been investigated as transparent conductive films (TCFs) to alternate indium tin oxide (ITO) films. One of important factors that makes TCF more conductive is the dispersion of SWNTs. However, SWNTs exist as a bundle due to a strong intertube van der Waals attraction. In order to obtain well dispersed SWNTs, efficient dispersants are firstly required. Here, poly[2-(dimethylamino)ethyl methacrylate]-co-polystyrene (PDMAEMA-co-PS) was synthesized and used as a polymeric dispersant for SWNTs in organic solvent. PDMAEMA-co-PS with different copolymer compositions was prepared by atom transfer radical polymerization (ATRP). With PDMAEMA-co-PS, SWNTs were effectively dispersed through non-covalent functionalization by ultrasonication in tetrahydrofuran (THF). Especially, the stability of dispersed SWNTs was optimized with PDMAEMA70-co-PS30. SWNTs coatings on poly(ethylene terephthalate) (PET) film and glass, were prepared via spin-coating method. Moreover, the heating treatment and chemical treatment were carried out as a post-treatment to decrease the sheet resistance without the change of transparency. Transmittance and sheet resistance of SWNTs/ PDMAEMA-co-PS films were obtained by UV-vis spectroscopy and four point probe measurement, respectively.

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$[\{Cu_2(Glu)_2(\mu\text{-bpa})\}?(CH_2CN)]_n$ (MOF)를 넣은 기체 분리 막에서 CO_2 선택도에 관한 MOF의 효과

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세종대 화학과 [1]이화여대 화학-나노과학과 [2]이화여대 화학과

Poly(2-ethyl-2-oxazoline)(POZ)에 CO_2 와 상호작용이 있다고 알려진 MOF($[\{Cu_2(Glu)_2(\mu\text{-bpa})\}?(CH_2CN)]_n$)를 혼합해 지지체(웅진) 위에 코팅하여 CO_2 기체의 분리 효율을 높였다. MOF 는 'glutarate 0.2mmol / 20ml water, Cu 0.1mmol / 20ml water, bpa 0.2mmol / 20ml meoh'로 각각의 용액을 만든 후 혼합한 다음 24 시간 동안 상온에서 반응시켜 필터로 걸러 제조하였다. MOF 제조 후 16.34wt% POZ/meoh 용액에 10wt% MOF 를 고르게 분산시킨 다음 막에 코팅한다. 코팅한 막의 기체투과도는 순수한 CO_2/N_2, CO_2/CH_4 를 'bubble flow meter'를 이용하여 측정하였다. 기체투과도 측정 후 두께와 MOF 의 분포가 막의 선택도에 미치는 상관관계를 고찰하기 위해 FESEM 을 이용하였다. FESEM 으로 막의 두께를 측정하고. EDX 을 이용하여 막의 표면에 MOF 의 분포도를 보기 위해 Cu 의 분포를 측정하였다. CO_2 는 MOF 와 상호작용으로 더 빠르게 투과되고, N_2, CH_4 는 상호작용 없이 통과되어 선택도가 높아졌다. CO_2/N_2 의 선택도는 POZ 가 2.2 에 비해 POZ 에 MOF 를 섞어 코팅한 막의 선택도는 5.6 으로 약 2 배정도 높아졌다. * bpa(1,2-Bis(4-pyridyl)ethane)

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The effect of silver and gold nanoparticles on dye-sensitized solar cells using solid-like electrolyte

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세종대 화학과

Dye sensitized solar cells have attracted much attention as the next-generation solar cells with low production costs and good efficiency for energy conversion. The solid-like electrolyte was prepared by dissolving a PMII and I_2 and a PEGDME, 9wt% silica nanoparticles of 0.014μm in acetonitrile. To improve the low efficiency of DSSCs using solid-like electrolyte, we introduced metal nanoparticles with polyester hydroxyl acetylene bis (hydroxymethyl) propanoic acid Dendron (Dendron) on DSSCs. Metal nanoparticles can contribute to the effective light absorption of DSSCs, both by the localized surface-plasmon resonance (LSPR) and by light scattering. The plasmonic resonance of silver and gold nanoparticles has been studied because they strongly interact with visible light. Because silver has the sharpest resonance peak by the LSPR effect has light scattering effect, dye absorbs well the light. We employed Dendron as electron donor when we made silver and gold nanoparticles by illuminating ultraviolet-visible light. The formation of silver and gold nanoparticles was confirmed using UV-Vis absorption spectroscopy and TEM. We confirmed the presence of elemental silver and gold nanoparticles by the analysis of EDX. Through the analysis of J-V curves, EIS, IPCE, we observed the effect of silver and gold nanoparticles on DSSCs. The v_{oc} and J_{sc} of the DSSCs introduced silver nanoparticles with Dendron was increased by 11%, 16%, respectively. Up to a 23% increase in the total power conversion efficiency was achieved.

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Effect of co-adsorbents using cyclodextrin on the TiO_2 layer for dye-sensitized solar cells

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세종대 화학과

The recombination phenomena which occurred at the surface of TiO_2 semiconductor nanoparticles are one of the main factors for the low performance of dye-sensitized solar cells. Much effort has been devoted to the surface modification of TiO_2 to improve the performance by forming the barrier layer using chemical co-adsorbents. Most of co-adsorbents layers were formed by the formation of chemical bond between the surface of TiO_2 and carboxylic acids attached to the co-adsorbents. In order to cover the full surface of TiO_2 nanoparticles, large amount of co-adsorbent is necessary, however significant amount of co-adsorbent addition would detach the dye molecules which have the same chemical interaction with TiO_2 layer. Therefore we studied to reduce the amount of attachment of low molecular weight chemicals while maintaining the full coverage of the surface of TiO_2 layer using the host-guest interaction between 4-methyl-1-cyclohexane carboxylic acid and cyclodextrins. The big size of cyclodextrin would provide the barrier layer with relative small amount of co-adsorbents attached on the TiO_2 nanoparticles. Then we compared to different size of cyclodextrin such as α and β-cyclodextrin. Up to a 21% increase in the power conversion efficiency are achieved with the addition of 4-methyl-1-cyclohexane carboxylic acid in TiO_2 layer, and the effect of the formation of guest-host interaction with cyclodextrins was investigated with and without the addition of α or β-cyclodextrin. This work was supported through the NRF grant funded from the MEST of Korea (No. 2011-0030278).

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LbL assembled sPPO membrane for fuel cell PEM applications

조창기

한양대 유기나노공학과

Fuel cell membrane was prepared by layer-by-layer(LbL) deposition between poly(diallyl dimethyl ammonium chloride) (PDDA) and sulfonated poly(2,6-dimethyl-1,4-phenylene oxide) (sPPO). Engineering plastics such as PPO and poly(ether ether ketone) (PEEK) have good thermal/mechanical properties. and their highly sulfonated analogs exhibit good proton conductivity but poor methanol permeability. LbL technique have advantage in control of ionic conductivity and permeability of membrane. So, the methanol permeability of sPPO or sPEEK with high degree of sulfonation was tried to be modified by LbL technique. Other properties of membrane were also investigated.

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Carbonization and Characteristics of Carbon Fiber Precursor from Poly(acrylonitrile-co-Dicyclohexylammonium-2-(Carboxymethyl)acrylate)

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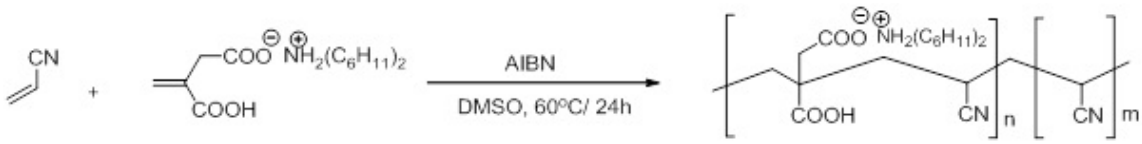
The P(AN-DCMA) copolymers with different dicyclohexylammonium-2-(carboxymethyl)acrylate (DCMA) contents (0.125 ~ 1.5 mol % in the feed) were polymerized using solution polymerization with 2,2′-azobis(isobutyronitrile) (AIBN) as an initiator. The DSC curves under nitrogen atmosphere indicated that the initiation temperature for cyclization of nitrile groups was reduced to around 201 oC. The heat release for cyclization reactions was decreased in comparison with those of PAN homopolymers. P(AN-DCMA) copolymers was stabilized by heating in air at 220 ~ 300 oC temperatures range and carbonized in an inert atmosphere at temperatures 1200 oC.



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Synthesis of characterization of polytungstic acid (PWA)/tetra-sulfonated block copolymer composite membrane for Polymer Electrolyte Membrane Fuel Cell (PEMFC)

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본 연구는 새로운 술폰화된 poly(biphenylsulfone ketone) 블록공중합체를 제조하여 polytungstic acid (PWA)와 혼합 후 이들의 특성들을 분석하여 고찰하였다. 신규 블록공중합체는 다음과 같이 합성하였다. 먼저, 친수성 고분자와 소수성 고분자를 합성하고 이 두 고분자를 몰비율 1 : 1 로 직접 공중합반응을 시킴으로써 새로운 블록공중합체를 합성하였다. 이렇게 합성된 블록공중합체를 PWA 를 중량비를 조절하여 10%, 20%, 30% 컴파지트 블록공중합체를 합성하였다. 합성한 블록코폴리머들은 1H NMR, FT-IR 및 GPC 를 통하여 고분자의 구조분석을 확인하였으며, DMSO 용매를 사용하여 각각 제막하였다. 상용의 Nafion-117 을 비교물질로 하여 열적 안정성을 확인하였는데, TGA 를 측정한 결과, 우수한 열적 안정성을 보여주었으며, 또한 막의 PWA 의 함량이 증가함에 따라 이온교환능력 (IEC)의 증가와 water uptake (물흡수도)의 감소하는 경향을 보여주었다. 30% 컴파지트 블록공중합체의 이온전도도는 90 ℃ 100 %RH 에서 96 mS cm-1 나왔으며, 같은 조건에서 Nafion 117 는 110 mS cm-1 로 측정되었다. 이는 PWA 의 acidic 한 성질로 이온교환채널의 확보를 통해 효과적으로 이온 전도도가 증가되었음 예측할 수 있었다. 따라서 이 고분자는 고분자 전해질 연료전지의 고체 전해질막으로 적용하기에 좋은 대체 물질로서 판단된다.

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Synthesis and characterization of new poly(arylene biphenylsulfone ether) block copolymers containing fluorenylidene unit

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본 연구는 새롭게 디자인하여 제조한 블록 공중합체를 후술폰화를 시켜 이들의 특성을 분석하여 고찰하였다. 블록 공중합체 합성은 다음과 같이 3 단계로 진행하였다. 먼저, 단량체인 4,4'-bis[(4-chlorophenyl) sulfonyl]-1,1-biphenyl 과 4,4'-(9-fluorenylidene) diphenol 을 사용하여 친수성 전구체를 합성한 다음, 단량체 bis(4-chlorophenyl) sulfone 과 4,4'-sulfonyldiphenol 을 사용하여 소수성 올리고머을 합성하였다. 앞에서 합성한 친수성 전구체와 소수성 올리고머를 공중합반응을 시켜 블럭공중합체를 합성하였다. 제조된 블럭공중합체에 chlorosulfuric acid 를 가한 후 실온에서 술폰화를 진행하였다. 블록 공중합체의 술폰화도(degree of sulfonation)는 친수성 올리고머(30%, 50%, 70%)의 비율을 조절함으로써 결정하였다. 합성한 블록 공중합체는 1H-NMR, FT-IR 및 GPC 를 통하여 폴리머의 구조분석을 확인하였으며, TGA 와 DSC 를 이용하여 이들의 열적 안정성을 확인하였다. 후술폰화된 공중합체는 NMP 용매를 사용하여 제막한 후, 이들의 산화 안정성, 물흡수도(water uptake), 이온교환용량(IEC), 양이온 전도도 및 표면 등을 분석하였다.

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Synthesis and characterization of tetrasulfonated block coploymers containing perfluorobiphenylene units

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본 연구에서 우리는 4,4'-bis[(4-chlorophenyl)sulfonyl]-1,1'-biphenyl 단량체에 sulfuric acid 를 첨가하여 술폰화된 단량체로 합성하였다. 이 합성된 단량체와 4,4'-(hexa-fluoroisopropylidene) diphenol 을 사용하여 우선 친수성을 갖는 고분자를 합성하였고, 또한 decafluorobiphenyl 과 4,4'-(hexafluoroisopropylidene) diphenol 을 사용하여 소수성을 갖는 고분자를 합성하였다. 합성된 소수성 고분자와 친수성 고분자는 각 단량체들에 큰 반응성으로 인하여 40000~50000 에 대체적으로 높은 분자량을 갖는 고분자들이 합성되었으며 이를 통해 합성된 블록 공중합체는 100000 이상의 값을 나타내고 있었다. 선술폰화(pre-sulfonation)방법으로 친수성 부분의 비율이 각각 30%, 50%, 70%로 조절함으로써, 세 종류의 새로운 블록 공중합체를 성공적으로 제조하였다. 이들은 DMSO(dimethyl sulfoxide) 용매를 사용하여 각각을 제막하였다. 합성한 블록 공중합체는 4 개 술폰기 단량체 단위를 가진 고분자로써 proton NMR, FT-IR, 및 GPC 분석을 통해 제조된 블록 공중합체의 구조적 특징과 술폰화도를 분석하였으며, TGA 와 DSC 의 열분석 장비로 200 ℃ 이상에서 질량감소가 일어남을 관측함으로써 합성된 물질의 열적 안정성을 확인하였다. 이 밖에도 술폰화도에 따른 이온교환능력 (ion exchange capacity), 물 흡수도 및 양이온 전도도를 확인하였다. Block copolymer 70%에서 가장 높은 값인 129 mS/cm (90 ℃, RH 100%)의 이온 전도도 성능을 얻을 수 있었으며 AFM phase image 를 통하여 합성된 공중합체가 Block copolymer 의 형태로 합성이 잘 되었는지 확인하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-64**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymerization and mechanical properties of elastomer using metallocene catalyst.

정성원

호남석유화학(주) 연구5팀

엘라스토머는 탄성을 가진 고부가가치 제품으로 차량 내부 소재, 충격보강재, 특수 접착제 등에 적용되며 그것의 독특하고 우수한 물성을 바탕으로 기존 소재를 대체할 뿐만 아니라 새로운 소재로 개발할 수 있는 물질이다.이번 연구에서는 당사의 촉매를 이용하여 여러 가지 조건에서 엘라스토머를 중합하였고 GPC, DSC 등의 분석을 통해서 기본 물성을 파악하였다. 또한 현재 양산되는 다른 제품과 비교하여 온도에 따른 Izod 수치, Haze 등의 분석을 통해서 중합품의 물리적인 특성들에 대해 살펴보았다.

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발표코드: **POLY.P-65**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Sensor based on Prussian Blue/ CNT-Graphene Multilayer Electrode for Determination of Hydrogen Peroxide

Yangjiao 이영관 조미숙

성균관대 화학공학과

AbstractElectrochemical sensor based on Prussian blue (PB) and CNT-graphene multilayer electrode was developed for H2O2 determination. CNT-graphene multilayer electrode was prepared by layer-by-layer assembly on ITO-coated glass: alternatively chemical dipping for CNT layer and electrodeposition for graphene layer. PB was deposited on the CNT-graphene multilayer electrode by self assembles technique. The surface morphology of the PB/CNT-graphene modified electrode was characterized by electron scanning microscopy. The PB/CNT-graphene sensor shows high electrochemical activity and excellent stability for H2O2 sensing in a linear dynamic detection range from 0.05 mM ~ 9.5 mM, and its sensitivity was 382.4 μA mM-1 cm-2. It has good selectivity in the presence of electroactive species such as ascorbic acid, dopamine, glucose, and uric acid.Key words: CNT, graphene, hydrogen peroxide, self-assemble

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photovoltaic Properties of Carbonyl-Functionalized Low Band-gap Polymers

Nguyen Thanh Luan 우한영[1]

부산대 나노융합기술학과 [1]부산대 나노기술대학 나노정보소재공학과

Conjugated polymers composed of dialkoxybenzo[1,2-b:4,5-b']dithiophene and thiophene bearing a carbonylalkyl group were designed, synthesized via Stile coupling reaction with high molecular weight (Mn) of 167 kDa for TCDT and 32 kDa for BDTCOT. The carbonylalkyl substituted thiophene with strong electron affinity was used as an electron acceptor group. The large intramolecular charge transfer (ICT) interaction induces a small band gap of the copolymers for large light harvesting ability. BDTCOT and TCDT exhibited low band gap 1.97 eV and 1.85 eV, with the highest occupied molecular orbital (HOMO) of -5.3 eV and -5.25 eV and the lowest unoccupied molecular orbital (LUMO) of -3.33 eV and -3.4 eV, respectively. The blends of these polymers with PCBM showed promising photovoltaic device properties for solar cell applications.

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

Fabrication of Porous Microparticle Scaffolds using Sintering and Centrifuge Methods for Tissue Engineering

김병혁 류동훈 김승범[1] 정영재[2] 이우경[2]

인제대 나노시스템 [1]인제대 나노시스템공학부 [2]인제대 나노공학부

A scaffold which supports structure environment that allows cells to migrate, proliferate and differentiate plays a crucial role in tissue engineering with specific cells, such as stem cells, fibroblasts, and chondrocytes to reconstruct damaged organs. To make a suitable scaffold, it has to have appropriate mechanical properties, as well as porosity, biodegradability and biocompatibility. Our research was conducted to develop scaffolds that have proper porosity, biodegradability, biocompatibility and mechanical properties. PLGA and PEG were used for biodegradability and biocompatibility. To obtain appropriate mechanical properties and porosity, double emulsion-solvent evaporation and solvent sintering-centrifugation methods were employed. The mean porous microparticle diameter and surface pore size were measured by averaging the diameter and pore size of each microparticle using SEM images. The porosity was measured by using Archimedes method. The mean diameter and surface pore size of porous microparticles, made from double emulsion-solvent evaporation method were 17.56 ± 5.89 um and 2.93 ± 1.26 um. After porous microparticles treated with water-miscible solvent in aqueous solution to sinter, the mean diameter of porous microparticles at 80%, 60%, 40% solvent/non-solvent solution (ethanol/water (v/v)) concentrations was 15.75 ± 4.94, 17.11 ± 5.52 and 16.33 ± 4.68 um, respectively, and the mean surface pore size was 1.74 ± 1.11, 2.09 ± 0.78, and 2.81 ± 0.74 um at each concentration. Porosities of scaffolds were 54.32 ± 5.3, 61.70 ± 6.2, 64.50 ± 6.0 % at each concentration, respectively. Sample A treated with 80% solution(ethanol/water) has the strongest mechanical property, although the mechanical properties couldn't be measured by the instrument.

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장소: 부산BEXCO

발표코드: **POLY.P-68**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Glycidyl tetrazolyl polymers(GTePs)

정지혜 신정아 임영권 이경희

국방과학연구소 4-2

Tetrazoles are nitrogen-rich compounds which have great potentials for energetic and pharmaceutical applications. Especially, tetrazole have high heat of formation(237kJ/mol) so it is expected as a good candidate for high energy density material(HEDM). Although molecular tetrazoles have been investigated extensively, the researches about polymer containing tetrazoles are still rare. Glycidyl tetrazolyl polymers(GTePs), polyether containing tetrazole pendants were synthesized by reaction of PECH with various tetrazoles using NaOH in DMSO. The structures of GTePs were confirmed by IR, 1H and 13C NMR spectral analyses. Thermal properties of the GTePs were evaluated using differential scanning calorimetry(DSC).

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발표코드: **POLY.P-69**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Aromatic and Aliphatic linkages of Hyperbranched Polyester Polymers on Thermal Properties in Thermal Printing System

장연임 최원호 안병관

가톨릭대 화학과

A novel class of hyperbranched polyester developers containing phenol groups as linear and terminal units for thermal recording/ printing papers were synthesized by the polycondensation of the controlled ratio of aromatic and aliphatic A2 (bifunctional) monomers with B3 (trifunctional) monomers. The thermal properties and developing properties of these polymers were systematically investigated.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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발표코드: **POLY.P-70**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Sunset Yellow FCF Coatable Polarizer

이상아 이종훈[1] 김대윤 이명훈 정광운[2]

전북대 고분자나노공학과 [1]전북대 유연인쇄전자공학과 [2]전북대 고분자.나노 공학과

Sunset Yellow FCF (H-SY) was self-assembled to oriented anisotropic films. To stabilize the oriented H-SY films and to minimize the possible defects generated during and after the coating, the photo-polymerization of acrylic acid (AA) monomers was carried out. Based on the experimental results of two-dimensional wide angle X-ray diffraction and selected area electron diffraction, H-SY crystalline unit cell was determined to be a monoclinic structure. The polymer-stabilized H-SY films showed good mechanical and chemical stabilities with maintaining a high polarizability. Additionally, patterned polarizers were fabricated by applying a photo-mask during the photo-polymerization of AA, which may open new doors for the practical applications in electro-optic devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2011K000776) of Korean government.

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발표코드: **POLY.P-71**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fullerene Striped Pattern in the Cholesteric Liquid Crystals

이상아 이종훈[1] 김대윤 정광운[2]

전북대 고분자나노공학과 [1]전북대 유연인쇄전자공학과 [2]전북대 고분자.나노 공학과

A fullerene derivative (C60RM) was newly designed and synthesized. Its chemical structure and phase behavior were investigated with combined techniques of microscopy, scattering and spectroscopy. C60RM striped pattern was successfully fabricated in an elastically anisotropic cholesteric liquid crystal medium. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

THE KOREAN CHEMICAL SOCIETY

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장소: 부산BEXCO

발표코드: **POLY.P-72**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

silicone 기반의 가교제를 이용한 에폭시 봉지재 합성

지애라 맹일호 김진권 PIAO LONGHAI

공주대 화학과

LED 봉지재는 LED 의 고출력, 고휘도 제품의 요구와 함께 LED 의 수명과 투과율에 밀접한 관계를 가지고 있어 그 역할이 더욱 중요해지고 있다. 에폭시는 낮은 가격대와 높은 굴절률을 갖추고 있지만 고온에 의한 황변현상으로 투과율이 떨어진다. silicone 은 투명도가 좋고 열안전성이 좋아 각 기업에서 각광받고 있는 봉지재 중 하나이다. 본 연구에서는 silicone 기반의 가교제를 이용하여 에폭시 봉지재를 가교시켰다. 구체적으로 에폭시 group 을 가진 사슬형의 silicone 과 선형 silicone 고분자 전구체를 합성했다. 이것을 silicone 기반의 가교제를 이용하여 가교시키고 투과율, 굴절률, 열안전성을 연구하였다. 이번 연구를 통해 합성된 봉지재는 투과율과 굴절률이 높고 안정적이며 고온에서도 변성되지 않고 안전하다.

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발표코드: **POLY.P-73**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electropun nanofiber containing the self-assembled Sunset-Yellow FCF nanocolumns

이종훈 김대윤[1] 이명훈[1] 정광운[2]

전북대 유연인쇄전자공학과 [1]전북대 고분자나노공학과 [2]전북대 고분자.나노 공학과

Chromonic nanofibers with the self-assembled Sunset-Yellow FCF were successfully fabricated by electrospinning techniques. Based on the thermal, microscopic and scattering experiments, it was realized that Sunset-Yellow FCF molecules formed a glassy columnar nematic (N) phase in the PVP/H-SSY nanofiber. When the PVP/H-SSY nanofiber was annealed above the T_g of PVP, the H-SSY nanocolumns further self-organized to crystals. The anisotropically oriented nanofiber mats embedding assembled nanocolumns may open new doors for the practical applications of the electrospun nanofibers in optical, electronic and electro-optic devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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장소: 부산BEXCO

발표코드: **POLY.P-74**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of dynamic chemical patterns with stimuli-responsive hydrogels

이현진 김도완 백슬기 윤진환

동아대 화학과

In this work, we have developed dynamic chemical patterns with visible-light responsive hydorgels.V visible-light responsive hydrogels can be prepared with temperature-responsive hydrogel incoporating ferrofluid. We have revealed the composite consist of thermal responsive hydrogel and magnetic nanoparticles show reversible volume transition in response to irradiation of visible light. Base on light-responsibility and creasing instability of hydrogel film, we have successfully demonstrated light-induced global or local switching of dynamic pattern. Preparation for spherical beads of various size is also discussed in this work.

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장소: 부산BEXCO

발표코드: **POLY.P-75**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Benzotriazole-Based Donor-Acceptor Type Semiconducting Polymers with Different Alkyl Side Chains for Photovoltaic Devices

김지훈 신원석[1] 강인남[2] 황도훈

부산대 화학과 [1]한국화학연구원 에너지소재연구센터 [2]가톨릭대 화학과

A series of low band gap polymers composed of benzotriazole and benzo[1,2-b:4,5-b’]dithiophene derivatives were synthesized using a Stille cross-coupling reaction for use in organic photovoltaic devices. Linear or branched alkyl groups were incorporated into the benzothiazole-based accepting monomer part, and alkoxy or alkylthiophene groups were introduced to benzo[1,2-b:4,5-b’]dithiophene-based donating monomer part. Changes in photo-physical properties of the polymers by the structural modification of the donor-acceptor type low band gap polymers were investigated. The synthesized polymers were soluble in common organic solvents, and the resulting polymer solutions could be used to form smooth and uniform thin films by spin-casting. The intra-molecular charge transfer interaction between the electron donating and electron accepting blocks in the polymeric backbone induced a broad absorption from 300 to 650 nm. Solution-processed field-effect transistors were fabricated and characterized using the polymers as p-type channel materials. Bulk hetero-junction photovoltaic devices were fabricated using the polymers with [6,6]-phenyl C71-butyric acid methyl ester (PC71BM) as the electron acceptor. One of the fabricated device showed the maximum power conversion efficiency of 3.20 % under AM 1.5 G (100 mW/cm2) conditions.

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장소: 부산BEXCO

발표코드: **POLY.P-76**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Immortal Copolymerization of CO_2/Propylene Oxide and Architecture of Various Block Copolymers.

이정재 이분열

아주대 분자과학기술학과

A highly active and relatively cheap catalyst for CO_2/propylene oxide (PO) copolymerization is developed. It was initially designed on the concept of binding two components or two metal centres, and later it was revealed that the high activity is due to an unusual binding mode of a cobalt(III) complex prepared from a Salen-type ligand tethered by four quaternary ammonium salts. This catalyst displays an excellent catalytic performance even in the presence of a large amount of protic compounds which enables us to efficiently perform "immortal polymerization" in CO_2/propylene oxide copolymerization. Precise control of molecular weight is achieved by feeding various protic compounds, adipic acid. Various three armed and star shaped polymeric structures are demonstrated by simply feeding three armed and four armed carboxylic acids. Respectively, by feeding bulk polymer contains OH or COOH in immortal polymerization, we have demonstratrated block and graft copolymerization. Addtional melting region with slightly higher glass transition temperature is introduced by feeding PE-monoalcohol or PEG. The PPC exhibits favorable properties such as clean incineration, printability, and adhesiveness. When it is processed to a film or sheet, it show good barrier property for both oxygen and water, but mechanically it is easily breakable (brittle). A sheet prepared from PPC-block-PEG of 8.3 w% PEG unit is not as brittle as that of PPC itself. It is flexible and stretchable as the conventional PE film. A sheet prepared from PPC-block-PS of 11 w% PS unit is translucent and tougher than PPC itself. These block copolymers containing ~10 w% common bulk polymer units can supplement demerits of PPC itself.

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발표코드: **POLY.P-77**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal rearrangement of the microporous polyurea molecular networks synthesized by the organic sol-gel method

문수영

광주과학기술원 신소재공학과

The 3D crosslinked polyurea network synthesized via organic sol-gel polymerization was thermally rearranged into polyisocyanurate by trimerization of decomposed isocyanates from urea groups(TAPM/HDI-TR). TAPM/HDI-TR showed high gas adsorption capacity and selectivity against CO2/N2 gas pair owing to removal of hydrogen bonding between urea group and primary amine decomposed from urea group . After thermal rearrangement network indicated structural stability by crosslinking system and thermal stability by isocyanurate moieties. The reversibility of the CO2 adsorption process at 25℃, 1bar by TGA cycling revealed ~6.5 wt% for single gas and ~4.5 wt% for mixed gas (CO2/N2 = 15/85). TAPM/HDI-TR based on solution processable organic sol-gel also can be processed into not only particles but also monolith and it may be applicable to CO2 adsorbent.

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장소: 부산BEXCO

발표코드: **POLY.P-78**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

pH-Sensitive Color Transition of Organic Polymer Films and Optimized Monomers Composition of the Transition

우희정 최미언 도정윤

부산대 화학교육과

수소이온 농도 검출 과정에서 액상 지시제의 시료 오염과 일회성 사용의 단점을 극복하고자 고분자 필름을 사용하였고 지시제의 용출을 막고 재현성 및 재사용을 위하여 지시제가 공유결합된 박막을 개발하고자 하였다. pH 감응 발색단으로 기존의 아조기를 포함한 methyl red(OMR, PMR) 유도체와 phenolphthalein 을 이용하여 고분자필름을 제조하고 특성을 평가하였다. 발색단의 광학적 특성 변화를 최소화하는 아크릴 및 아크릴 아마이드 유도체 제조를 하였다. 친수성 박막을 얻기 위하여 극성 물질로서 acrylic amine, acrylic acid 등을 도입하고 함량을 조절하였고 발색단의 전이 특성과 pH 를 고려하여 최적의 함량과 비율을 결정하였다. 넓은 영역의 pH 변화에 따른 변색을 유도하기 위하여 혼합발색단을 사용하였고 이를 흡수분광분석을 통하여 관찰하였다. 제조된 필름의 특성을 온도 변화, 검출시간, 용매종류 등 다양한 조건에서 비교하였다. 조건에 따른 색상변화의 시각적 효과를 증가시키기 위해 무색의 발색단 구조를 도입하였고 액상과 필름상의 변색 특성을 비교하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-79**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Radiolytical Synthesis of Anion Exchange Membranes with quaternized DABCO Moiety

손준용 고범석 신준화

한국원자력연구원 첨단방사선연구소 공업환경연구부

Anion exchange membranes with DABCO (1,4-diazabicyclo[2,2,2]octane) were synthesized via radiation graft polymerization of vinylbenzyl chloride onto poly(ethylene-alt-tetrafluoroethylene) film and subsequent quaternarization with DABCO. Further modifications were also carried out through quaternarization with trimethylamine and iodomethane. The prepared anion exchange membranes were characterized by FT-IR, TGA, DSC, SEM-EDX, and UTM. Physico-chemical properties such as ion exchange capacity, water uptake, ionic conductivity, and chemical stability were discussed in detail. The results indicate that anion exchange membranes having mono-quaternary ammonium moiety of DABCO are chemically, thermally, and mechanically stable compared to ETFE-g-PVBTMA anion exchange membrane which is frequently synthesized for solid alkaline fuel cell application.

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장소: 부산BEXCO

발표코드: **POLY.P-80**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

고분자를 이용한 유기태양전지 투명전극용 실버 나노와이어 전극의 최적화

조현수 박상혁

공주대 화학과

최근 저비용, 유연성 등의 장점을 가진 유기전자재료에서 다양한 최적화 연구가 진행되고 있다. 현재 널리 사용중인 ITO 전극은 그 전기적 특성은 우수하나 공정 및 원료비가 비싸고 유기전자재료 특유의 유연성을 저해하는 특성을 가지고 있다. 이러한 이유로 ITO 전극의 대체 물질의 연구 및 개발이 활발히 이루어 지고 있다. ITO 를 대신할 새로운 산화 전극으로 연구중인 실버 나노-와이어는 그 전기적 특성이 ITO 에 비해 낮을 뿐만 아니라 전극과 유기전자재료 물질과의 연결이 원활하지 않다. 우리는 실버 나노-와이어와 유기전자재료 사이에 고분자를 코팅하여 유기전자재료 물질과의 연결을 원활하게 하여 기존 실버 나노-와이어 전극에 비해 향상된 성능을 이끌어 낼 수 있음을 확인하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-81**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reversible control of intramolecular crosslinking of molecular brushes

이지은

울산대 화학과

A series of PBIEM-PB-PEGMA molecular brushes was synthesized by ATRP (Atom Transfer Radical Polymerization) of 4-Vinylphenylboronic acid and Di(ethylene glycol) methyl ether methacrylate using PBIEM-Br macroinitiator as an initiator.We started from making the macroinitiator PBIEM-Br by ATRP. Then boronic acid be protected with 1,3-propandiol and we have synthesized brush polymer like this. After polymerization, protection parts of the end of boronic acid were deprotected by DOWEX? resin to recovery hydroxy group. These brushes can be crosslinked intramolecularly by the addition of the crosslinker and recovered to the original state by the change of pH. This process can be reversibly controlled. We characterized the reversible crosslinking behavior by 1H NMR, GPC and AFM.

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장소: 부산BEXCO

발표코드: **POLY.P-82**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of bulk-heterojunction solar cells based on small molecule containing multiphenyl donor and benzo[2,1,3]thiadiazole acceptor

김슬기 박상혁

공주대 화학과

In order to develop high efficiency organic photovoltaic materials that exhibit promising electronic properties, electroactive small molecules have recently received attention as alternatives to polymers. A novel class of donor-acceptor type small molecules for electron donating active layers for bulk-heterojunction solar cells were synthesized and investigated. The thermal, optical and electronic properties of the molecules were examined by themogravimetric analysis (TGA), differential scanning calorimetry (DSC), UV-vis absorption, and cyclic voltammetry (CV). The synthesis, characterization and photovoltaic properties of low band gap small molecules will be discussed.

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장소: 부산BEXCO

발표코드: **POLY.P-83**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and evaluation of novel acceptor-donor-acceptor type conjugated molecules for organic photovoltaics

전수지 박상혁

공주대 화학과

During the last decade, organic semiconductor materials have been developed as a novel class of optoelectronic materials with applications including both light-emitting diodes and photovoltaics. Organic photovoltaics possess many advantages such as light-weight, low cost, facile fabrication for large area, and mechanical flexibility. However, there are still obstacles to achieve high power conversion efficiencies (PCE) because of the mismatch between the solar spectrum and the spectra of organic materials used in active layer. To overcome this absorption limitation, synthesizing new low band gap materials is proposed to improve PCE of organic solar cells. Generally, low band gap molecules consist of D (electron-donating unit) and A (electron-accepting unit) alternative structure. In this work, we have synthesized new low band gap A-D-A type molecules, and their optical and electrochemical properties will be presented along with their application to organic solar cells. The oligomers were characterized by Infrared(IR), Proton nuclear magnetic resonance(H-NMR), elemental analysis(EA), and mass spectra(MS). Their thermal properties were investigated by differential scanning calorimetry(DSC).

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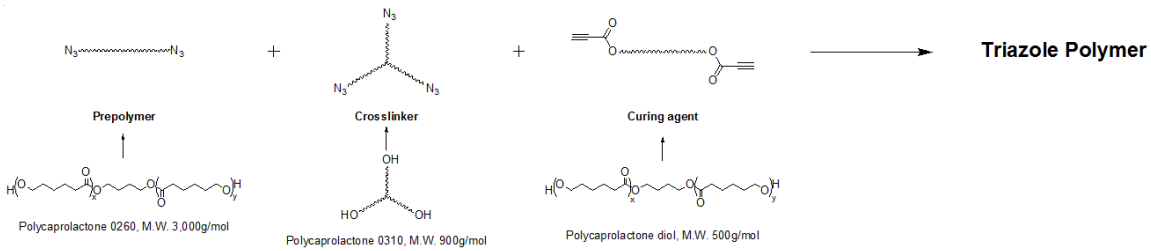
장소: 부산BEXCO
발표코드: **POLY.P-84**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study on the Triazole Crosslinked System from Endcapped Azides and Alkynes

김경태 전홍배 민병선[1]

광운대 화학과 [1]국방과학연구소 1기술연구본부 6부 로켓추진기관부

Recently, a triazole crosslinked system was used for a new solid rocket propellant binder in which azide groups in the polymer react with alkyne groups of a dipolarophile curing agent. In this study, the twelve triazole crosslinked polymers were prepared by the mixing of a diazide prepolymer, a triazide crosslinker and various dipolarophile curatives under C≡C/N_3 equivalent ratio of 1.1, and were degassed in a rotary evaporator during 30 minutes under 55℃. All the mixtures were cured at the oven under 52℃ during 7 days, and the curing reactivity was investigated by the measurement of FT-IR spectra everyday. Among a similar form of dipolarophile curing agent types, using carbonyl group acting as electron withdrawing group is close to triple bonds accelerated the reaction very significantly. This result clearly demonstrate that 1,3-dipolar cycloaddition reaction depends on each chemical structure adjacent to the azide groups and alkyne groups.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-85**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Paraffin wax를 이용한 Phase Change Material 합성

민동진 PIAO LONGHAI

공주대 화학과

Phase Change Material (PCM)이란 고체에서 액체로 변할 때 열을 흡수하고 액체에서 고체로 변할 때는 열을 방출하면서 주변온도의 급격한 변화를 막아주는 물질을 칭한다. Paraffin wax 는 지금까지 알려져 있는 여러 PCM 중에서 상대적으로 상 변화 온도 설정이 가장 용이하고 무기물에 비하여 매우 안정하며 인체에 무해하다는 장점이 있다. 본 연구에서는 paraffin wax 를 이용하여 고분자 중합반응을 통해 gel type 의 PCM 을 합성하였다. 그리고 Differential Scanning Calorimetry (DSC)를 이용하여 잠열을 분석함과 동시에 중합 조성이 PCM 의 성능에 어떤 영향을 미치는가에 대하여 연구하였다.

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장소: 부산BEXCO

발표코드: **POLY.P-86**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Modulus improvement of carbon nanotube reinforced polystyrene nanofiber composite

김한수 신관우[1]

서강대 화학과 [1]서강대 화학과 및 바이오융합과정

Electrospining is one of the attractive methods in order to form well-aligned fibers on the substrates. As-spun fibers are comparatively weak due to the residual solvents which have the low vapor pressure and high boiling point such as Dimethylformamide. In this experiment, however, annealed fibers dried during 1 h at 60℃ have higher modulus than as-spun fibers have. Solvent evaporation was also investigated by Thermal gravimetric analysis. Optimized condition for the Modulus of polystyrene (PS) nanofibers was found by varying concentrations of carbon nanotubes (CNTs) in the PS nanofibers. UV initiator also functions as a reinforcing agent to cause reactions between CNTs in the PS nanofibers by exposing 312 nm wavelengths during 1 h. Modulus of all types of fibers was measured by simple equation and machine by making use of a computerized spring-balance and step-motor setup. Optical microscopy and SEM images were used to measure number and diameter of fibers.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of fluorophore based pH and temperature dependent polymer films

최미언 우희정 도정윤

부산대 화학교육과

A fluorophore is a fluorescent chemical compound that can re-emit light upon light excitation. A conventional fluorophores such as fluorecein and rhodamine contain several combined aromatic groups, or plane or cyclic molecules with several π bonds. The absorbed wavelengths, energy transfer efficiency, and time before emission depend on both the fluorophore structure and its chemical environment, as the molecule in its excited state interacts with surrounding molecules. Emission wavelength and intensity of the fluorophores have been considered for pH, temperature and media detection. We prepared fluorescent polymer films by using acrylic monomers of the fluorophore. Acrylic amine and acrylic acid monomers were introduced for rapid proton transfer into polymer film. The higher content of amine monomer and acid monomer was required for fluorocein and rhodamine analogue, respectively. The content of fluorophore was minimized with less than 5% for stable hydrophilic polymer film. The combinative use of acid and base sensitive fluorophores provides a fluorescent film to be active in a wide pH range. Optical characterization of single and duel fluorophore attatched polymer films is discussed with pH and temperature dependence.

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장소: 부산BEXCO

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface-induced phase transition behaviors of the rod-disc liquid crystal

이종훈 김대윤[1] 이상아[1] 정광운[2]

전북대 유연인쇄전자공학과 [1]전북대 고분자나노공학과 [2]전북대 고분자.나노 공학과

Surface-induced phase transition behaviors of a rod-disc (cyanobiphenyl-triphenyl) liquid crystalline (LC) molecule (RD12) were investigated by changing the surface chemistry and the physical interactions. Upon varying the thickness of the LC cells and their surface chemical and physical conditions, the RD12 phase transition behavior was dramatically changed. The nematic (N) phase of RD12 in the LC cell with a low cell gap and polyimide (PI) rubbed surface could be preserved and the crystallization of RD12 was completely suppressed. Based on the systematic experimental observations, 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 (2012K001428) of Korean government.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent anion chemosensors based on 2-amino-6-nitrobenzothiazole derivatives

최상현 박상혁

공주대 화학과

Fluorescence sensing is a rapidly developing field of research and technology. Its target is nearly the whole world of natural and synthetic compounds being detected in different media including living bodies. The selective recognition of anions by artificial receptors has recently attracted much attention because anions play a role in many chemical and biological processes. Flourescene is an important detection method because of its simplicity and high detection limit. In this study, novel fluorescent anion chemosensors based on 2-amino-6-nitrobenzothiazole derivatives were synthesized. The anion binding properties of them will be investigated by fluorescent method with various anions.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Theta-Shaped and Separation of Branched Polystyrene via Selective Precipitation.

김혜원 정종화[1] 이수경[1]

부산대 기판학과 [1]부산대 고분자공학과

Multicyclic polymers exhibit distinct physical properties, such as lower hydrodynamic volume and radii, reduced viscosity and different glass-transition temperatures. However, due to the synthetic difficulty and separation problem, obtaining pure form of multicyclic polymers remains challenging.In this report, we describe the synthesis three-arm star polystyrene using ATRP and “Click” reaction. After “Click” reaction, theta-shaped and branched polystyrene were simultaneously formed. Prepared theta-shaped and branched polymer can be easily separated by selective precipitation owing to their solubility difference. Separated multicyclic polystyrenes were characterized by GPC, MALDI-TOF MS, 1H NMR and FT IR analysis.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Nile Red-loaded Nanostructures via Protein-Polymer Conjugation

이채연 백현종

부산대 고분자공학과

Polymeric micelles have emerged as a novel promising colloidal carrier for the targeting of poorly water soluble drugs and nanoparticles. Herein we describe a one pot method for encapsulation of Nile Red into micellar aggregates using nickel complexed (nitrilotriacetic acid)-end-functionalized polystyrene (Ni-NTA-PS) and histidine-tagged green fluorescent protein (His-tagged GFP) in water/DMF (DMF 4 vol %). When Ni-NTA-PS and Nile Red dissolved in DMF was added slowly into PBS buffer containing His-tagged GFP, GFP coated micellar aggregates were formed and Nile Reds were encapsulated inside the micellar aggregates at once. The formation of micellar aggregate was confirmed by transmission electron microscopy (TEM) measurement and dynamic light scattering (DLS) study. Encapsulation of Nile Red was confirmed by photoluminescence (PL) spectroscopy and fluorescent microscopy.

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장소: 부산BEXCO

발표코드: **POLY.P-92**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of fluorescent chemosensors for cyanide detection

김승언 박상혁

공주대 화학과

Sensors based on fluorescent molecules appear to be particularly attractive due to simplicity and high detection limit of the in a number of the fluorescence. The development of selective optical signaling systems for anions has received considerable attention for recent few decades due to their important roles in biological and environmental processes. Especially, cyanide is a detrimental anion causing poisoning in biology and environment. In this work, various fluorescent colorimetric sensors based on fluorescent small molecules have been developed to detect cyanide ion.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Thermosensitive Polypeptide Aqueous Solution

정소영 문효정[1] 정병문[1]

이화여대 바이오융합과학과 [1]이화여대 화학나노과학과

A temperature-sensitive biodegradable poly(L-alanine)-based diblock copolymers were synthesized. Polymers were characterized by 1H-NMR, DLS, CD, TEM. Thermal properties were investigated by Rheometer. The number average molecular weights of each block of the triblock copolymers were calculated in the 1H-NMR. The polymer aqueous solutions undergo sol-to-gel transition as the temperature increases and show different modulus depending on the composition and temperature. Based on dynamic light scattering and circular dichroism spectra, the change in size of molecular assemblies and secondary structure of the polypeptide were studied as a function of temperature.

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장소: 부산BEXCO

발표코드: **POLY.P-94**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and characterization of synthetic hydrogel with FG-rich peptides tomimic the nuclear pore complex

류동훈 김병혁 김승범[1] 정영재[2] 이우경[2]

인제대 나노시스템 [1]인제대 나노시스템공학부 [2]인제대 나노공학부

Nuclear pore complexes (NPCs) act as effective and robust gateways between the nucleus and the cytoplasm. NPCs permeability barrier is formed by a meshworkof FG nucleoporin filaments interacting weakly via hydrophobic attraction between FG motifs. FG-rich polymers were synthesized by attaching the FG sequence peptides to the hydrophilic polymer backbone. Used poly(ethyleneimine) (PEI) in this study was synthesized by substitution GFSFG peptide for the side chain of the polymer. Thereby, hydrogel mimicking NPCs can be fabricated. The FG-hydrogel showed the specific permeability.

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장소: 부산BEXCO

발표코드: **POLY.P-95**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Well-Defined 4-Arm Star Polymeric Pigment Dispersants by Atom Transfer Radical Polymerization

김병재 정지혜[1] 정종화 김진구[2] 정기석[3] 백현종

부산대 고분자공학과 [1]국방과학연구소 4-2 [2]이리도스(주) [3]솔베이코리아(주) 신규사업개발팀

Polymeric dispersants have been applied to academic research and various fields of industry, such as paints, inks, CNTs, displays, cosmetics, etc. The chemical structure of polymeric dispersants for pigment is important to improve dispersion stability and prevent aggregation or flocculation of pigment in organic or aqueous solvent system. Polymeric dispersants should contain both anchoring group that interact with pigment surface and stabilizing group that provide entropic stabilization. In this study, we describe the synthesis of 4-arm star polymeric dispersants which containing quaternized (2-dimethylamino)ethyl methacrylate (DMAEMA) and benzyl methacrylate (BzMA) as anchoring group and oligo(ethylene oxide)methyl ether methacrylate (OEOMA) as a stabilizing group by atom transfer radical polymerization (ATRP). The resulted star polymer was characterized by GPC and ^{1}H NMR. We studied dispersibility and dispersion stability by DLS and turbiscan.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-96**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Application of Novel Photoacid Generator Bound Polymer for Electron Beam Lithography Resist

강하나 정진혁 이해원

한양대 화학과

Photoacid generator (PAG) have been widely used as a key component for chemically amplified polymer resist due to its high quality of swelling property and lithographic performance. PAG bound polymer resist has been important issue for solving the problems such as PAG aggregation and acid migration with the use of PAG blended resist. A novel monomer having a triphenylsulfonium salt methylmethacrylate (TPSMA) moiety as a PAG was synthesized and copolymerized with methyl methacylate (MMA) for electron beam lithography. Poly(MMA-TPSMA) were characterized to render high resolution, thermal stability, and sensitivity. These PAG bound polymer successfully applied for fabrication of nanoscale patterns.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-97**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functionalization of Carbon Nanotubes Combining Non-covalent and covalent methods Using Polymeric Dispersant and Quaternization of Amine Group for Introduction to Initiating Sites of Atom Transfer Radical Polymerization

이태헌 김봉수 백현종

부산대 고분자공학과

Carbon nanotubes (CNTs) have unique properties for engineering applications. In this study, CNTs were functionalized through combination of non-covalent and covalent methods. CNTs were dispersed using polymeric dispersants and introduced to initiating site via amine quaternization in dispersants. Poly(2-dimethylamino ethyl methacrylate-*co*-Styrene) (Poly(DMAEMA-*co*-St)) were polymerized via atom transfer radical polymerization (ATRP) , poly(quaternized (2-dimethylamino ethyl methacrylate)-*co*-Styrene) (poly(QDMAEMA-*co*-St)) were prepared by quaternization of poly(DMAEMA-*co*-St) with *p*-(chloromethyl)benzyl 2-bromoisobutylate (BBiB) in order to introduce initiating site for atom transfer radical polymerization (ATRP). The functionalized CNTs were dispersed and observed by transmission electron microscopy (TEM), atomic force microscopy (AFM). Raman spectroscopy was carried out to confirm the defect of functionalized CNTs.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-98**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

고강성 난연 폴리아미드 나노복합재

조영민

호남석유화학(주) 연구3팀

일반적으로 폴리아미드 수지는 내열성 및 기계적 특성이 우수한 엔지니어링 플라스틱으로서 각종 기계 및 전기전자, 자동차 부품용으로 널리 사용되고 있으며 이러한 특성을 바탕으로 무기계 섬유상, 무기분말 등을 첨가하여 강도, 내열성 및 치수 안정성 등을 강화시켜 산업적으로 널리 사용되고 있다. 그러나 폴리아미드 수지는 수분흡수율이 높아 수분이 흡수되었을 경우 강도의 저하는 물론 치수의 변형, 성형 가공상의 문제점들을 야기하며 난연성이 없는 문제점이 있다. 이러한 문제점으로 인하여 각종 기계, 전기전자, 자동차 부품에서 요구되는 물성들, 즉 강성, 치수안정성, 내열성, 난연성 등의 제반 특성들을 충분히 만족시킬 수 없다. 따라서 본 발명은 In-situ 중합법에 의해 유기화된 층상점토화합물이 고분산된 폴리아미드 나노복합재를 이용하여 난연성, 고강성, 치수안정성, 내열성, 성형성, 내흡습성이 우수한 고강성 난연 폴리아미드 나노복합재를 제조하였다. 제조한 고강성 난연 폴리아미드 나노복합재는 ASTM 규격으로 시편을 성형하여 기계적, 열적 특성을 측정하였으며 UL94 규격으로 난연성을 평가하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-99**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SYNTHESIS OF POLY (PROPYLENENE CARBONATE) AND THERMOPLASTIC POLYURETHANES HAVING FLAME RETARDING PROPERTY

KodiyanVarghese Jobi 이분열

아주대 분자과학기술학과

A preparative method for a ?ame-retarding poly(propylene carbonate) (PPC) was demonstrated by employing diphenylphosphinic acid (Ph2P(O)(OH)), phenylphosphonic acid (PhP(O)(OH)2),or phosphoric acid (P(O)(OH)3) as a chain transfer agent in the immortal CO2/propylene oxide copolymerization catalyzed by a highly active catalyst, a cobalt(III) complex of a Salen-type ligand tethered by four quarternary ammonium salts . High turnover frequencies of 10 000?20 000 h-1(700?1300 g-polymer per g-cat?h) were maintained even in the presence of a large amount of the protic chain transfer agent ([?OH]/[Cat], 1600?200). Directly after the copolymerization using PhP(O)(OH)2 as a chain transfer agent, thermoplastic polyurethane (TPU) was formed by adding a stoichiometric amount of toluene-2,4-diisocynate. The TPU also was not in?ammable. Low-molecular-weight poly(propylene carbonate)s bearing ?OH groups at both ends (PPC-diols) are prepared by feeding protic chain-transfer agents (1,2-propanediol, terephthalic acid, 2,6-naphthalenedicarboxylic acid, and phenylphosphonic acid) in the CO2/propylene oxide copolymerization catalyzed by a highly active Salen?Co(III) complex tethered by four quaternary ammonium salts. The generated low-molecular-weight PPC-diols are used in situ for the formation of thermoplastic polyurethanes through subsequent feeding of diisocyanates (4,41-methylenebis(phenyl isocyanate), 1,4-phenylene diisocyanate, and toluene 2,4-diisocyanate). By varying the structure of the fed diisocyanate and chain-transfer agent, the glass transition temperature of the polyurethane can be tuned in the range 40?60 0C. A high glass transition temperature of up to 60 0C, which is 200C higher than that of high-molecular-weight PPC itself (400C), is attained when 2,6-naphthalenedicarboxylic acid (as the chain-transfer agent) and 4,41 -methylenebis(phenyl isocyanate) are employed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-100**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Analysis of dPS-*b*-PEtHA Diblock Copolymer Films using AFM and SIMS

이지혜 강민화[1] 이연희

KIST 특성분석센터 [1]과학기술연합대학원대 나노및바이오표면과학

The microphase separation processes of deuterated polystyrene-*block*-poly(ethyl hexylacrylate) (dPS-*b*-PEtHA) copolymers were investigated using Atomic Force Microscopy (AFM) and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS). A series of the diblock copolymers were prepared by spin coating from toluene solutions onto a silicon substrate (2000 rpm for 60 s). The different molecular weight copolymer films were produced with thickness and different annealing conditions. Surface pattern formation and the film thickness were observed by using AFM. TOF-SIMS depth profiling was obtained for the lamellar morphology of symmetric dPS-*b*-PEtHA which is found to orient parallel to the surface of the substrate. Elemental and molecular depth profiles measured in the negative ion mode by a Cs+ primary ion beam demonstrate variations in hydrogen, deuterium, carbon, oxygen, hydrocarbons and deuterated hydrocarbons within the diblock copolymer according to the depth.

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장소: 부산BEXCO

발표코드: **POLY.P-101**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Polystyrene Nanoparticles Containing Copper Phthalocyanine

정종화 이윤정 김병재 김진구[1] 정기석[2] 백현종

부산대 고분자공학과 [1]이리도스(주) [2]솔베이코리아(주) 신규사업개발팀

Metallophthalocyanines (MPc) have two-dimensional and 18 π electrons conjugated structure. Due to their optical and electrical properties, MPcs have attracted in numerous applications. Even with vast application, they are hardly soluble in organic solvents from their strong π-π interactions. However, the combination of MPc and polymer gives not only solubility in organic solvent but also a variety of choice of monomers that could be changed according to its applications. In this study, copolymers having phthalonitrile groups were synthesized via RAFT polymerization. Polystyrene nanoparticles containing copper phthalocyanines were prepared by cyclotetramerization of phthalonitrile groups on precursor copolymers at diluted condition. The formation of CuPc from the precursor copolymers was confirmed using UV/Vis. spectroscopy. The shape of polymeric phthalocyanine nanoparticles was observed by TEM and AFM. And their size was measured using DLS.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-102**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermosensitive poly(N-isopropylacrylamide-co-acrylic acid) nanogel and gold nano rod complex containing photosensitiezer for cancer therapy

정영재 류동훈[1] 김병혁[1] 김승범[2] 윤일[3] 이우경

인제대 나노공학부 [1]인제대 나노시스템 [2]인제대 나노시스템공학부 [3]인제대 PDT 연구소

Thermosensitive poly(N-isopropylacrylamide-co-acrylic acid) nanogels were prepared by emulsion polymerization. Gold nano rods which show the maximum absorption wavelength at 750nm were fabricated by electrochemical synthesis method. Gold nano rods and photosensitizer were incorporated into the prepared nanogels by incubating in water for 1 days at room temperature. LCST of the nanogel was measured by UV-vis spectroscopy. The nanogels became clear under LCST and cloud above LCST. The nanogels containing photosensitizer and gold nano rods also demonstrated similar results as the nanogels without photosensitizer and gold nano rods. This nanogels seem to be a promising drug delivery carrier that is effective for cancer therapy.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-103**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photovoltaic Efficiency Enhancement by the Generation of Embedded Silica Passivation Layer along the P3HT/PCBM Interface Using an Asymmetric Block Copolymer Additive

한민구 박지웅

광주과학기술원 신소재공학과

We report a novel concept enabling the generation of an embedded passivation layer along the 3-dimensionally intertwined interfaces between the nanoscopic domains of P3HT and PCBM in the polymer bulk hetero-junction solar cells. We used an asymmetric block copolymer of a P3HT block and a short tail. The tail blocks are segregated in the interfacial region of nanoscopic donor/acceptor domains and thermally transformed to a layer containing silica-like residues of sub-nanometer thickness. The additional interfacial thin layer generated in this way was shown to act perfectly as a block layer effectively depressing the recombination of charge carriers, affording 50~100 % enhancement of the power conversion efficiency over he devices without the copolymer.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **POLY.P-104**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dye/Peroxalate Aggregated Nanoparticles with Enhanced and Tunable Chemiluminescence for Biomedical Imaging of Hydrogen Peroxide

이용덕 김세훈[1]

경희대 화학과 [1]KIST 의과학연구센터

Hydrogen peroxide (H2O2) is an endogenous molecule that plays diverse physiological and pathological roles in living systems. Here we report multimolecule integrated nanoprobes with the enhanced chemiluminescence (CL) response to H2O2 that is produced in cells and in vivo. This approach is based on the nanoscopic coaggregation of a dye exhibiting aggregation-enhanced fluorescence (AEF) with a H2O2-responsive peroxalate that can convert chemical reaction energy into electronic excitation. The coaggregated CL nanoparticles (FPOA NPs) with an average size of～20 nm were formulated by aqueous self-assembly of a ternary mixture of a surfactant (Pluronic F-127) and concentrated hydrophobic dye/peroxalte payloads. Spectroscopic studies manifest that FPOA NPs as a reagent-concentrated nanoreactor possess the signal enhancement effect by AEF, as well as the optimized efficiencies for H2O2 peroxalate reaction and subsequent intraparticle energy transfer to the dye aggregates, to yield greatly enhanced CL generation with a prolonged lifetime. It is shown that the enhanced CL signal thereby is capable of detecting intracellular H2O2 overproduced during immune response. We also demonstrate that the densely integrated nature of FPOA NPs facilitates further intraparticle CL energy transfer to a lowenergy dopant to red shift the spectrum toward the biologically more transparent optical window, which enables the high-sensitivity in vivo visualization of H2O2 associated with early stage inflammation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-105**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

PHOTOSWICHABLE FLUORESCENT POLYMER NANOPARTICLES FOR BIOIMAGING

정근수 이용덕[1] 박솔지[2] 김세훈[3] 박종래

서울대 재료공학부 [1]경희대 화학과 [2]경희대 이학부/화학과 [3]KIST 의과학연구센터

A number of fluorescent nanoprobes have been reported to achieve high resolution bioimaging. We have developed a new type of fluorescent organic nanoparticles composed of densely integrated conjugated polymers and a diarylethene derivative. The nanoparticles were prepared via colloidal in situ polymerization in aqueous micelles containing highly concentrated photochromic molecules. By varying the monomer structure, the fluorescence color of the nanoparticles was readily tuned from visible to near-IR which is the spectra range favorable for bioimaging. Regardless of color, the fluorescence signal was stably and reversibly switched on and off by the irradiation of UV/visible light, through the effective nanoscopic energy transfer. Reversible photoswitching of in vivo fluorescence imaging demonstrate the potential of the rationally designed hybrid organic nanoparticles for advanced bioimaging applications.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-106**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of *watermelon-shaped* Polystyrene via ATRP and "Click Chemistry"

이수경 정종화 김혜원[1] 전홍배[2] 백현종

부산대 고분자공학과 [1]부산대 기판학과 [2]광운대 화학과

Synthesis of cyclic polymers has recently been attracting attention because cyclic structures are possible to have unprecedented properties such as high glass-transition temperatures and lower hydrodynamic volume. However, due to the synthetic difficulty and separation problem, synthesis of multicyclic polymers remains challenge. To overcome these problems, ATRP and “Click” reaction are introduced to synthesis of multicyclic polymers. “Click” reaction is highly efficient in cyclization of polymer due to high reactivity and low possibility to side reactions. Selective fractionation was used to separate cyclic and branched polymer. In this study, *watermelon-shaped* and *branched* polystyrene were synthesized simultaneously by intermolecular “Click” reaction between an azido-terminated polystyrene (*star*-PS-N_3)$_6$ and 6-alkynyl coupling agent in diluted solution. The structure of separated watermelon-shaped polystyrene was determined by MALDI-TOF MS, ^{1}H NMR and FT-IR.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-107**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyethylene imine-based Nanoparticles for Drug Delivery and Bioimaging

박솔지 정근수[1] 김세훈[2] 박종래[1]

경희대 이학부/화학과 [1]서울대 재료공학부 [2]KIST 의과학연구센터

The uses of therapeutic molecules are limited by the lack of selectivity to malignant cells, and cationic polymers with positive charge are considered as a promising category due to their strong cellular interaction resulting good cellular uptake. Therefore, polyethylene imine (PEI)-based nanoparticles with positively charged surface have been suggested as a nano-platform for effective drug delivery. Here we prepared hydrophobically modified PEI for an effective drug carrier by direct conjugation of octadecane bromide to the backbone of PEI, followed by preparation of PEI nanoparticles with hydrophobic core and positively charged surface in aqueous media. Further, the surface properties of positively charged PEI nanoparticles were readily modified with polyethylene glycol (PEG), a neutral and biocompatible polymer, to control the surface properties. All the nanoparticles were labeled with Cy5.5, a near-infrared fluorescent (NIRF) dye, and loaded with green fluorescent dyes as a model drug. Efficient cellular and in vivo tumor imaging with surface-controlled PEI nanoparticles demonstrate that the PEI nanoparticles hold great potential for drug delivery.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-108**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyelectrolyte multilayers onto the gold nanoparticle to control the release rate of photosensitizer

김승범 류동훈[1] 김병혁[1] 정영재[2] 이우경[2]

인제대 나노시스템공학부 [1]인제대 나노시스템 [2]인제대 나노공학부

Recent studies have shown that GNPs accumulated in tumor sites and could produce heat and selectively ablate tumors by absorbing externally applied NIR light. In this study, photosensitizers were complexed with GNP to enhance the effect of anticancer therapy. Photosensitizers(PS) with (+) charge were prepared and incorporated into GNP multilayer complex by the layer-by-layer preparation method using poly(styrene sulfonate)(PSS) as negative polymer layer and PS as positive layer. Each layer by layer coating step was characterized with UV?vis, FTIR spectroscopies, and Zeta potential measurements. The complexes had spherical morphology and showed larger size and higher drug contents with increasing polyelectrolyte layers. More studies such as in vitro release test and in vitro cell viability test need to be investigated to evaluate the ability of complexs to carry a PS and biocompatibility.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **POLY.P-109**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of a Photo-cleavable PS-PMMA Block Copolymer Using a Bifunctional Living Radical Polymerization Initiator Bearing an ortho-Nitrobenzyl (ONB) Group

문봉진 이정현[1]

서강대 화학과 [1]서강대 화학

These days, block copolymers are finding more values in fabricating nano-scale devices because the patterns and dimension derived from the block copolymer template can be easily and precisely controlled by varying the block size and polymer architecture. When a photo-cleavable group is introduced to the block copolymer, the resulting polymer provides greater potential in such applications because the selective removal of one domain after the self-assembly becomes much easier by simple light irradiation, which is otherwise quite challenging process. In this presentation, we have designed and synthesized a new photo-cleavable initiator that has two-orthogonal initiating groups. The initiator is based on a photo-cleavable ortho-nitrobenzyl (ONB) group and bears both ATRP- and NMRP-initiation sites. Introduction of an ONB group to the initiator enables us to obtain a photo-cleavable copolymer. Using the initiator, two kinds of living radical polymerizations, NMRP and ATRP, have been performed to give PS-ONB-PMMA with low polydispersity. Since ONB groups would be located at the interface of PMMA and PS, it will enable us to achieve selective cleavage and removal of PMMA by UV irradiation followed by rinsing with selective solvent. The resulting porous polystyrene membrane will have large surface area and can be applied in various fields.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **POLY.P-110**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of counter ions on drying patterns of partially neutralized poly(styrene-ran-methacrylic acid) ionomers

유정아 김준섭[1] 고광환[2]

조선대 과학교육학부(화학) [1]조선대 응용화학소재공학과 [2]조선대 첨단부품소재공학과

In previous paper we reported that the micro morphology of dried thin films of randomly copolymerized poly(styrene-ran-methacrylic acid: PSMA). The morphology was depended on the mol% of methacrylic acid(MA) and degree of neutralization of MA as well as solvent[1]. We also found the dried film showed cracks with wavy Y shape, Y and T mixtures, and T shape depending on mol% of MA and the degree of neutralization[2]. To investigate further, mathacrylic acid groups in PSMA were neutralized with $Ca(OH)_2$ as well as NaOH. The copolymers were dissolved in DMF, and solutions were placed on slide glasses and dried. According to SEM images, aggregates of PSMA-Na are directed radially outward along the substrates surface, while those of PSMA-Ca are directed inward to the center of the drop. The closer look of the deposition structures vary depending on the counter cation, MA mol% and the degree of neutralization.1) Jeong-A Yu, Yu-Ri Park, and Joon-Seop Kim Journal of Nanoscience and Nanotechnology 2010, 10, 3586-3589.2) Jeong-A Yu, Kwang-Hwan Ko and Joon-Seop Kim2010 International Chemical Congress of Pacific Basin Societies 2010, TECH-109.In previous paper we reported that the micro morphology of dried thin films of randomly copolymerized poly

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

납이온만을 선택적으로 감지하는 펩타이드를 이용한 바이오센서 개발

한유정 조미숙 Su Wenqiong 이영관

성균관대 화학공학과

본 연구에서는 납이온만을 선택적으로 감지하는 펩타이드를 이용하여 전기화학적 센서를 개발하였다. 펩타이드는 Thr-Asn-Thr-Leu-Ser-Asn-Asn 와 같은 아민기로 구성되어 있다. 금 전극을 mercapto propionic acid (MPA)용액에 담가 자기조립법으로 전극상에 MPA 층을 형성하였다. 펩타이드의 NH2 기와 MPA 의 COOH 기가 결합하여 펩타이드가 MPA/Au 전극상에 고정되었다. 전극의 개질화 단계는 [Fe(CN)6]3/4-의 존재 하에 전기화학적 임피더스(electrochemical impedance spectroscopy, EIS)로 확인하였다. 제작한 peptide/MPA/Au 전극으로 네모파 전압전류법(square wave voltammetry, SWV)을 이용한 분석으로 다양한 농도의 납이온을 검출하였다. 개발한 센서의 납이온 감지범위는 10 nM?1?M 이고 민감도는 0.027μAnM-1cm-2 이다. 다른 중금속 이온들 중에서 peptide/MPA/Au 센서는 탁월한 선택도를 보였다. 본 센서는 식수 또는 혈액내의 납이온 검출에 이용 가능성을 제시한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Hyperbranched Polyester Materials for Thermal Printing System

최원호 장연임 안병관

가톨릭대 화학과

A novel class of hyperbranched polyesters with phenol groups as linear and terminal units which react with leuco dyes for a coloring process in thermal recording/ printing system were synthesized and their hyperbranched structure was characterized by ^{1}H-NMR spectroscopy. The reaction properties of leuco dye with these developer polymers were investigated and compared with a conventional developer material, bisphenol A (BPA).

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발표코드: **POLY.P-113**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of graphene oxide and graphene/chitosan composite materials and their properties

박규한

단국대 나노바이오의과학

Abstract 키토산은 다당체의 일종으로 키틴의 탈아세틸화에 의해 제조되며 생체적합성, 항미생물성, 생분해성 및 금속이온 흡착능 등의 기능성이 밝혀짐에 따라서 섬유고분자 산업, 의공학, 기술 분야에서 시작하여 이에 대한 연구도 국내외적으로 활발하게 진행되고 있다. 또한 그래핀은 열적, 전기적, 기계적 특성이 좋아 탄소나노튜브만큼 많은 영역에서 그 응용을 기대하고 있으며 약물전달체에 응용한 한 예로써 새롭게 부각되고 있다.본 연구에서는 수용성 키토산 나노입자의 제조, 특성 및 그래핀과 복합재료의 특성에 대하여 알아보고자 하였다. 먼저 Hummer 방법에 따라 산화그래핀 (GO)을 제조하고 다시 GO 를 하이드라진으로 환원하여 그래핀을 제조하였으며 키토산을 알라닌 NCA 와 그라프트 공중합시켜 수용성 키토산 공중합체(Cts-NCA?L-Ala)를 각각 얻었다. 제조한 샘플은 FT-IR, XRD, DSC, NMR, SEM 등을 이용하여 확인하였다. GO 의 비율은 키토산 공중합체의 각각 1%와 3%(w/w) 사용하였으며 글리옥살을 이용하여 가교된 Cts-NCA?L-Ala/GO 복합재료 필름을 제조하였다. 또한 RGO 의 경우는 상기와 동일하고 Cts-NCA?L-Ala 와 글리옥살로 가교시킨 필름을 그 위에 0.1, 0.5, 1%, 3%(w/w) 를 다시 코팅하였다. 가교된 Cts-NCA?L-Ala/GO 및 Cts-NCA?L-Ala/RGO 복합필름의 인장강도, 전기전도성, DSC, 수분 흡습성 및 생분해성를 비교분석 측정하였다.

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발표코드: **IND.P-114**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

CO_2absorption using aqueous hydrazines and hydrazides.

정태영 이은옥 김영준

충남대 화학과

The absorption of CO_2 into the aqueous hydrazines and hydrazides was studied by using vapor-liquid equilibrium(VLE) apparatus at 333K. The results show that the CO_2absorption rate of aqueous hydrazine monohydrate was 1.5 times faster than that of aqueous monoethanolamine(MEA). The CO_2 absorption capacity of aqueous hydrazine monohydrate and alkylhydrazines was similar to that of aqueous MEA. The CO_2 absorption rate of aqueous hydrazides was very slow and the CO_2 absorption capacity was smaller than that of aqueous MEA.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study of Calcium Binding Properties of Polyacrylic Acid and Acrylate Copolymers.

최민배 김세미[1] 빈혜선[1] 박종목[1] 이병민[1] 강호철[1]

한국화학연구원, 충북대 공업화학과 [1]한국화학연구원

Conventional chelating agents such as EDTA(Ethylenediaminetetraacetic acid) and phosphates cause environmental problem such as eutrophication, because these materials are containing nitrogen or phosphorus. In order to overcome environmental problem, polyacrylic acid derivatives has been synthesized. The average molecular weight of the polymer was controlled from 1,800 to 64,000 and analyzed by GPC. In order to increase calcium binding capacity, various acrylate copolymers containing acrylic acid, maleic anhydride, mono-alkyl maleate, nonylphenol and/or taurine has been synthesized. Calcium binding capacity of polyacrylic acid derivatives and acrylate copolymers has been studied by calcium selective ion electrode. As a result, calcium binding capacity of synthesized acrylate copolymers are very higher than traditional chelant such as EDTA, TPP and NTA.

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장소: 부산BEXCO

발표코드: **IND.P-116**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synergistic Solvent Extraction of Europium and Yttrium with Fatty Acid and Crown Ether.

김세미 이은수[1] 빈혜선[1] 김정훈[1] 허남호[2] 강호철[1]

한국화학연구원, 경북대 응용화학과 [1]한국화학연구원 [2]경북대 응용화학과

The separation of europium and yttrium have been carried out by using various fatty acid with different carbon chain length. On the basis of experimental data, the recovery of europium is 60% and that of yttrium is 3% when 0.2M tetradecanoic acid is used as extractant under the optimized condition. In order to improve the separation of europium and yttrium, crown ether and PEG have been used as additive. The study for synergistic effect of extraction has been studied with several experimental condition, ⅰ)pH, ⅱ)concentration of additive, ⅲ)fatty acid.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The reactions of sorbiol to isosorbide by using various acid catalysts.

빈혜선 김세미[1] 이은수[1] 최민배[1] 강호철[1]

한국화학연구원, 과학기술연합대학원대 [1]한국화학연구원

Isosorbide derived from biomass is important for the industrial raw material. And it is produced through dehydration of sorbitol by using acid catalyst. We have compared the processes in presence of acid catalyst by changing various parameters such as catalyst, catalyst concentration, solvent and reaction temperatures. As the results of the experiments using heterogeneous catalysts, the selectivity of isosorbide is 84.2% when we use sulfated copper oxide calcined at 650℃. And the selectivity of sorbitan is 68.7% when we use zirconium oxide at 170℃.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Multiple Gold Nanoparticles- or Gold Nanoclusters-Doped Silica Nanoparticles

박준성 장민훈 유효종[1]

한림대 화학과 [1]한림대 자연과학대학 화학과

Multiple gold core@silica shell nanoparticles (Multi Au@SiO_2 NPs) were successfully synthesized through a reverse (water-in-oil) microemulsion method. The microemulsion was prepared by mixing a surfactant (Brij35), co-surfactant, organic solvent, and water. Multiple gold nanoparticles with a maximum diameter of 2 nm were doped into a silica matrix during the growth process. Control of the diameters of the gold nanoparticles within the silica matrix was achieved by varying the amount of cationic gold precursors. The size of the Multi Au@SiO_2 NPs was also controlled in the reverse microemulsion process employing Brij35 by varying the water to Brij35 ratio. This is a novel and simple synthetic approach for generating hybrid gold-silica nanomaterials by doping multiple gold nanoparticles into a silica matrix. We also present the incorporation of gold 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.

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발표코드: **IND.P-119**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of efficient mixed host system for deep blue phosphorescent organic light emitting devices

위경량 김성관 강상욱

고려대 소재화학과

We report on the systematic investigation of the relationship between hole mobility of host materials and device performance to maximize the power efficiency. Three different materials with different hole mobility were used as host materials of iridium(III)[bis(4,6-difluorophenyl)pyridinato-N,C2′]tetrakis(1-pyrazolyl)borate (FIr6) based deep blue phosphorescent organic light-emitting device (PHOELD). Host material, tris(4-(N-carbazolyl)phenyl)methylsilane (MCBP), with higher hole mobility (1.1 × 10?3 cm2 V?1 s?1), can accommodate more electron current carried by an n-type host, bis(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)dimethylsilane (SiTAZ), than the other p-type hosts with lower hole mobility, maintaining the charge balance between hole and electron current. As a result, the optimized device shows high external quantum efficiency (EQE) of 19.0%, high power efficiency of 23.5 lm/W, low efficiency roll off, and deep blue color coordinates of (0.15, 0.23).

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

Hydrogen storage system based on dehydrogenation of metal hydride: The effect of Pd nanoparticles on the decomposition of borohydrides in homogeneous solution

김성관 윤창원[1] 강상욱

고려대 소재화학과 [1]KIST 연료전지센터

Complex hydrides such as borohydrides (BH4?) attracted considerable attention due to their high storage capacities. Among them, LiBH4 with a high theoretical storage capacity of 18.5 wt.% of H2, has been considered as a good candidate for on-board applications. However, extraction of hydrogen from LiBH4 suffers due to the onset temperature of LiBH4 decomposition of ca. 400 °C and only half of the hydrogen being released below 600 °C. Consequently, recent research has focused on the catalyzed dehydrogenation of borohydrides (BH4?) in order to lower the H2 evolution temperature and to increase the hydrogen desorption capacity. This is mainly due to the various complicated interactions involved in the solid state reactions in general: e.g. (a) chemical reactions of reactants and catalyst; (b) physical interactions in the solid state transformations, such as nucleation and growth, phase transformation and diffusion of molecules and atoms.In the present study we carried out the reactions under the homogeneous condition in solution phase. Tetraglyme (TG) was used as a solution matrix for homogeneous dehydrogenation because of its high boiling point (270 °C), the thermal stability and the solubility of borohyrides. We show the pressure change upon heating of LiBH4 solutions without additives. While the solid LiBH4 exhibits an decomposition at 400 °C, the onset temperatures of LiBH4 in TG are 250 °C. However, the molar ratio of released H2 to starting LiBH4 is about 3.4:1, which is larger than the nominal ratio (1.5:1). We attributed the excessive hydrogen to the side reaction of NaH or Al with the TG solvent.It is known that a transition metal species enhances the dehydrogenation of LiBH4 in solid state. We carried out the dehydrogenation in solution in order to examine if the palladium nanoparticles (PdNPs) enhances the reaction under homogeneous condition as in solid state. The results show that the PdNPs enhances the reaction in solution, the onset temperature of LiBH4 with PdNPs in TG

is 220 °C. One and two-dimensional solid-state 11B-NMR spectra of the LiBH4 spent fuel (LiBHx) sorted out all non-equivalent boron sites and classified them into B3 (SP2)and B4 (SP3) borons and the SP2 boron sites are rather similar to SP2 boron of B-O coordination. In addition, there are significant amount of organic species co-precipitated with LiBHx.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Practical hydrogen storage system based on dehydrogenation of ammonia borane for fuel cell unmanned aerial vehicles (FCUAV)

김성관 윤창원[1] 강상욱

고려대 소재화학과 [1]KIST 연료전지센터

On-board hydrogen storage system with a 5.5 total system-wt% which enables a 300 mile driving range will be a milestone for the realization of a hydrogen economy. Various hydrogen storage materials have been proposed, and developed to meet the corresponding material based gravimetric target, 9 material weight percent H2 released (mat-wt% H2) which are mapped to the DOE (U.S. Department of Energy) technical targets. Among potential storage materials, ammonia borane (NH3BH3, AB) seems to be the most promising one by virtue of its high gravimetric hydrogen storage capacity, 19.6 wt%. To achieve the storage capacity over 9 mat-wt% H2, AB solid or semi-solid state is suggested to be the best option and it will likely be necessary to develop heterogenous catalyst system to come along. Here, we report the tetraglyme (TG)-mediated, size-controlled synthesis of Palladium nanoparticles (PdNPs). Those PdNPs were easily redispersed in a minimum amount of TG with AB and shown to be highly active catalysts for AB dehydrogenation. Most importantly, TG-mediated PdNPs were applied for the generation of H2 from AB/TG semi-solid state system, and recorded high hydrogen storage system {10.01 mat-wt % H2 [mat-wt % H2 = H2-wt/(AB+TG+PdNPs-wts)]} completing hydrogen release in 30 min at 80 ?C.

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

Nano-emulsification of Pseudo-ceramide through Co-assembly with Glycolipid Biosurfactants

김민경 정은선

한양대 응용화학과

It has been known that ceramide molecules in the stratum corneum layer form a thin lipid membrane with other biocomponents, including lipids, cholesterol, and free fatty acids. This membrane, which is either parallel or curved, plays an essential role in fulfilling epidermal barrier function by protecting trans-epidermal water loss as well as influx of environmental irritants. However, in usual complex formulations, ceramide molecules display strong intermolecular attractions, thus leading to serious phase separation from the system. This unique behavior of ceramide hampers much wider application in industry. This study introduces a robust and straightforward method for fabrication of stable pseudo-ceramide nanoparticles through co-assembling with a biosurfactant. The biosurfactant considered in this study is the mannosylerythritol lipid. It has a unique molecular structure consisting of a mannosylerythritol as a hydrophilic part and two alkyl chains with different number of carbons as hydrophobic moieties. We have found that this biosurfactant can assemble with pseudo-ceramide molecules due to the hydrophobic attraction, while its asymmetric molecular geometry disturbs formation of perfect lamellar structure of ceramide molecules. This allows us to obtain a very fine dispersion of ceramide nanoparticles in water. We show how our biosurfactant affects ceramide nano-particulation by observing phase miscibility, particle morphology, and suspension stability.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SAPO-34 분자체의 합성 및 부탄올 탈수 반응

전종원 정성화

경북대 화학과

다양한 입자 크기를 갖는 SAPO-34 분자체를 마이크로파와 전기 가열 방법으로 합성하였다. 또한 카본 블랙을 주형물질로 활용하여 메조 세공을 갖는 SAPO-34 분자체도 합성하였다. 이러한 SAPO-34 분자체는 질소 흡착, 수분 흡착, XRD 및 전자현미경으로 특성을 조사하였다. 이들은 부탄올의 탈수 반응에 의한 부텐 제조에 적용되었으며 특히 촉매 수명에 미치는 입자 크기, 메조 세공 및 친수/소수성의 효과에 대해 조사하였다. 본 발표에서는 이러한 SAPO-34 분자체의 합성, 특성연구 및 부탄올 전환 반응에 대해 설명할 것이다.

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발표코드: **IND.P-124**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Porous iron-benzenetrycarboxylate (MIL-100-Fe) loaded with Cu+ species: A new adsorbent for thiophenes in liquid fuel

Nazmul Abedin Khan 정성화

경북대 화학과

Removal of sulfur-containing compounds from fuels like diesel and gasoline to a low level before utilization has become a great challenge [1]. MIL-100-Fe, one of the typical metal-organic frameworks [2, 3], has been used for the first time as support materials for Cu+ species, which were obtained from one-step synthesis of Cu2O particles at low temperature. The Cu+-loaded MOFs were evaluated as efficient adsorbents for the liquid-phase adsorption of benzothiophene (BT) [4]. The effect of Cu+ loading on the adsorption kinetics and maximum adsorption capacity (Q0) for the adsorption of BT was also studied. The maximum adsorption capacity (Q0) increased with increasing copper loading up to a Cu/Fe (wt./wt.) ratio of 0.07 in Cu+-loaded-MIL-100-Fe, resulting in an increase in the Q0 by 14% compared with the virgin MIL-100-Fe without Cu+ ions. Since the surface area and pore volume decrease with the loading of copper, the increased Q0 over the Cu+-loaded MIL-100-Fe adsorbents suggests specific favorable interactions (probably by π-complexation) between Cu+ and BT. Acknowledgement 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 (grant number 2012004528). References[1]V.C. Srivastava, RSC. Adv. 2 (2012) 759. [2]G. F?rey, Chem. Soc. Rev. 37 (2008)191.[3] P. Horcajada, S. Surbl?, C. Serre, D.-Y. Hong,Y. -K. Seo, J.-S. Chang, J. -M. Gren?che, I. Margiolakid, G. F?rey, Chem. Commun. 27 (2007) 2820.[4] N.A. Khan, S.H. Jhung, J. Hazard. Mater. (2012) in press; DOI: 10.1016/j.jhazmat.2012.08.025.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-125**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Liquid-phase dehydration of 1-phenylethanol to styrene over sulfonated D-glucose catalyst

HASAN ZUBAIR 정성화[1]

경북대 대학원 화학과 [1]경북대 화학과

Styrene is a very important raw material in the modern chemical industry since this chemical is widely used in the production of various polymers, copolymers, synthetic rubbers, plastics and resins, etc [1, 2]. In this study, carbon-based solid acid catalysts were prepared from renewable resources like D-glucose which were utilized for the dehydration of 1-phenylethanol to produce styrene for the ?rst time. The catalysts were prepared facilely in one-step where carbonization and sulfonation were done simultaneously in one-pot synthesis. The carbon-based catalyst showed 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 [2].Acknowledgement This study was supported by a grant (B551179-10-03-00) from the cooperative R&D Program funded by the Korea Research Council Industrial Science and Technology, Republic of Korea. References[1]J.A. Maci?-Agull?, D. Cazorla-Amor?s, A. Linares-Solano, U. Wild, D.S. Su, R. Schl?gl, Catal. Today 102?103 (2005) 248?253.[2] Z. Hasan, J.-S. Hwang, S.H. Jhung, Catal.Commun.26 (2012) 30?33.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-126**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Purification of MFB from industrial waste to available high-value green resources and synthesis of OB-1 from MFB

함미정 김기림 **Dagvajantsan Oyunerd** 김석찬

국민대 화학과

MFB is a by-product generated from process of DMT, base material PET. The quantity of PET is getting increased every year. MFB which is a by-product of DMT is getting increased , too. About MFB mixture waste of 70~80% is produced, 2,000 MT/year. Currently, MFB is no place to apply. Many companies Which produce DMT are dealing with MFB, is collected MFB and incinerated by the service. This kind of incineration has some problems such as odor, lots of CO2 and cost and it leads to environmental pollution. And we synthesize to high-value green resources, OB-1(optical brightner), using by MFB.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-127**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of ether group on the electrochemical stability of zwitterionicimidazolium compounds

김희환

경희대 화학과

The cathodic stability of the zwitterionic imidazolium compounds was significantly enhanced by the introduction of an ether group at 1 or 2-position on the imidazolium ring. The cycle performance tests showed that the initial cell capacity was maintained almost unchanged up to 100 cycles at 0.5 and 1 C when 2.5 wt.% of 2-butoxymethyl-1-methylimidazolium-3-propylsulfonate or 2-butoxymethyl-1-butylimidazolium- 3-propylsulfonate was added to the model electrolyte (1 M LiPF6 in ethylene carbonate, dimethyl carbonate and ethylmethyl carbonate (1/1/1 v/v/v)). Structures of zwitterionic compounds and their interactions with lithium ions were theoretically investigated.

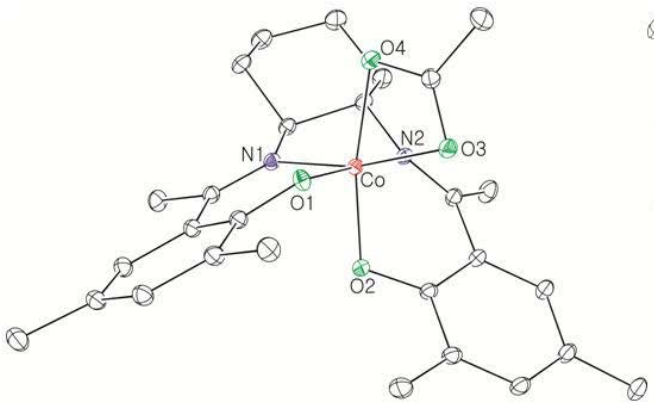
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **IND.P-128**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

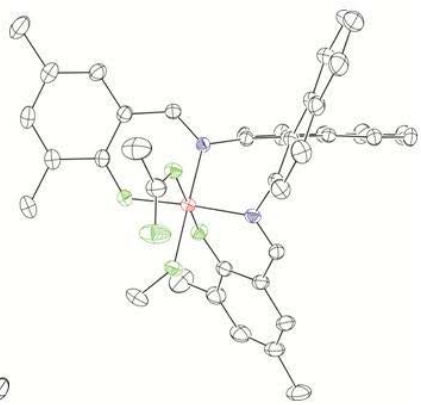
Ligand Variation for Highly Active Catalyst for CO2/epoxide Copolymerization forming cis-β conformation

전종엽 이분열

아주대 분자과학기술학과

A highly active catalyst for CO2/epoxide copolymerization was developed in our group. It contains cobalt metal in center of salcy-type ligand tethered by four quaternary ammonium salts. Contrary to the well-known salcy-type ligand metal symmetric framework, the (salcy)Co(III) complex adopt an unusual cis-β configuration, especially in the presence of a chelating additional donor. We found this information by growing single crystals of analogue complex. It bears methyl group instead of complex substituent which is hampering the growth crystal. We have tried to synthesis several variant ligands which readily form cis-β conformation. However these modified catalysts did not show any activity for CO2/PO copolymerization. The interasting phenomenon was that these catalysts adopt the cis-β configuration even in DMSO. It means cis-β conformation of those catalysts is so stable that it can not act as catalyst.





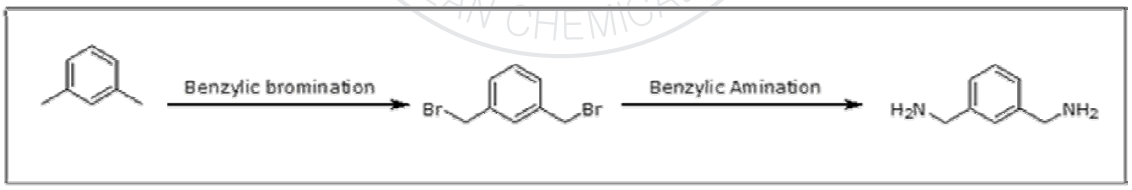
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **IND.P-129**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of meta-xylene diamine with facile amination of m-xylene through halogenation

이재명 하형호[1] 김근식[2] 곽지훈

순천대 화학과 [1]순천대 약학대학 약학과 [2]케이에스랩 부설연구소

Meta-xylene diamine, which has the aromatic and aliphatic properties together, is a useful material for the epoxy curing agent and a raw material for polyurethane, refractory material, synthetic resin, etc. Usually, it is produced by hydrogenation through isophthalonitrile industrially. However this method requires very high pressure, high temperature and excess of ammonia, and produces many kinds of side product. Thus, we develop a preparation method of meta-xylene diamine with a facile amination through halogenation of meta-xylene. We present this preparation method in detail.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-130**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

젖산으로부터 아크릴산 합성에서 인산칼슘 촉매의 반응특성

조한아 박정우 김형록[1] 장종산[2] 한요한[3]

한국화학연구원 바이오리파이너리 [1]한국화학연구원 그린화학연구본부 [2]한국화학연구원 그린화학촉매연구센터 [3]한국화학연구원 그린화학연구단

바이오플랫폼 화합물인 젖산을 탈수반응하여 아크릴산을 제조하는 촉매의 반응 특성을 조사하였다. 알콜의 탈수에 의한 올레핀 합성에서 인산칼슘 촉매의 산성과 염기성 및 반응조건에 따라 탈탄산반응 및 수소화분해 반응 등의 부반응이 일어나기 쉽고, 생성물인 아크릴산의 고온에서의 높은 중합성으로 촉매의 비활성화가 문제가 되므로 고선택성 및 고안정성을 가진 촉매와 적합한 반응조건에서의 운전이 요구된다. 본 연구에서는 인산 칼슘 촉매를 사용하여 반응온도, 반응압력, 반응물공급속도 및 장기 반응안정성에 대한 조사를 수행하여, 각 반응조건의 효과를 조사하고, 적합한 반응조건을 선택하여 약 500 시간의 반응에서 젖산 전환율 90% 이상, 아크릴산 선택도 70% 이상의 안정된 반응성을 보임을 확인하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

NEW TYPES OF CYCLO-OLEFIN POLYMER EMPLOYING TRICYCLOPENTADIENE AND DICYCLOPETANDENE

김성훈 이분열

아주대 분자과학기술학과

Over the past few decades, cyclo-olefin polymers prepared by ring opening metathesis polymerization and subsequent hydrogenation have received considerable attention because of their attractive properties which are suitable for use as optical-grade materials. [1] In this work, employing the TCPD and DCPD as a monomer, new types of cyclo-olefin polymer can prepared by ring opening metathesis polymerization. Ring opening metathesis polymerization of TCPD and DCPD is performed using a catalytic system of W(=NPh)(2,6-Me2-phenolate)4/n-BuLi. Afterwards, all the remain double bonds are hydrogenated using the catalytic system, Ni(acac)2/triisobutylaluminium. Molecular weight can be controlled by the amount of 1-octene.

Entry	DCPD (mol%)	TCPD (mol%)	**1-Octene** [c] **(eq)**	Yield (%)	T_g (°C)[d]	M_w[e] **(×10^{-3})**	M_w/M_n
1	80	20	**100**	91	126	**199**	3.1
2	80	20	**125**	95	128	**185**	3.2
3	80	20	**150**	90	124	**132**	2.9
4	65	35	**100**	89	143	**231**	3.2
5	65	35	**125**	92	144	**212**	3.1
6	65	35	**150**	94	147	**176**	3.3

[a]Polymerization conditions: sum of DCPD and TCPD = 19 mmol, cyclohexane solvent = 4 times the total weight of DCPD and TCPD, catalyst = W(NPh)(2,6-Me_2-phenolate)$_4$ (14.5 mg, 0.019 mmol), [Cat]:[*n*-BuLi] = 1:2, 80°C, 6 h. [b]Hydrogenation conditions: catalyst = Ni(acac)$_2$ (29 mg, 0.114 mmol) activated with Al(iBu)$_3$ (87 mg, 0.44 mmol) in cyclohexane (10 g), H_2 = 35 bar, 80°C, 6 h. [c]Mole ratio of [1-octene]/[cat]. [d]Glass transition temperature determined on DSC after hydrogenation. [e]Determined on GPC using the polystyrene standard

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일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **IND.P-132**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal Effect of Nitrogen Dopping on Electrical Properties of Styrene-acrylonitrile (SAN)-based Porous Carbons for Electrodes of EDLCs

이지한 박수진

인하대 화학과

In this work, the electrochemical properties of nitrogen dopped styrene-acrylonitrile based carbons (N-SANs) were investigated in electric double-layer capacitors (EDLC). We prepared Styrene-acrylonitrile (SAN) copolymer from copolymerization of styrene and acrylonitrile. And then we conducted carbonization and KOH activation for using electrodes. Nitrogen functional groups of N-SANs were prepared by thermal decomposition with urea as a function of heat temperature. N-dopping treatments were carried out with different temperatures to confirm the optimal thermal conditions. The crystalline and structural features were investigated by X-ray diffraction (XRD). The surface properties of the N-SANs were characterized by X-ray photoelectron spectroscopy (XPS). The textural properties of N-SANs were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. And their electrochemical behaviors were confirmed by cyclic voltammetry (CV).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-133**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The development of environmental friendly biodegradable detergent

김아나 유영 김석찬

국민대 화학과

The detergent used in the existing industry is harmful to the human body and induces the environmental contamination that is the second-order product. The biodegradable material is done with the starting material and several kinds of detergents are synthesized and the new detergent development of the kind is developed with the target through each biodegradability and toxicity test.

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일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **IND.P-134**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The One-step Synthesis of N,N-Dialkyl-p-Phenylenediamines and Evaluated the Oxidation Stability for Biodiesel

안경룡 전근 신승림 신종일 이상오 박수열

한국화학연구원 계면화학공정연구팀

Biodiesel is composed saturated and unsaturated long-chain fatty acid ester. When exposed to air during storage, autoxidation of biodiesel can cause degradation of fuel quality. One approach for increasing resistance of fatty derivatives against is to treat them with oxidation inhibitors, i.e. antioxidants. p-Phenylenediamine derivatives are useful stabilizers for polymers, particularly as antioxidants and antiozonants for rubbers, plastics, foods, and oils. The synthesis method involves several steps in the past. Therefore, simpler route are desirable. This report, however, discloses the first one-step reactions of dione with primary alkylamines in the presence of air for direct, convenient and green preparatations of N,N'-dialkyl-p-phenylenediamines. The studies have investigated the oxidation stability of a various antioxidants on biodiesels.

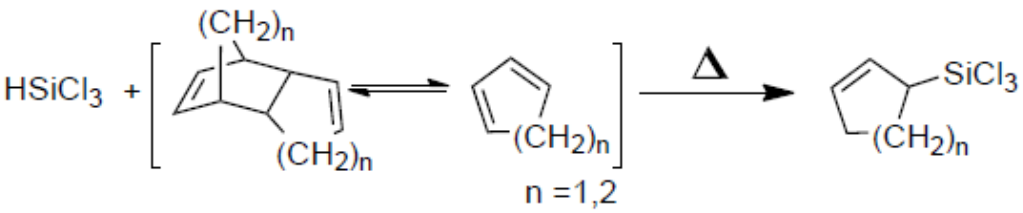
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **IND.P-135**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal Reaction of Cyclic Alkadiene with Trichlorosilane. Preparative and Mechanistic Aspects

정동의 한준수[1] 유복렬[2]

고려대 [1]KIST 물질구조제어연구단 [2]KIST 나노재료센터

The thermal reactions of trichlorosilane (1a) with cyclic alkadienes such as cyclopentadiene (2a), 1,3-cyclohexadiene (2b), and 1,4-cyclohexadiene (2c) were studied at temperatures ranging from 170 °C to 250 °C. In this reaction, the hydrosilylation rate increased as the reaction temperature was raised using an equimolar ratio of 1a to 2a. The reaction of 2a with 1a at 250 °C afforded 2-cyclopentenyltrichlorosilane (3a) as the major hydrosilylation product within 1 h in good yield (82%). This reaction also works when dicyclopentadiene (2a′) was used as a reactant instead of 2a. In a large scale preparation (2a′, 0.19 mol) under the same conditions, 3a was obtained in 82% isolated yield. It is significant to note that 2a′ can be used for the hydrosilylation, with no requirement of a cracking step under our thermal conditions. While the reaction of cyclohexadienes with 1a under the same conditions gave a mixture of three hydrosilylation products in moderate yields, along with other unsaturated C6 components, such as benzene and cyclohexene. In the thermal reaction of cycloalkadienes with 1a, the five-membered-ring diene 2a undergoes both a hydrosilylation reaction with 1a as well as a [4+2] cycloaddition reaction, leading to the hydrosilylation product 3a in good yield. While the six-membered ring dienes, 2b and 2c, undergo four different types of reactions, including hydrosilylation, [4+2] cycloaddition, dehydrogenation, and hydrogenation in competition to give the hydrosilylation products, hexane, and benzene, respectively. The reaction rates of cyclic alkadienes under our thermal conditions increase in the following order: 2c << 2b < 2a.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-136**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

무용의 MFB를 이용한 PABA의 합성

김경덕 정효진 유영 김석찬

국민대 화학과

p-Xylene 을 산화시켜 DMT 를 얻는 과정에서 발생하는 부산물인 MFB 혼합물을 가지고 분리 정제하고 Hoffmann degradation 을 통해 PABA 를 합성였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-137**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Carbon Paper as Gas Diffusion Layer for Fuel Cells by Wet Processing

이지한 박수진

인하대 화학과

In this work, we prepared the carbon paper from chopped carbon fibers for using gas diffusion matrix (GDM) in polymer electrolyte membrane fuel cells (PEMFCs) by wet processing. The process of making carbon paper consists of below three steps. ‘Dispersion of chopped carbon fiber’, ‘Preparation of carbon fiber web’, ‘Impregnating of phenol resin’. In whole process, we focused on two steps. First step is dispersion of carbon fiber, five kinds of surfactants were using in the first step to find optimal surfactants for carbon fiber dispersion. The other is the effect of the content of phenol resins on the electrical properties of carbon paper. We used 0.1 g of 6 ㎜ chopped carbon fibers for making carbon paper preform with 5 x 5 ㎠ size. Various contents of phenol resin were impregnated and estimated. The dispersion states of carbon fibers were investigated by scanning electron spectroscopy (SEM) and the electric resistivity of carbon paper was measured using two probe techniques.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **IND.P-138**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Cp(cyclopentyl)-substituted oligosiloxanes with a molecular weight that can be controlled

박은경 한준수[1] 강윤경 유복렬[2]

상명대 화학과 [1]KIST 물질구조제어연구단 [2]KIST 나노재료센터

Synthesis of silanols bearing Cp (cylcopentyl) groups was performed. Cp-substituted silanetriol, $CpSi(OH)_3$ was prepared by the hydrolysis of $CpSiCl_3$, and can be handled without special care in the air. The versatility of this silanol is amply demonstrated as a starting material of various silanols with novel frameworks. Also, the condensation of (cyclopentyl)trichlorosilane using trimethylchlorosilane as a end-capping agent afforded stable oligosiloxanes that combined with end-capping agent. When (cyclopentyl)trichlorosilane was treated with vinyl-substituted silane as a end-capping agent, oligosiloxanes were obtained that can be combined with other siloxane compounds. In this way, siloxane compounds with a variety of properties such as high refractive index, high thermal stability, etc were obtained. all these novel silanols and oligosiloxanes were determined by NMR, IR, GC-MS.

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장소: 부산BEXCO

발표코드: **IND.P-139**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal Reaction of Allyl chloride with Trichlorosilane and their Mechanistic Aspects.

정영애 한준수[1] 강윤경 유복렬[1]

상명대 화학과 [1]KIST 물질구조제어연구단

Thermal reaction of allyl chloride with Trichlrosilane was studied without catalyst at temperatures ranging from 170 to 250℃.In the reaction, the hydrosilylation reaction rate increases as the reaction temperature increases.The reaction of allyl chloride with Trichlorosilane at 250℃ for 1h afforded predominantly hydrosilylation and Si-C coupling products such as allyl tirichlorosilane, trichloro(3-chloropropyl)silane, 1,3-bis(trichlorosilyl)propane and (2-(5-(trichlorosilyl)-2-(trichlorosilylmethyl)pentyl) propane-1,3-diyl)bis(trichlorosilane). Thermal Si-C coupling reaction of Chloropropane with Trichlorosilane in order to investigate the its mechanism. The thermal reaction of Chloropropane with Trichlorosilane took place to give Si-C coupling products such as Trichloropropane, Tetrachlorosilane, etc. It was confirmed that Chloropropane of chloro was decomposed at a specific temperature.When 6-chloro-1-hexene was used instead of allyl trichlorosilane under same condition, the yields of hydrosilylation and Si-C coupling products were very similar to those obtained from the reaction of Allyl chloride with Trichlorosilane.It is expected that the thermal reaction of Allyl compounds with Trichlorosilane is Radical reaction. We will investigate the mechanism of this reaction.

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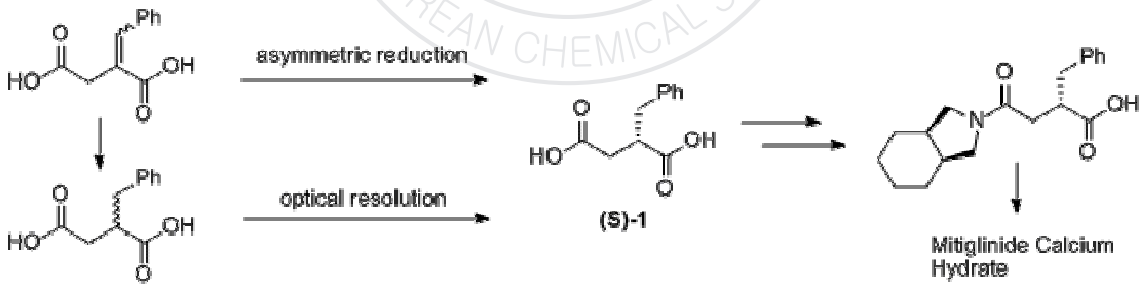
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of synthetic procedure of Mitiglinide, a drug for type II diabetes

이강우 권현지 오세한[1] 김학원[1]

경희대 화학과 [1]경희대 응용화학과

Mitiglinide is a drug for the treatment of type 2 diabetes. Although numerous enantioselective synthetic methods for Mitiglinide have been reported, most of these approaches employed chiral auxiliaries, chiral substrates, or enzymatic resolution, which cannot be readily applied to large scale production. Herein, we present a novel approach to the synthesis of Mitiglinide, via resolution or asymmetric reaction, which is regarded as one of the most efficient synthetic processes for large scale production in the points of view of economical and environmental aspects.



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장소: 부산BEXCO

발표코드: **IND.P-141**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of silafluorene derivatives for sensing and OLED applications

이성기 엄성용 김성룡 손홍래

조선대 화학과

In recent years, photoluminescence polysilole has been a topic of interest because of ther unusual electrical and optical properties. silafluorene is synthesized and evaluated for white O-LED applications. These compounds are of interest as light emissive layers, as they possess relatively low LUMO energy levels while maintaining high HOMO-LUMO optical gaps. Differential scanning calorimetry measurements reveal that these silafluorene compounds have advantages of thermal stability above 300 oC. Organic light-emitting diodes have been fabricated using thermal evaporation technique. They emit blue to bluish-white light with an excellent diode behavior under the forward bias. The synthesis, spectroscopic characterization, and fluorescence quenching efficiencies of silafluorene were reported. The synthesized compounds were characterized by 1H and 13C NMR spectroscopy. Absorption and emission spectra for these compounds were obtained by using UV-Visible and fluorescence spectroscopy in solution. Their emission behaviors and quantum yield for these compounds were investigated both in the solid and colloid state. Our results indicated that both compounds were used as the 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 silafluorene derivatives were synthesized and their photonic behaviors were investigated. 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.

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발표코드: **IND.P-142**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Silicon Nanowire Wrapped withMicrowave-Exfoliated Graphene Oxide via Hydrosilylation

신동희 신기루 김종준 손홍래

조선대 화학과

Silicon nanowire (SiNW) have been synthesized using wet chemical etching of bulk siliconwafers (p-Si(100)) with a mask of silver nanoparticles that are deposited by wet electrolessdeposition. The etching of SiNWs is based on subsequent treatments in chemical solutions suchas 0.04 M aqueous solutions of silver nitrate (AgNO3) followed by 5 M hydrofluoric acid and30% hydrogen peroxide (H2O2). Graphene oxide was obtained by ball milling carried out in aball-mill machine in the presence of graphite and stainless steel balls and followed by themodified Hummers' process. Activated microwave-exfoliated graphite oxide (MEGO) wasprepared and used for the composite materials of silicon nanowires and grapheme oxide viahydrosilylation. The silicon nanowire-graphene composite materials were characterized byXRD, TEM, and FE-SEM. A specific surface area (SSA) was measured by theBrunauer?Emmett?Teller (BET) method. Detailed information for the composite materials willbe discussed.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

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Sensor Based on Functionalzation of Silole

김성룡 이성기 엄성용 손홍래

조선대 화학과

we have synthesized the siloles derivatives to develop a new optical probe for florescence turn off detection biomolecules. 1-methyl-1-hydro-2,3,4,5-tetra- phenyl silole were derived with allylamines to give amine functionalized silole via hydrosilylation. Amine-functionalized silole were further derived with biotin to give biotin-functionalized silole. These biotin-functionalized molecules were used for the detection of biomolecules such as avidin and streptavidin through the quenching of photoluminescence. Our results indicated that biotinylated-silole nano aggregate are highly sensitive and selective to detect the avidin/streptavidin without any other interference.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

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

Synthesis and Optical Characterization of Silicon Nanoparticles

조보민 손홍래

조선대 화학과

Various reaction conditions, such as quantity of reducing agent and reaction time wereinvestigated with the aim of finding a simple, optimized synthetic route for the synthesis ofluminescent silicon nanoparticles (SiNPs). Si NPs were synthesized from the reaction ofethylenediammonium chloride and magnesium silicide via a low temperature solution route.Optical characterizations of silicon nanoparticles were achieved by using ultraviolet-visible(UV-Vis) and photoluminescence (PL) spectroscopy. As the reaction time longer, siliconnanoparticles grew and their emission wavelength shifted to the longer wavelength. Themonotonic shift of the photoluminescence as a function of excitation wavelength resultedfrom the excitation of different sizes of nanocrystals that had different optical transitionenergies.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

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장소: 부산BEXCO

발표코드: **IND.P-145**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection etection of nerve agent stimulants based onphotoluminescent porous silicon interferometer

김성웅 조보민 김성룡 손홍래

조선대 화학과

Novel porous Si exhibiting dual optical properties, both Fabry-P?rot fringe (optical reflectivity) and photoluminescence, were developed and used as chemical sensors. Porous Si samples were prepared by an electrochemical etch of p-type silicon under the illumination with a 300 W tungsten filament bulb for the duration of etch. The surface of porous Si was characterized by FT-IR instrument. The sensing experiments using fresh and containing a copper (II) catalyst dual PSi for the detection of nerve agents such as triethyl phosphate (TEP), dimethyl methylphosphonate (DMMP), and diethyl ethylphosphonate (DEEP) have been achieved. Both reflectivity and photoluminescence were simultaneously measured under the exposure of Organophosphonate nerve agents. These surface-modified samples showed unique respond in both reflectivity and photoluminescence with various Organophosphonate nerve agents. 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

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **IND.P-146**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1,1-Difunctional Germafluorene for the OLED

엄성용 이성기 김성룡 손홍래

조선대 화학과

Various functionalized germaflourenes have been synthesized and optical and electronic characterizations were investigated. The compounds were synthesized by a stepwise reactions from 1,2,4,5-tetrabromobenzene to 2,2'-dibromobisfluorene with germanium tetrachloride in THF at row temperature. The germafluorenes were characterized by 1H-NMR, 13C-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. hese compounds are of interest as light emissive layers, as they possess relatively low LUMO energy levels while maintaining high HOMO-LUMO optical gaps. Dierential scanning calorimetry measurements reveal that these Metallafluorene compounds have advantages of ther-mal stability above room temperature regions. Organic light-emitting diodes have been fabricated using thermal evaporation technique which emit blue light with an excellent diode behavior under the forward bias. 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.

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장소: 부산BEXCO

발표코드: **IND.P-147**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Optical Characterization of Full Color Stop Band Based on Rugate-Structured Porous Silicon

정성은 김강빈 엄성용 손홍래

조선대 화학과

The reflection band characteristics of rugate porous silicon (PS) and the effect of an etching time for the formation of rugate photonic structure were investigated. The reflection band of rugate PS shifted to shorter wavelength by about 30 nm as the etching time increased. The effect of frequency for the formation of rugate PS was investigated. The reflection band characteristics of 17 rugate PS samples according to the frequency change were investigated. All parameters but etching frequency were fixed. The values of Ai, B, and t were 11.55 and 63.05 mA and 1000 s, respectively. The frequencies, ki, varied from 0.22 to 0.38 Hz. and the effect of a frequency for the reflection band characteristics of rugate PS were investigated. Rugate PS exhibited a linear dependence between the reflection wavelengths and the etching frequencies.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

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발표코드: **IND.P-148**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Silicon Quantum Dots showing High Quantum Efficiency

백상수 정성은 김강빈 손홍래

조선대 화학과

Quantum efficiencies of silicon quantum dots have been investigated from the reaction ofmagnesium silicide and ammonium chloride. The change of quantum yield and opticalcharacterization of silicon quantum dots are measured depending on the reaction time. Highlyluminescent silicon quantum dots were obtained as the reaction time longer. Absorptionmeasurement indicated that the Si NPs consisted of only silicon and hydrogen atom. Opticalcharacterizations of silicon quantum dots were measured by ultraviolet-visible (UV-Vis) andphotoluminescence (PL) spectroscopy. The size distribution and orientation of silicon quantumdots were measured by TEM and XRD. TEM image displays the spherical silicon quantum dotswith the size of 2-4 nm.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

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발표코드: **IND.P-149**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anisotropic Multi-spot DBR Porous Silicon Chip for the Detection of Human Immunoglobin G

안지훈 신기루 신동희 손홍래

조선대 화학과

Asymmetric porous silicon multilayer (APSM)-based optical biosensor was developed to specify human Immunoglobin G (Ig G). APSM chip was generated by an electrochemical etching of silicon wafer using an asymmetric electrode configuration in aqueous ethanolic HF solution and constituted with nine arrayed porous silicon multilayer. APSM prepared from anisotropic etching conditions displayed a sharp reflection resonance in the reflectivity spectrum. Each spot displayed single reflection resonance at different wavelengths as a function of the lateral distance from the Pt counter electrode. The sensor system consisted of the 3 ? 3 spot array of APSM modified with protein A. The system was probed with an aqueous human Ig G. Molecular binding and specificity was monitored as a shift in wavelength of reflection resonance.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

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장소: 부산BEXCO

발표코드: **IND.P-150**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Gradient Optical Filter Containing Anisotropic Bragg Nanostructure

김강빈 안지훈 신동희 손홍래

조선대 화학과

New gradient optical filters containing asymmetric Bragg structure were prepared from the distributed Bragg reflector (DBR) porous silicon (PSi). Anisotropic DBR PSi displaying a rainbow-colored reflection was generated by using an asymmetric etching configuration. Flexible anisotropic DBR PSi composite films were obtained by casting of polymer solution onto anisotropic DBR PSi thin films. The surface and cross-sectional images images of anisotropic DBR PSi composite films obtained with cold field emission scanning electron microscope indicated that the average pore size and the thickness of porous layer decreased as the lateral distance increased. As lateral distance increased, the reflection resonance shifted to shorter wavelength. 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

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장소: 부산BEXCO

발표코드: **IND.P-151**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of Photoluminescence Efficiency of n-Type Porous Silicon by Controlling of an Etching Time and Applied Current Densities

신기루 김종준 백상수 손홍래

조선대 화학과

Photoluminescence properties and surface morphologies of porous silicon were investigated by controlling of etching times and applied current densities. FE-SEM image of porous silicon surface indicated that the porous silicon prepared at currents below 200 mA/cm2 exhibited very stable and even surface. However the porous silicon prepared at currents above 300 mA/cm2 displayed the cracked surface of porous silicon. This cracked surface was collapsed to give cracked domains at currents over 500 mA/cm2. Photoluminescence of porous silicon was investigated by controlling of etching times and applied current densities in the range from 50 sec. to 900 sec. and from 50 mA/cm2 to 800 mA/cm2, respectively. Photoluminescence intensity of porous silicon increased gradually during etching process, reached maximum, and then decreased as the etching time increased. Porous silicon showed the best photoluminescence efficiency was prepared at currents of 200 mA/cm2 and etching time of 300 sec.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

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장소: 부산BEXCO

발표코드: **IND.P-152**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of New Synthetic Route for the Polysilafluorenes via Dehydro-coupled Polycondensation

김종준 백상수 정성은 손홍래

조선대 화학과

1,1-Dihydrosilafluorenes were synthesized and their electronic and photonic behaviors have been investigated. The synthesized compounds were characterized by 1H and 13C NMR spectroscopy. Absorption and emission spectra for these compounds were obtained by using UV-Visible and fluorescence spectroscopy in solution. Their emission behaviors and quantum yield for these compounds were investigated. Polymers of silafluorene, poly-1,1'-silafluorene, via dehydrocoupling polycondensation using catalysts such as H2PtCl6, Rh(PPh3)3Cl, and Pd(PPh3)4. The polysilafluorenes obtained from various conditions were characterized by gel permeation chromatography(GPC). Comparison of optical behaviors of polysilafluorene by the measurement of fluorescence life time and quantum efficiencies were achieved. Detailed experimental results will be discussed.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

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발표분야: 무기화학

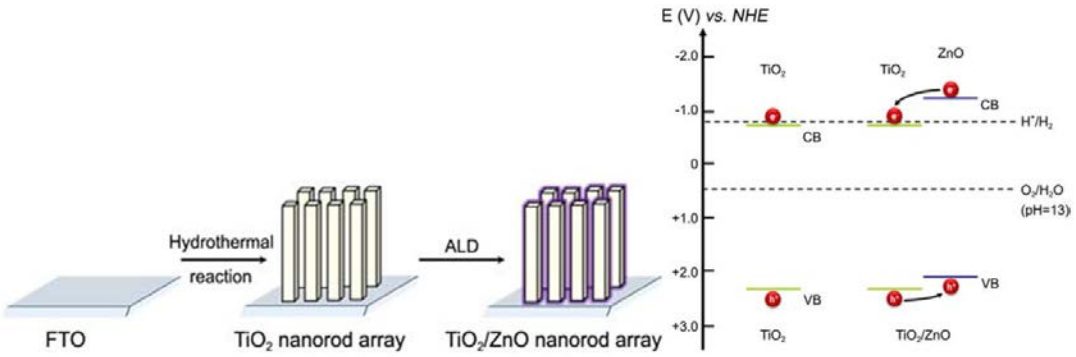
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Dimensional Core/Shell Structured TiO_2/ZnO Heterojunction for Improved Photoelectrochemical Performance

지인애 방진호 이용우

한양대 응용화학과

A wide variety of strategies have been developed in order to enhance the photocatalytic activity of TiO_2. Fabricating nanostructures of TiO_2 - such as nanowires, nanotubes, nanoplates, or porous spheres - is a representative example among the sustained efforts. we have recently developed a simple hydrothermal synthetic route, where single-crystalline TiO_2 nanorods grow directly on optically transparent electrode (OTE). Despite the successful demonstration of the TiO_2 nanorods as a photoanode, its catalytic activity in the photoelectrochemical water splitting is quite low mainly because the crystal structure of the TiO_2 nanorods is rutile. Because the Fermi level of the rutile-phase TiO_2 is less favorable than that of anatase-phase counterpart for H_2 generation, thereby requiring much higher bias voltage. We report hereby the fabrication of core/shell structured TiO_2/ZnO nanorod array via atomic layer deposition (ALD) technique. The newly developed TiO_2/ZnO heterojunction significantly improved its performance in the photoelectrochemical water splitting cell due to the beneficial synergetic effects of the heterostructured nanocomposite. Further, we demonstrated that the TiO_2/ZnO photoelectrode could be utilized as an oxide substrate for a semiconductor-sensitized solar cell to boost up its energy conversion efficiency.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-154**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic properties of the surface modified Manganese ion doped ZnS nanocrystals

박상현 황청수

단국대 화학과

Water-dispersible ZnS:Mn nanocrystals were synthesized by capping their surfaces with polar aminoacids (e.g. Val, Ala, Ser and Thr), mercaptopropionic acid (MPA), mercaptoacetic acid (MAA) and polyethyleneglycol (PEG) molecules. The resulting surface modified ZnS:Mn nanocrystals were optically characterized by UV-Visible and room temperature solution photoluminescence spectroscopies. Further physical characterization works were performed by XRD, HR-TEM, EDXS, FT-IR, and ICP-AES analyses. Finally, photocatalytic activities of the prepared ZnS:Mn nanocrystals were evaluated by their degradation ability of methylene blue molecules under UV light irradiation, Degree and rate of the degradation were measured and calculated by using UV-Visible absorption spectroscopy.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Triarylboranes with Indole and Phenol: B/H Hybrid Receptors for Fluoride

이민형 성우영

울산대 화학과

To enhance the fluoride binding affinity of triarylborane, we have designed novel B/H hybrid receptors containing both a Lewis acidic boron center and a hydrogen bond donor such as NH and OH group. 7-Mes_2B-1-H-indole (1) and 2-Mes_2B-phenol (2) were prepared and characterized by X-ray diffraction studies. Both compounds showed enhanced fluoride binding affinity due to the presence of XH-F (X = N, O) hydrogen bond which assists B-F dative bond. The details of synthesis, characterization, and fluoride binding properties of 1 and 2 will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Fe^{2+} Ion Recognition Using a Fluorescent Pyridinyl-benzoimidazole-derived Ionophore

노진영 현민영 배정미 윤성호[1] 김철

서울과학기술대 정밀화학과 [1]국민대 생명나노화학과

Fluorescent organic molecules that respond to changes in the Fe^{2+} concentration with selectivity to other abundant di-valent metal ions will offer the ability to understand the dynamic fluctuations of the Fe^{2+} ion in interesting media. The use of 6Br-ppmbi, derived from 2-pyridin-2-yl-benzimidazole, for metal ion-selective fluorescence recognition was investigated. Screening of the main group and transition metal ions showed exclusive selectivity for Fe^{2+} ions even in the presence of competing metal ions. In addition, the requirement for low concentrations of probe molecules to detect certain amounts of Fe^{2+} ions make this sensor unique compared to previously reported Fe^{2+} ion sensors.

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Nonheme Cobalt-Catalyzed Olefin Epoxidation: Participation of Multiple Active Oxidants

배정미 황인홍 송은주 김경범 김철

서울과학기술대 정밀화학과

We have synthesized and characterized the mononuclear nonheme Co^{III} complex 1 supported by a chelate ligand having two deprotonated amide moieties, which catalyzes a wide range of olefin epoxidations by MCPBA, via multiple active oxidants, Co^{V}=O, Co^{IV}=O, and Co^{III}-OOC(O)R. It is proposed that 1 shows partitioning between heterolytic and homolytic cleavage of the O-O bond to afford both a less accessible Co^{V}=O and Co^{IV}=O (or Co^{III}-coordinated ligand radical) intermediates responsible for the stereospecific olefin epoxidation and radical-type oxidations, respectively. Moreover, under extreme conditions, where the concentration of an active substrate is very high, the Co-OOC(O)R (3) might be a possible reactive species for epoxidation. This proposal was explained after a reactivity study in which PPAA was used as a mechanistic probe. These results and other results recently reported by our group reveal the important role that supporting chelate ligands having dianionic charge, via deprotonation of the two amide moieties, play in influencing the formation of high-valent metal-oxo species.

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **INOR.P-158**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and catalytic properties of (π-allyl) Pd pseudohalide containing NHC(N-heterocyclic carbene) ligand

김용주 김현경 이정현[1] 이순원[2]

강릉원주대 화학과 [1]KIST 천연의약센터 [2]성균관대 화학과

Various (π-allyl) Pd cazides having NHC ligands were obtained from the reactions of bis(π-allyl) Pd azides with 2 equiv. of NHC ligand. Also, several (π-allyl) Pd siothiocyanates having a NHC ligand were obtained from the reactions of (π-allyl) Pd chloride with 1.2 equiv. of KSCN in aquous solvent. The isolated complexes were characterized by spectroscopic analyses and some of X-ray diffraction study. Treatments with Dimethyl acetylene dicarboxylate to the (π-allyl) Pd-NHC azide caused the formation of tetrazolalto (π-allyl) Pd-NHC complexes. Also, Suzuki-Miyaura cross C-C coupling reactions using the some of various (π-allyl) Pd pseudhalogeno complexes underwent. Experimnetal details will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Structures, and Properties of New Dinuclear Phosphido (or Chloro)-bridged Palladium(II) Azido Complexes

김용주 최근영 이선계 **ZHENG ZHENNU**[1] 이순원[1]

강릉원주대 화학과 [1]성균관대 화학과

Phosphido- and chloro-bridged palladium(II) complexes were obtained from the reactions of [Pd(?-PPh2)(PPh2H)Cl]2 with various phosphines (PEt3, PMe3, PMe2Ph). Treatments of [Pd(?-PPh2)(PPh2H)Cl]2 with excess NaN3 in aquous solvent caused coresponding dinucelar azido complexes, [Pd(?-PPh2)(PPh2H)(N3)]2 Also, reactions of Na2PdCl4 with L2PdCl2 (L=PEt3, PMe2Ph) produced [Pd(?-Cl)(PR3)Cl]2 in quantitative yields. Their chemical properties toward nucleophiles or electrophiles were examined.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-160**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Synthesis of Highly Active Iron Carbide/CMK-3 Nanocatalysts by Melt-Infiltration Process for High Temperature Fischer-Tropsch Synthesis Reaction

박지찬

한국에너지기술연구원 청정연료연구단

Fischer-Tropsh (FT) reaction is a method for production of hydrocarbons from synthesis gas. Especially, high temperature Fischer-Tropsch (or HTFT) reaction has been operated at temperatures of 330°C-350°C by using an iron-based catalyst. The iron-based catalyst has been prepared by various ways such as co-precipitation and wetness impregnation with various supports such as carbon, silica, alumina, and other metal-oxides as well as additional promoters like Ru, Cu, and K to enhance the activity and selectivity of catalysts. In the present work, we newly introduce iron carbide/CMK-3 catalysts which are synthesized by melt infiltration process under the controlled aging temperature and the loading amounts of hydrated metal salts and subsequent ex-situ activation step. The obtained iron carbide/CMK-3 catalysts were successfully employed as active nanocatalysts for HTFT reactions. It is anticipated that these iron carbide-based nanocatalysts could serve as good candidates for HTFT reaction to produce gasoline (C5-C12) with high yields, selectively.

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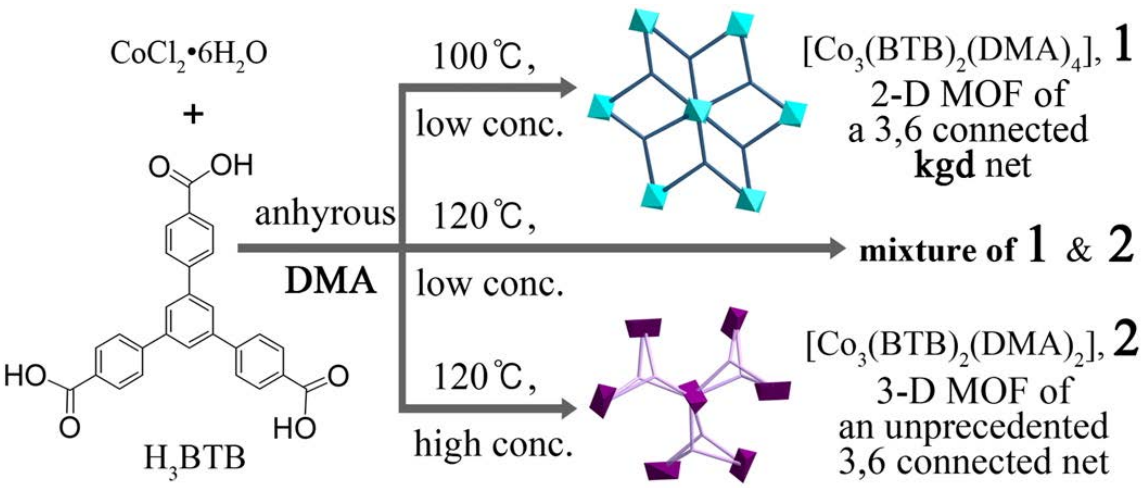
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

2-D and 3-D metal?organic frameworks of 3,6-connected net topologies based on a triscarboxylate and a linear trinuclear $Co_3(COO)_6$

김동욱 **Song xiaokai**[1] 오민학 나명수

울산과학기술대 친환경에너지공학부 [1]한양대 응용화학과

The solvothermal reactions of cobalt(II) chloride hexahydrate and 1,3,5-benzenetribenzoic acid (H_3BTB) in anhydrous N,N'-dimethylacetamide (DMA) led to two 3,6-connected metal?organic frameworks (MOFs) with different net topologies depending on reaction temperatures and reactant concentrations. MOF $[Co_3(BTB)_2(DMA)_4]$, 1, with a linear trinuclear cobalt carboxylate cluster, $Co_3(COO)_6$ and an inversion point symmetry with "compressed trigonal antiprismatic" 6-connectivity, is a two-dimensional (2-D) layered structure of a 3,6-connected kdg net topology. However, the same linear trinuclear cobalt carboxylate cluster, $Co_3(COO)_6$, with a twofold point symmetry with "compressed trigonal prismatic" 6-connectivity leads to the three-dimensional (3-D) network of 2, with an unprecedented 3,6-connected net topology with a point symbol $(4^3)_2(4^3?12^{12})$.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-162**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new strategy to construct core-shell heterostructural metal-organic frameworks via selectively post-synthetic modifications of framework metal ions

Song xiaokai 김혜현[1] 김동욱[1] 정석[1] 나명수[1]

한양대 응용화학과 [1]울산과학기술대 친환경에너지공학부

A new strategy to construct core-shell heterostructural metal-organic frameworks (MOFs) was demonstrated here. The post-synthetic replacement of metal ions (i.e. transmetalation) in a family of highly porous isostructural MOFs, M6(BTB)4(BP)3 (where M = Zn(II) (1), Co(II) (2), Cu(II) (3), and Ni(II) (4), BTB = 1,3,5-benzenetribenzoate, and BP = 4,4'-bipyridyl) with an ith-d net topology has been investigated. This series of isostructural MOFs with different framework metal ions have different framework stabilities. The MOFs having similar thermodynamic stabilities of metal ions, 1 and 2, could convert to each other via reversible and complete transmetaltion. While soaking thermodynamically less stable MOFs, 1 and 2, in DMF solution containing Cu(II) and Ni(II) ions, led to thermodynamically more stable MOFs, 3 and 4, respectively, no reverse transmetalation reaction was observed. Notably, the transmetalation process is occurring heterogeneously with site selectivity in a single crystal. Therefore, by simply controlling the soaking time, either a homogeneous framework structure via complete transmetalation of the framework metal ion or a core-shell heterostructure via selective transmetalation mainly constrained to the external shell region of a crystal could be achieved. The fully transmetalated MOFs showed significantly improved framework stabilities compared with the parent MOFs suggested by N2 sorption studies. Surprisingly, a marked improvement in the framework stability was observed, even in the selectively transmetalated Co(II)/Cu(II)- and Co(II)/Ni(II)-core-shell heterostructures. Although the frameworks are partially transmetalated, the framework stability of not only the external shell region but also of the internal core region was significantly affected.

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발표코드: **INOR.P-163**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Light- and photo-induced [2 + 2] cycloaddition of metal-directed assembly of metal(II) benzoates

황인홍 강주혜 노진영 송은주 김현 김철 김성진[1] 김영미[1]

서울과학기술대 정밀화학과 [1]이화여대 화학-나노과학과

We report here the syntheses, structures, thermal stabilities, and photoluminescence of four novel M^{II} coordination polymers (1-Mn, 3-Ni, 4-Cu, and 6-Cd), and comparison of coordination geometries of metal ions including the previously known compounds 2-Co and 5-Zn. Their structures show various coordination modes depending on metal ions: a tetragonal pyramidal (five-coordinate) Cu^{II} ion, a trigonal-bipyramidal (five-coordinate) Zn^{II} ion, octahedral (six-coordinate) Mn^{II}, Co^{II}, and Ni^{II} ions, and a pentagonal-bipyramidal (seven-coordinate) Cd^{II} ion. 1-Mn and 5-Zn show ladder-type double chains, 2-Co does a simple linear chain, 3-Ni does a two-dimensional sheet, 4-Cu does a chain containing paddle-wheel dinuclear units, 6-Cd does a thick one-dimensional structure containing newly generated [2 + 2] addition product 4pycb ligands. Since different structures provide different coordination polymers for each metal ion, it is clear that selection of appropriate metal ions can control the structure of coordination polymers.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Eu3+-Doped Silica@Coordination Polymer Core-Shell Structures and Hollow Gd2O3:Eu Microspheres

손주희 이희정 오문현

연세대 화학과

There is much interest in lanthanide activated phosphor materials for useful applications in electroluminescent displays, optical devices, and bio-imaging. In special, Eu3+-doped rare-earth oxides are attractive phosphors for use in optical devices. Here, we report a synthetic method based on the solvothermal reaction for the construction of highly uniform Eu3+-doped luminescent silica@coordination polymer core-shell microspheres through the growth of coordination polymers onto the silica surface. The subsequent calcination and etching processes resulted in the production of doping ratio-controlled luminescent hollow Gd2O3:Eu microspheres.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In situ-generated metal oxide catalyst during CO oxidation reaction transformed from redox-active metal-organic framework -supported palladium nanoparticles

김진영 이경주 주상훈[1] 김지만[2] 문희리

울산과학기술대 친환경에너지공학부 [1]울산과학기술대 나노생명화학공학부 [2]성균관대 화학과

The preparation of redox-active metal-organic framework (ra-MOF) -supported Pd nanoparticles (NPs) via the redox -couple -driven method is reported, which can yield unprotected metallic NPs at room temperature within 10 min without the use of reducing agents. The Pd@ra-MOF has been exploited as a precursor of an active catalyst for CO oxidation. Under the CO oxidation reaction condition, Pd@ra-MOF is transformed into a PdOx-NiOy/C nanocomposite to generate catalytically active species in situ, and the resultant nanocatalyst shows sustainable activity through synergistic stabilization.

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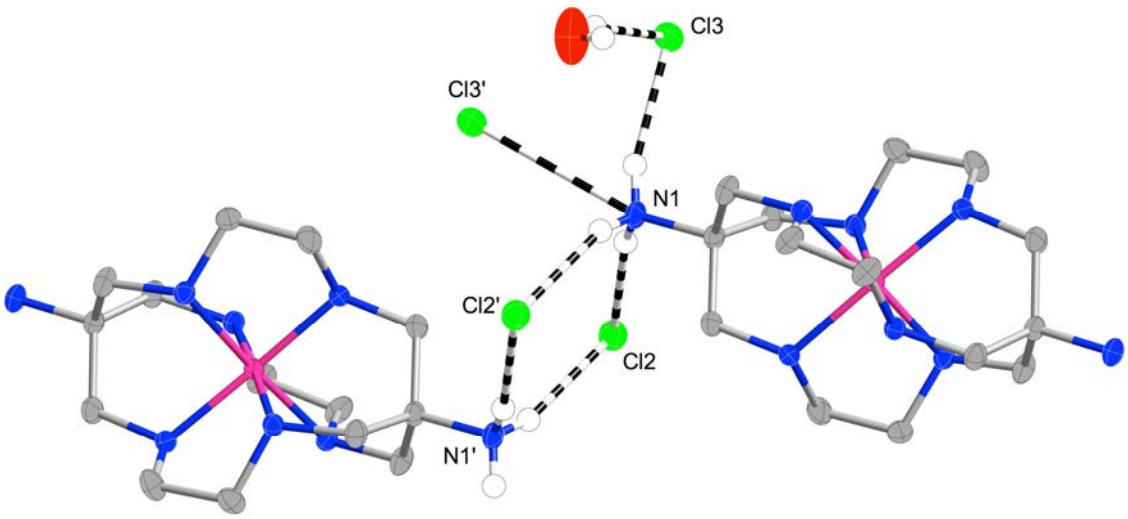
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrogen-bonding properties of polyamine complexes incorporating pendent nucleophiles

원미선 우아림[1] 조정환 김양[2]

고신대 화학신소재학과 [1]고신대 화학과 [2]고신대 화학 신소재학과

In the case of pendent ammonio groups, not only do they appear to be good H-bond donors but they are frequently involved in contacts suggestive of hyperdenticity at N. As part of a programme of chemical synthesis concerning both macrocyclic and macrobicyclic (sarcophagine) ligands and their complexes, we have been concerned in particular with the introduction of simple pendent groups, such as hydroxyl, onto these species. We present herein an analysis of several crystal structures bearing upon the issue of the hydrogen bonding capacity and the nucleophilicity of both pendent amino and hydroxyl groups.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-167**

발표분야: 무기화학

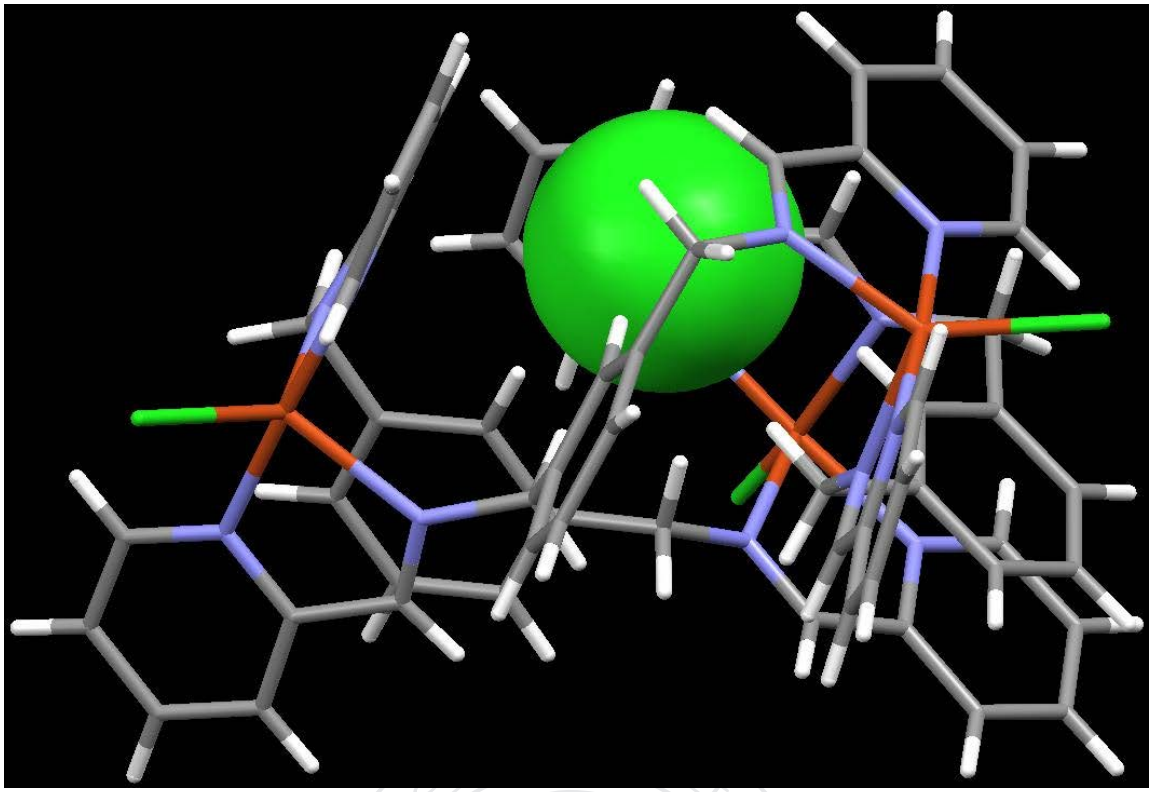
발표종류: 포스터, 발표일시: 수 16:00~19:00

Di- and tri-nuclear Cu(II) complexes incorporating the isomeric Schiff base ligands

우아림 원미선[1] 조정환[1] 김양[2]

고신대 화학과 [1]고신대 화학신소재학과 [2]고신대 화학 신소재학과

Di- and trinuclear Cu(II) complexes incorporating the isomeric Schiff base ligands being incorporated two separated α-diimine coordination domains have been synthesised and their X-ray structures and variable temperature magnetic properties determined. A chloride anion is encapsulated in the structure being bound by six non-classical hydrogen bond interactions. Variable temperature magnetic susceptibility measurements indicated the presence of weak antiferromagnetic behaviour for dinuclear species and weak ferromagnetic behaviour for trinuclear one



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-168**

발표분야: 무기화학

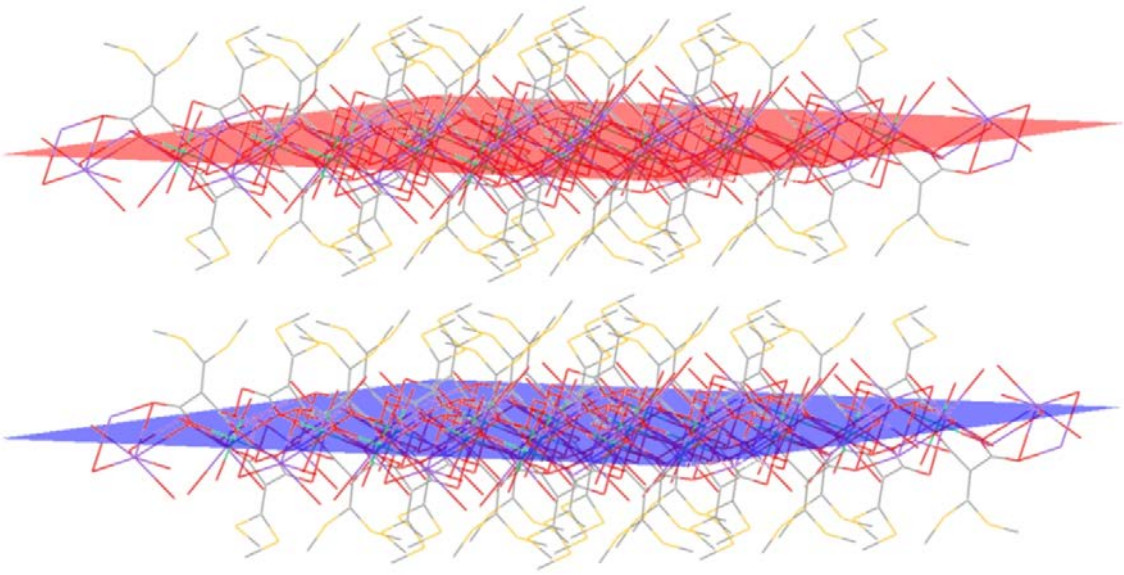
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Structural Properties of 2D Anionic Nickel(II) and Magnesium(II) Complexes Containing Bis(alkylthio)ylidenemalonato Ligands

김성민 정옥상

부산대 화학과

Nickel(II) and magnesium(II) complexes of bis(alkylthio)ylidenemalonato ligands were synthesized in aqueous solution. Their crystal structures were confirmed by single crystal X-ray crystallography. These complexes in solution are discrete anionic structures with K^+ as couter-cations whereas their structures are 2D sheets linked by K^+ and water molecules. The substituents of the ligands affected the inter-layer distance. For nickel(II) complexes, magnetic properties were monitored. Behavior of solvated water molecules were checked by thermogravimetry analysis.



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발표코드: **INOR.P-169**

발표분야: 무기화학

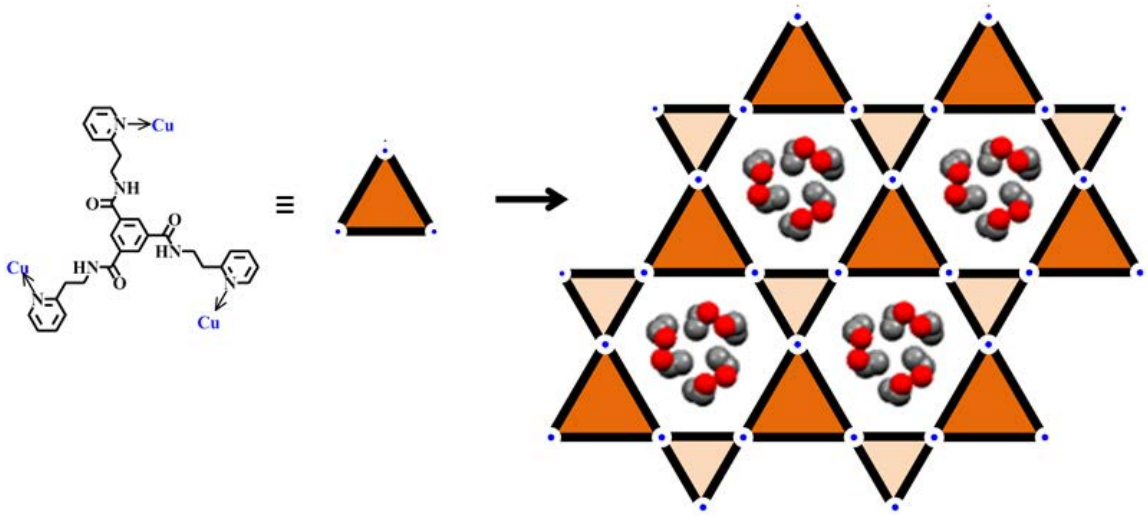
발표종류: 포스터, 발표일시: 수 16:00~19:00

Kagome-type Networks Via Tridentate Ligand For an Alcohol Reservoir

이해리 정옥상

부산대 화학과

Self-assembly of CuX_2 (X^- = 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. Notably, two slightly different kinds of triangles exist in the two-dimensional (2D) infinite structure in the solid state. The nano-sized hexagons with diagonal distance Cu⋯Cu = 25.172(1) Å for [$Cu_3Cl_6L_2$] and 25.405(1) Å for [$Cu_3Br_6L_2$] are occupied by six ethanol molecules (6EtOH@[$Cu_3Cl_6L_2$]) and by a mixture of three ethanol and three methanol molecules (3MeOH·3EtOH@[$Cu_3Br_6L_2$]) indicating that the hexagon is an effective reservoir for small alcohol molecules. The interlayer distances are very short (3.606(1) Å for 6EtOH@[$Cu_3Cl_6L_2$]; 3.560(1) Å for 3MeOH·3EtOH@[$Cu_3Br_6L_2$]), and are comparable to that of graphite (3.35 Å). In the present study, the temperature-dependent morphology change of the crystals was monitored in order to confirm the solvent-desorption and decomposition procedures.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-170**

발표분야: 무기화학

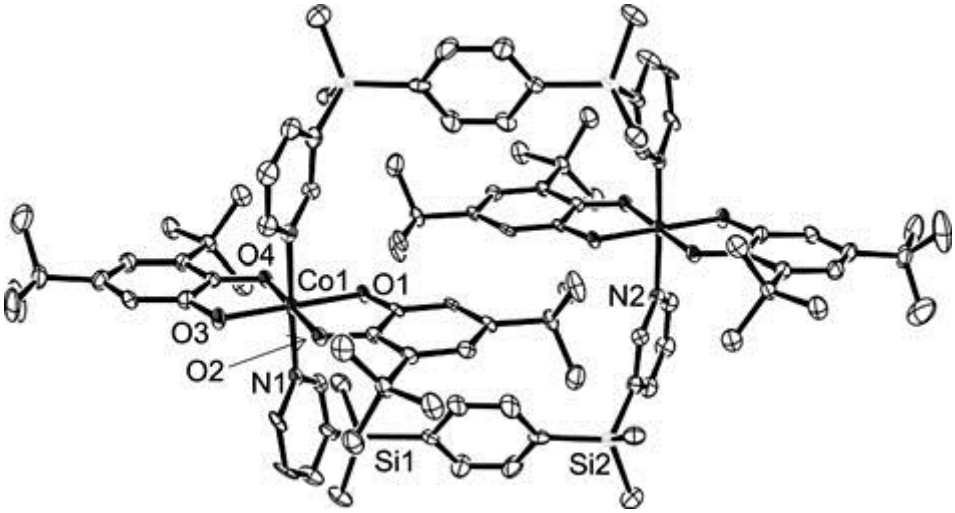
발표종류: 포스터, 발표일시: 수 16:00~19:00

Bistable Molecular System via Intramolecular Electron Transfer. Cyclodimeric 1,2-Semiquinonato/Catecholatocobalt Complex Containing

문소연 정옥상

부산대 화학과

Metal complexes containing 1,2-semiquinonato (sq^-, S =1/2) and catecholato (cat^{2-}, S = 0) ligands have shown an unique bistability via the intramolecular electron transfer between the metal and the ligand around room temperature. Different valence states of the bistable complexes have significantly different charge and spin distributions, and consequently, show different optical, electric, and magnetic properties. This has been very rominently elucidated for the cobalt complexes where temperature- and photodependent equilibria between the [Co^{III}] and [Co^{II}] valence tautomeric species have been demonstrated both in solution and in the solid state. Such electronic-labile complexes have been utilized as potential building blocks for molecular electronic devices,6-8 and are very sensitive to environment such as temperature, solvent, state, and photo-energy. Even though some dicobalt valence tautomeric systems were reported, but the corresponding cyclodimeric cobalt complexes remain unexplored. In order to construct new cyclodimeric cobalt complexes, 1,4-bis(dimethyl-3-pyridylsilyl)benzene (L) as a bridged bidentate ligand was provided. Herein we report the synthesis, structure, and physicochemical properties of unprecedented cyclodimeric valence tautomeric cobalt complex. The cyclodimeric cobalt complex was characterized based on pectral, magnetic, and X-ray crystallography.



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장소: 부산BEXCO

발표코드: **INOR.P-171**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Coordination Cages versus Spherical Morphology using Tridentate Ligands

노태환 정옥상

부산대 화학과

In order to validate the formation and behavior of cage containing a flexible tridentate ligand, we report cage compounds, $[Pd_3(L1)_2](X)_6$ (Pd = $(Me_4en)Pd(II)$; X^- = BF_4^- and ClO_4^-; L1 = 1,3,5-tris(isonicotinoyloxyethyl)cyanurate) via construction of a new C_3-symmetric potential triangular component with *cis*-protected ditopic $(Me_4en)Pd(II)$ as a corner linker. A single water molecule is nestled within the new cage, and is reversibly adsorbed and desorbed via a combination of the adequate space, polar environment, and conformational flexibility of the cage. Thus, the duality of liberal and restrictive properties of a single water molecule has been discussed based on spectroscopic data. In Suzuki-Miyaura C-C cross-coupling reactions, the cage complex shows significant catalytic activity along with the effects of the isolated single water molecule. On the other hand, reaction of $(bpy)Pd(PF_6)_2$ (bpy = 2,2'-bipyridine) with 1,3,5-tris(nicotinoyloxyethyl)cyanurate (L2) in acetone, and followed by addition of water and solvent evaporation allows to form amorphous spherical morphology consisting of $[(bpy)Pd(L2)]_2(PF_6)_4$ without any template or additive. In contrast, the reaction and slowly evaporation in acetone for 1 month yield single crystals consisting of $[(bpy)_3Pd_3(L2)(\mu^3\text{-}HPO_4)](PF_3(OH)_3)\cdot(OH)_3$. The formations of spherical morphology and cage-shaped single crystal appear to be primarily associated with the kinetic and thermodynamic control, respectively. The present compounds were characterized by IR, ^{19}F and ^{31}P NMR, and thermal analyses.

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발표분야: 무기화학

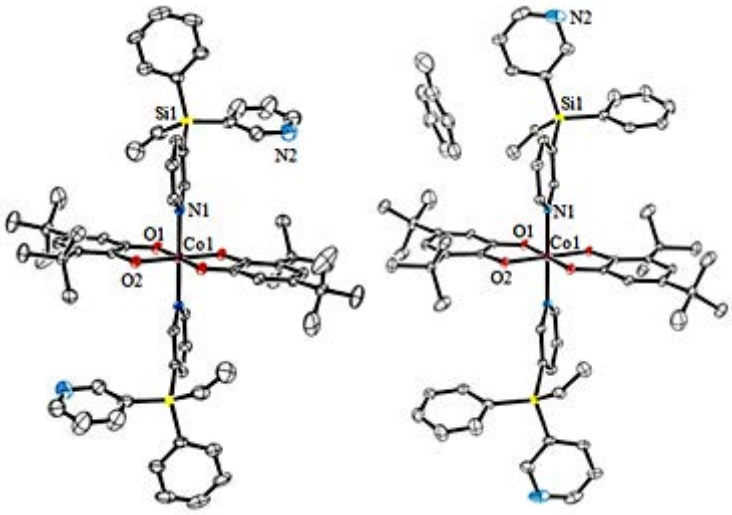
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1,2-Semiquinonato/catecholatocobalt Complexes Containing Bis(3-pyridyl)-phenylvinylsilane and Effects of Solvation

홍우식 정옥상

부산대 화학과

Recrystallization of [Co(3,5-dbbq)$_2$(L)$_2$] (3,5-dbbq = 3,5-di-*tert*-butyl-1,2-benzoquinone; L = bis(3-pyridyl)-phenylvinylsilane) from diethyl ether at -20 ℃ produces *trans*-[Co(3,5-dbbq)$_2$(L)$_2$] while the recrystallization from toluene at -20 ℃ gives *trans*-[Co(3,5-dbbq)$_2$(L)$_2$]·2PhMe. The complex exists as *trans*-[Co^{III}(3,5-dbsq)(3,5-dbcat)(L)$_2$] (3,5-dbsq = 3,5-di-*tert*-butyl-1,2-semiquinonato; 3,5-dbcat =3,5-di-*tert*-butylcatecholato) in the solid state at 173 K. Differences in charge distribution between *trans*-[Co(3,5-dbbq)$_2$(L)$_2$]and *trans*-[Co(3,5-dbbq)$_2$(L)$_2$]·2PhMe have been observed based on the effective magnetic moments and IR spectra of the complexes along with their X-ray crystal structures.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-173**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A chemical model of cysteine dioxygenase; the oxygen atom transfer reactivity of Cr(III)-superoxo species

우재영 조재흥[1] 남원우[2]

이화여대 바이오융합과학과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과

Oxygen-coordinating metal intermediates, such as metal?superoxo, ?peroxo, and ?oxo species, are frequently invoked as plausible oxidants in the oxidation of organic substrates. Previously, we found that an end-on Cr(III)-superoxo complex bearing a macrocyclic ligand, $[Cr^{III}(14\text{-TMC})(O_2)(Cl)]^+$ (1) (14-TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane), is capable of activating weak C-H bonds and oxidizing O-H bond. We recently studied about the oxygen atom transfer (OAT) reaction of the superoxo complex by using P-oxidation and S-oxidation substrates; the latter of reactions is mimicking the catalytic cycle of cysteine dioxygenase. Kinetic studies reveal that 1 is able to conduct OAT reactions and possesses an electrophilic character. In addition, a Cr(IV)-oxo complex, $[Cr^{IV}(14\text{-TMC})(O)(Cl)]^+$, is formed during the OAT reactions indicating that the terminal oxygen of the superoxo group in 1 is transferred to organic substrates.

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발표코드: **INOR.P-174**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ring Size Effect on O_2 Activation in the Chromium-O_2 Complexes bearing Macrocyclic Ligands

한정은 조재홍[1] 남원우[2]

이화여대 바이오융합과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과

Mononuclear metal-dioxygen species, such as metal-superoxo and -peroxo complexes, are critical components of processes leading to practical substrate oxidative transformations in enzymatic reactions. Previously, some of us reported an end-on Cr(III)-superoxo complex with a 14-membered macrocyclic ligand, $[Cr^{III}(14\text{-TMC})(O_2)(Cl)]^+$ (14-TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane), and its reactivity in C-H bond activation (e.g., electrophilic reactivity). In this work, a side-on Cr(IV)-peroxo complex, $[Cr^{IV}(12\text{-TMC})(O_2)(Cl)]^+$ (12-TMC = 1,4,7,10-tetramethyl-1,4,7,10-tetraazacyclododecane), was synthesized by changing ring size of the mycrocyclic ligand, and characterized with X-ray crystallography and spectroscopic methods such as UV-vis absorption, electrospray ionization mass, EPR, and resonance Raman. Compared to the Cr(III)-superoxo species, the Cr(IV)-peroxo complex was not reactive in electrophilic reactions but was capable of deformylating aldehydes via a nucleophilic reaction. These results indicate the significance of supporting ligands in regulating the stability, geometric and electronic structure and reactivity of metal-O_2 intermediates that have been shown to have biological as well as synthetic usefulness in biomimetic reactions.

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발표코드: **INOR.P-175**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Olefin Epoxidation by Cobalt(II) with Peracids: Role of an Active Oxidant Co^{II}-Acylperoxo Species

현민영 강주혜 김현 김경범 김철

서울과학기술대 정밀화학과

The present work described a new method for the fast epoxidation of a wide range of olefins using MCPBA as terminal oxidant and using a commercially available $Co(ClO_4)_2$ as a catalyst. The selectivity for the formation of epoxides was generally excellent enough to afford epoxides in high yields almost irrespective of electronic and/or steric variation of the substrates. Moreover, this catalytic system features a minimally allylic oxidation reaction. In particular, terminal olefins, which are normally least reactive to electrophilic oxidants and typically require long reaction times, were found to undergo fast conversion and high yields. These results suggest that the system $Co(ClO_4)_2$/MCPBA in CH_3CN is particularly suitable to achieve high yields in alkene epoxidations under simple and mild conditions, and that high activity and stability can be achieved without resorting to more extreme strategies such as very electron-deficient or complicated ligands.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

2-Thiopheneacetic acid directed fabrication of Au nanostuctures as SERS-active substrates

신혜선 허성

한국외국어대 화학과

Surface-enhanced Raman spectroscopy (SERS) has been one of the powerful tools for signal amplification and detection since its discovery in 1977. Not only overcomes it the several limitations of normal Raman scattering, but also enables us to open a new era of molecular detection based on spectroscopic technique. Special architectures of metallic substrates, normally silver, gold, or even sometimes copper, are required for Raman signal enhancement since they have appropriate values of the dielectric constant to support the localized electron oscillations, or localized surface plasmon resonance (LSPR). With the increasing interests on the proper metal substrates for SERS application, three-dimensional morphology control to generate effective and adequate hot spots creating strong electromagnetic field is getting exceptional attentions. Here we report 2-thiopheneacetic acid directed fabrication of rosette-like Au nanostructures with highly textured acute surfaces which give high SERS-activity. The rosette-like Au species with triangular topography exhibited evident SERS enhancements for the detection of methylene blue (MB) and crystal violet (CV). The detection limits of each were 10^{-9} M and 10^{-7} M, respectively.

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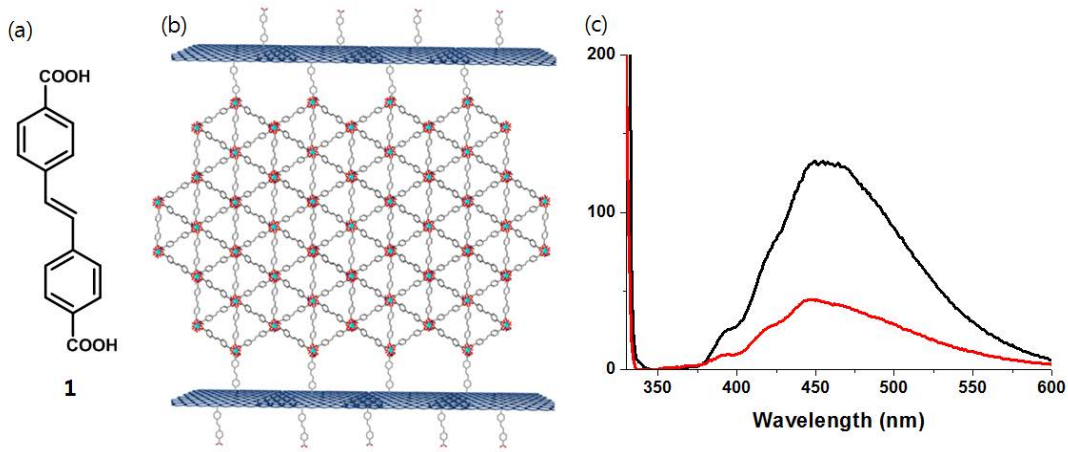
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure- Directing Role of Graphene Oxide-Based Metal Organic Framework for Explosive Detection

이지하 정종화

경상대 화학과

The azobenzoic acid derivative was attached into the surface of reduced graphene oxide. The azobenzoic acid-functionalized graphene oxide (A-GO) was used as a structure-directing template to prepare a metal-organic framework (MOF) structure MOF/A-GO composites were prepared at different concentration of ligand 1 in the presence of Zn^{2+} and were characterized by FT-IR, XPS, SEM, TGA and powder XRD. The MOF/A-GO composites showed the crystalline structures. MOF/A-GO composites form 2D structure. They exhibited the strong emission. When DNT was added to MOF/A-GO composite, the strong emission was quenched rapidly. As a result, MOF/A-GO composites can act as chemosensors, such as for the case of DNT molecule detection using a strong fluorescence enhancement.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-178**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization and Reactivity of Mn(IV)-Peroxo and Its Conversion to Mn(V)-Oxo

홍승우 박지영[1] 이용민[2] 박영준[1] 남원우[3]

이화여대 화학나노과학부 [1]이화여대 바이오융합과학과 [2]이화여대 기초과학연구소 [3]이화여대 화학과

Manganese-dioxygen adducts, including manganese-peroxo ($Mn-O_2$) and manganese-oxo (Mn=O) species, have been invoked as central intermediates in catalytic oxygen atom transfer reactions using porphyrin as well as in photosynthetic oxygen evolution. In order to stabilize higher oxidation state of metal center of the complexes, the supporting ligand should not be oxidized and required strong binding ability. TAML (tetraamidomacrocyclic ligand) is one of the best supporting ligand because it has shown to stabilize Fe(V)-oxo intermediate for the first time. In this context, we prepared $[Mn^{III}(TAML)]^-$ as a starting complex and upon addition of artificial oxidant such as peracetic acid and PhIO (iodosylbenzene), we were able to generate Mn(V)-oxo intermediate. Interestingly, the addition of potassium superoxide to the starting complex gave rise to Mn(IV)-peroxo intermediate which was converted to Mn(V)-oxo intermediate upon addition of benzoyl chloride.

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발표코드: **INOR.P-179**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, X-ray structures, and controlled ring opening polymerization behavior of *L*-lactide using titanium complexes chelated by tetradentate diamine-diethanolate ligand

김소한 고민정[1] 이준승[1] 김영조

충북대 화학과 [1]전남대 화학과

네자리 리간드인 살란, 살렌, 살라렌, 살로판은 [ONNO] 형태를 가지는데, 이들을 이용한 4 족 금속 화합물에 대한 합성 및 응용성 연구는 지금까지도 활발히 진행되고 있다. 하지만, 지방족 살란 리간드가 배위된 금속 화합물에 대한 연구는 다른 [ONNO]형태의 리간드에 비해 아직까지 많이 알려져 있지 않다. 이에 ($HOCMe_2CH_2NMeCH_2CH_2NMeCH_2CMe_2OH$) ($LH_2$)형태의 새로운 지방족 살란 리간드가 도입된 타이타늄 화합물들에 대한 합성, 구조 분석에 대한 결과를 발표하고자 한다. 더불어 합성된 화합물을 촉매로 사용하여 생분해성 고분자인 폴리락타이드의 리빙중합에 대한 결과도 보고하고자 한다.

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발표코드: **INOR.P-180**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Phan Complexes as Catalysts for Mukaiyama Aldol Addition of Aldehydes and Ketones with TMS Enolates

김소한 John. G. Verkade[1] 김영조

충북대 화학과 [1]Iowa State University, U.S.A

Mukaiyama Aldol 반응은 알데하이드 또는 케톤을 TMS enolate 를 사용하여 탄소-탄소 결합 형성을 통해 베타-하이드록시 카르보닐계의 화합물을 얻는 중요한 유기 합성 방법 중에 하나라고 알려져 있다. 이러한 Mukaiyama Aldol 반응에는 다양한 촉매가 사용된다고 알려져 있는데, 본 학술발표에서는 새로운 인계 촉매인 P(NRCH2CH2)3N 화합물을 합성하고, 이를 촉매로 사용하여 저온에서 다양한 종류의 알데하이드와 케톤의 Mukaiyama Aldol 반응에 응용한 예들에 대해 발표하고자 한다.

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발표코드: **INOR.P-181**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mukaiyama Aldol Reactions Catalyzed by a Trimeric Organo Aluminum(III) Alkoxide

김소한 John. G. Verkade[1] 김영조

충북대 화학과 [1]Iowa State University, U.S.A

Mukaiyama Aldol 반응은 알데하이드 또는 케톤을 TMS enolate 를 사용하여 탄소-탄소 결합 형성을 통해 베타-하이드록시 카르보닐계의 화합물을 얻는 중요한 유기 합성 방법 중에 하나라고 알려져 있다. 지금까지 Mukaiyama Aldol 반응에 사용되어진 알루미늄 화합물은 매우 제한적으로 알려져 있다. 특히 사용된 촉매는 단핵, 이핵 알루미늄만이 알려져 있고, 알루미늄 금속이 세 개 이상 존재하는 화합물의 예는 전무하다. 따라서 Mukaiyama Aldol 반응 촉매로 사용될 수 있는 신규 삼핵 알루미늄 화합물을 합성하고, 그 구조를 단결정 X-선 구조분석을 통해 밝히고자 한다. 더불어, 합성된 삼핵 알루미늄 화합물을 Mukaiyama Aldol 반응 촉매로 이용한 예들에 대해 발표하고자 한다.

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발표코드: **INOR.P-182**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimizing Hemocompatibility of Surfactant-Coated Silver Nanoparticles in Human Erythrocytes

우현제 박강현 윤부현[1]

부산대 화학과 [1]부산대 생명과학과

Several recent biological science studies have been focused on nanotechnology and nanomaterials due to their potential use in biomedicine. Drug delivery systems are an example of biomedical applications utilizing nanoparticles. Silver nanoparticles (AgNPs) can be used for these drug delivery systems. However, the effects of cytotoxicity caused by AgNPs are not fully understood. Determining the optimal characteristics to facilitate the biocompatibility of AgNPs is an important subject for application. In the present study, human erythrocytes were used as an in vitro model to examine the size, dose, and coating surfactant-dependent cytotoxicity of AgNPs. Our results demonstrated that polyvinylpyrrolidone (PVP) was a more suitable surfactant than polyethylene glycol (PEG) for AgNPs capping. In addition, we determined the appropriate particular size and dosage of AgNPs to reduce human erythrocytes hemolysis. Membrane damages including hemolysis, potassium efflux, protein leakage, and alterations in cell shape and membrane fragility were minimized with 100-nm AgNP particles. This study provides novel insights into AgNPs cytotoxicity and a basis for utilizing AgNPs for diagnostic and therapeutic applications.

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발표코드: **INOR.P-183**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Helical Arrangement of Gold Nanoprtcles by Nanofiber

정성호 정종화

경상대 화학과

터피리딘기를 갖는 트리포달 형태의 젤레이트 1 을 합성 하여 하이드로젤을 제조하였다. 하이드로젤의 특성은 TEM, AFM, FT-IR 및 CD 분광기를 이용하여 연구하였다. 특히 하이드로젤에 D-혹은 L-형태의 알라딘 유도체를 첨가하여 키랄특성에 대해서 연구를 수행하였다. 그결과 키랄성 알라딘 유도체를 포함하는 하이드로젤은 나선형 파이버를 나타내었다. 특히 나선형 파이버에 금나노입자를 첨가한 결과 금 나노입자는 나선형태로 배열하였다. 즉 나선형 나노파이버를 이용하여 금 나노입자를 나노구조로 배열 할 수 있었다.

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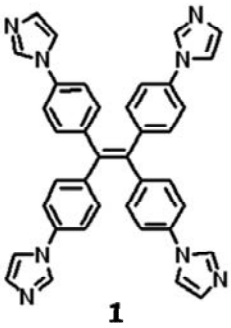
발표코드: **INOR.P-184**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

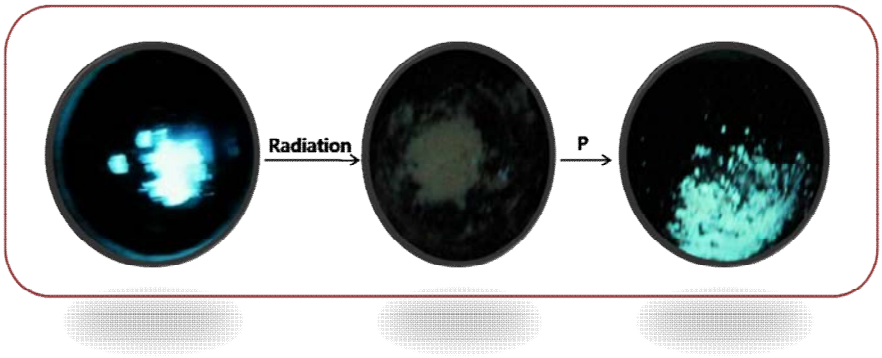
이미다졸기를 갖는 페닐유도체를 이용한 MOF제조 및 형광특성 연구

김가영 박선홍 정종화

경상대 화학과

금속-유기골격형 리간드로 이미다졸기를 갖는 화합물 1 를 두 단계 반응을 통해 합성하였다. 화합물 1 은 녹색 발광특성을 나타내었으며, 흥미롭게도 UV 빛을 조사한 결과 광이합체 반응이 진행되어 발광특성이 사라졌다. 광이합체반응에 의해서 생성된 화합물에 적당한 압력을 가한 결과 다시 발광특성이 나타났다. 따라서 화합물 1 은 UV 빛과 압력에 의해서 발광특성 제어가 가능했다. 그리고 화합물 1 에 전이금속을 첨가할 시 MOF 형태의 초분자 젤의 제조가 가능했다.





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장소: 부산BEXCO

발표코드: **INOR.P-185**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

그라핀과 파이렌 유도체를 활용하여 G-Quadruplex DNA를 검출하는 형광센서의 제조

문승진 정종화

경상대 화학과

일반적으로 G-quadruplexes 는 일가 양이온에 의해서 안정한 구조를 유지하며 네 가닥 DNA 로써 구아닌을 바탕으로 형성되어 있다. G-quadruplexes 은 telomere 의 암 세포 성장 및 제어 유전자 발현에 중요한 역할을 한다. 다양한 종류의 quadruplex 구조에 대한 높은 선택성과 신속하고 간단한 검출을 위해서는 독성이 없어야 하고 민감해야 하며, quadruplex DNA 의 생물학적 역할에 대한 검출방법이 간편해야 한다. 따라서, 본 연구에서는 파이렌 유도체 (JY-1)와[1] 그라핀를 이용하여 G-quadruplexes DNA 를 검출하고자 하였다. 그라핀 표면에 파이렌 유도체를 고정화 시킨 후, 다양한 DNA 와 선택적인 상호작용에 대한 연구를 형광분광기를 이용하여 수행하였다. 그 결과, 그라핀-파이렌 복합체는 구아닌 3 개 이상을 가지고 있는 DNA 와 선택적으로 결합하여 약 545nm 에서 강한 형광 스펙트럼을 나타내었다. 이는 파이렌 유도체가 구아닌기와 강한 상호작용으로 인해 파이렌 유도체의 ∏-∏stacking 상호작용을 하기 때문이다. 또한, 그라핀-파이렌 복합체는 약 20pM 의 DNA 를 감지할 수 있었다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-186**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Right-and Left-Handed Graphene Oxides Composites

박소현 문승진 정종화

경상대 화학과

Graphen oxide 는 Hummer 법에 의해서 graphite 로부터 제조하였다. Graphene oxide 는 HR-Raman 과 AFM 을 이용하여 분석하였다. 그 결과 graphene oxide 의 전형적인 D-band 는 1352cm^{-1} 에서 나타났고 G-band 는 1602cm^{-1} 에서 나타났다. 그리고 AFM 을 이용하여 관찰한 결과, 표면 두께는 약 1.0 nm 정도였다. 따라서 Hummer 법에 의해서 Grapene oxide 가 잘 제조되었음을 알 수 있었다. 이렇게 제조된 GO 를 정전기적 상호작용에 의해서 나선형 실리카 나노튜브에 고정화 시켰다. 그리고 GO 가 고정된 나선형 실리카 나노튜브는 전자 현미경을 이용하여 표면 특성을 체계적으로 연구하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-187**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

피리딘을 기반으로 하는 하이드로겔의 질소 치환 위치에 따른 특성 연구

안진호 김태호 박선홍 정종화

경상대 화학과

일반적으로 겔을 형성하는 주요한 분자간 힘에는 수소결합, 파이-파이 상호작용, 반 데르 발스 인력, 이온-쌍극자 상호작용 등이 있다. 따라서 본 연구에서는 피리딘 3 개가 구조에 포함된 파라 및 메타 치환체를 합성하였다. 두 종류의 젤레이터를 합성하여 젤 형성에 필요한 분자간 힘에 대하여 체계적으로 연구하였다. 특히 젤과 결정상태에서 분자 배열에 대한 비교연구를 단결정, PXRD 를 이용하여 수행하였다. 그 결과 젤 상태에서 분자 배열은 결정상태에서와 매우 유사하였다. 또한 젤의 안정도를 분자간의 상호작용을 통하여 분석한 결과 파라 치환체가 메타 치환체보다 더욱 강한 결합을 형성하고 있었다. 그리고 두 종류의 젤 상태에서 파이-파이 스팩킹이 형광특성에 미치는 영향을 조사한 결과 파라 치환체가 상대적으로 약한 파이-파이 스팩킹 상호작용을 통하여 강한 형광특성을 보였다.

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장소: 부산BEXCO

발표코드: **INOR.P-188**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of simonkolleite using sonochemical method

김아영 이수근

대구경북과학기술원 나노바이오연구부

Simonkolleite was synthesized using the sonochemical method with zinc chloride and hexamethylenetetramine as its starting materials. These Simonkolleite crystals have a flat plate-like morphology. The morphology still remains after calcination process which transforms simonkolleite into zinc oxide. The photocatalytic activities of the zinc oxide(flat plate shaped) in degradation of methylene blue was demonstrated and compared with the rod shape zinc oxide which was synthesized using sonochemical method. The structural and morphological properties of simonkolleite were characterized by X-ray diffraction(XRD) and scanning electron microscopy(SEM).

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

나프탈렌기를 갖는 리간드들을 이용한 Pb^{2+} 센서에 대한 연구

이진혁 박선홍 정종화

경상대 화학과

본 연구에서는 형광단으로써 나프탈렌기를 갖는 리간드 1 을 네 단계를 통하여 간단하게 합성하였다. 물에 대한 리간드 1 의 용해도를 증가시키기 위해서 pH 에 민감한 영향을 미치는 카르복시산을 도입하였으며, 특히 Pb^{2+} 의 결합자리로써 삼차 아민을 도입하였다. Pb^{2+} 에 대한 리간드 1 의 발광특성은 pH 7.4 수용액에서 형광 분광기를 이용하여 연구하였다. 그 결과 리간드 1 의 발광특성은 Pb^{2+} 첨가 시 548 nm 의 발광밴드가 급격하게 감소하였다. 이는 리간드 1 이 Pb^{2+} 과 결합하기 때문이다. 반면에 리간드 1 수용액에 다른 금속이온을 첨가 시 에는 어떤 형광 스펙트럼의 변화가 나타나지 않았다. 따라서 리간드 1 은 Pb^{2+} 과 선택적으로 결합함을 알 수 있다. 또한 녹색의 리간드 1 수용액에 Pb^{2+} 이 첨가됨으로써 무색으로 변화 하였다. 이는 리간드 1 은 Pb^{2+} 에 대한 발색 센서로도 활용 가능함을 의미한다.

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-190**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] 이광자 분자센서를 이용한 Zn(II) 센서에 대한 연구

이준규 박선홍 이재영[1] 정종화

경상대 화학과 [1]건양대 나노바이오화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Template Synthesis of Poly(macrocyclic) Nickel(II) and Copper(II) Complexes

이윤택 강신걸 정수경[1]

대구대 화학과 [1]김포대학 호텔조리학과

Although various types of polyaza macrocyclic ligands and their complexes have been prepared and investigated, examples of polynuclear polymer complexes containing 14-membered macrocyclic units are limited in number. New polynuclear poly(hexaaza macrocyclic) nickel(II) and copper(II) complexes have been prepared by the simple one-pot reaction of ethylenediamine and formaldehyde in the presence of the metal ion. The polymer complexes contain fully saturated 14-membered hexaaza macrocyclic units (1,3,6,8,10,13-hexaazacyclotetradecane) that are linked by *N*-$(CH_2)_2$-*N* chains. Synthesis, characterization, and chemical properties of the polymer complexes are presented.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Reactivity of Various Tetraaza Macrocycles Bearing *N*-Benzoyl Pendant Arm(s)

장보우 강신걸

대구대 화학과

Mono-, di-, and tetra-*N*-benzoylated derivatives (L^2, L^3, and L^4, respectively) of the macrocycle 3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (L^1) have been prepared by the reaction of L^1 with benzoyl chloride. The macrocycles were characterized by mass, IR, and NMR spectra. The reaction of the functionalized macrocycles with nickel(II) and copper(II) salts has been examined under various experimental conditions. The reactivity of the *N*-benzoylated derivatives is different from that of other functionalized derivatives of L^1. Synthesis, characterization, and chemical properties of L^2, L^3, and L^4 are presented.

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발표코드: **INOR.P-193**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Tris(macrocyclic) Nickel(II) Complexes Derived from Nitrile and Cyclic Amines

장보우 이윤택 강신걸

대구대 화학과

The cyanomethyl pendant arms of $[NiL^1]^{2+}$ (L^1 = 2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) react with the secondary amino group of 1,4,8,11-tetraazacyclotetradecane (A), 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacylotetradecane (B) or 3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (C) to yield the tris(macrocyclic) compound $[NiL^2]^{2+}$, $[NiL^3]^{2+}$, or $[NiL^4]^{2+}$, respectively. The pendant arms of the tris(macrocyclic) compounds contain A, B, or C. The tris(macrocyclic) compounds reacts with nickel(II) ion to form $[NiL^1]^{2+}$ and $[Ni(L)]^{2+}$ (L = A, B, or C). Synthesis, characterization, and chemical properties of $[NlL^2]^{2+}$, $[NiL^3]^{2+}$, and $[NiL^4]^{2+}$ are presented.

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발표코드: **INOR.P-194**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Macrocyclic Nickel(II) Complexes Bearing *N*-Aminomethyl Pendant Arms

방순무 강신걸 곽지훈[1]

대구대 화학과 [1]순천대 화학과

New di-*N*-functionalized macrocyclic nickel(II) complexes $[NiL^1)]^{2+}$ (L^1 = 2,13-bis(aminomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) and $[NiL^2]^{2+}$ (L^2 = 1,8-bis(cyanomethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacylotetradecane) have been prepared by the metal-assisted reduction of $[NiL^3]^{2+}$ (L^3 = 2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) or $[NiL^4]^{2+}$ (L^4 = 1,8-bis(cyanomethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacylotetradecane) using sodium borohydride under mild conditions. Synthesis, characterization, and chemical properties of the functionalized macrocyclic complexes are presented.

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발표코드: **INOR.P-195**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Reaction of Diamines with Two *N*-Cyanomethyl Pendant Arms of a Macrocyclic Nickel(II) Complex

방순무 강신걸

대구대 화학과

Ethylenediamine and 1,3-diaminopropane readily react with two cyanomethyl groups of $[NiL^1(OAc)]^+$ (L^1 = 1,8-bis(cyanomethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacylotetradecane) to yield $[NiL^2]^{2+}$ or $[NiL^3]^{2+}$ bearing two amidine functional pendant arms. On the other hand, prechloric acid salts of the diamines react selectively with one of the two cyanomethyl groups of $[NiL^1(OAc)]^+$, forming $[NiL^4]^{2+}$ or $[NiL^5]^{2+}$ bearing one cyanomethyl and one amidine pendant arms. The intra-molecular reaction of the two functional pendant arms of $[NiL^4]^{2+}$ and $[NiL^5]^{2+}$ produces the macrobicyclic complex $[NiL^6]^{2+}$ and $[NiL^7]^{2+}$, respectively, in which the two amidine groups are linked together by an ethylene or propylene chain.

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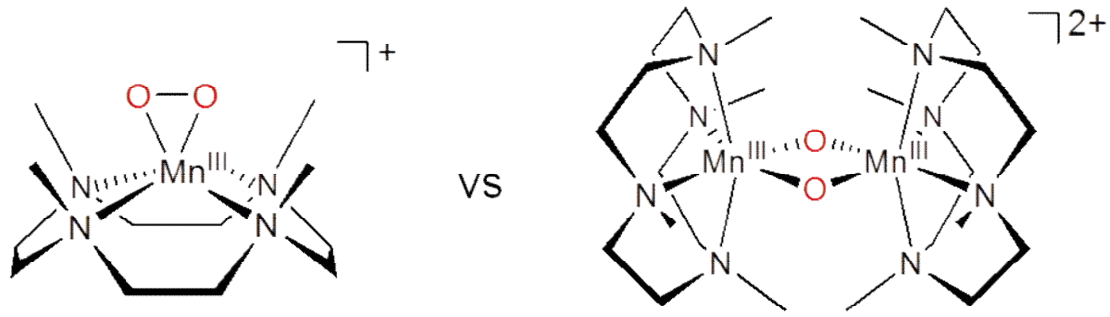
발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization and Reactivity of Mononuclear Mn(III)-Peroxo and Bis(μ-oxo)Mn(III)$_2$ Complexes Bearing the Same Macrocyclic Ligand

강현아 조재홍[1] 남원우[2]

이화여대 바이오융합과학과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과

Metal-active oxygen adducts are key intermediates detected in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. Some of us reported the structural and spectroscopic characterization and reactivity of mononuclear Mn(III)-peroxo complexes as biomimetic complexes. A number of bis(μ-oxo)Mn(III)$_2$ species have also been prepared and investigated as model complexes of photosystem II. However, there have been no studies on direct comparison between the mononuclear Mn(III)-peroxo species and the bis(μ-oxo)Mn(III)$_2$ species. Here, we report the differences in the structure and reactivity of the active oxygen complexes (i.e., $[Mn^{III}(12\text{-TMC})(O_2)]^+$ vs $[Mn^{III}(12\text{-TMC})(O)]_2^{2+}$; 12-TMC = 1,4,7,10-tetramethyl-1,4,7,10-tetraazacyclododecane) on the basis of the detailed comparison of these systems with the same ligand.



$[Mn^{III}(12\text{-TMC})(O_2)]^+$ $[Mn^{III}(12\text{-TMC})(O)]_2^{2+}$

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-197**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization and reactivity of a mononuclear non-heam manganese(III)-hydroperoxo complex

소희 조재홍[1] 남원우[2]

이화여대 바이오융합과학과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과

In biomimetic studies, a number of Mn-O_2 adducts have been synthesized and characterized and their reactivities in the oxidation of organic substrates have been extensively investigated. The synthesis and spectroscopic characterization of side-on peroxide Mn^{III}complexes bearing non-heme ligands and their reactivity was reported already. In this work, $[Mn^{III}(14\text{-TMC})(OOH)]^{2+}$ complex was prepared and characterized with spectroscopic methods such as UV-vis absorption and resonance Raman spectroscopy. The intermediate performed oxygen atom transfer (OAT) reaction with *para*-substituted-thioanisoles and then a negative ρ value (-5.0) is obtained. These results indicate the electrophilic character of $[Mn^{III}(14\text{-TMC})(OOH)]^{2+}$ in OAT reaction.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Diameter-controlled synthesis of thiol-functionalized hollow silica spheres through simple variation of water-ethanol Ratio

박지훈 최인성

KAIST 화학과

We report, herein, a synthetic method for thiol-functionalized hollow silica spheres as modulating their diameter. To incorporate thiol-functional groups in silica shell, 3-mercaptopropyl triethoxysilane (MPTES) was used along with tetraethyl orthosilicate (TEOS). The solvent composition (water-ethanol ratio) proved to be the prime factor to control diameter of silica spheres. It is noted that there is a critical ratio where silica spheres turn to hollow. After the critical ratio, the diameter of hollow silica spheres was decreasing as the water-ethanol ratio increased. As a result, we synthesize the hollow silica spheres ranging from submicrometer to one-micrometer size. Our method is a lot more simple than the conventional method, so it is highly applicable to a myriad of applications, including drug-delivery, photonic crystal, catalysis, and so forth.

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Changes of Electronic States of Heteroleptic Ru(II) Bipyridine Complexes by Remote Substituents

위경량 김성관 강상욱

고려대 소재화학과

We prepared a series of new heteroleptic ruthenium(II) complexes, Ru(NCS)2LL′ (3a?3e), where L is 4,4′-di(hydroxycarbonyl)-2,2′-bipyridine and L′ is 4,4′-di(p-X-phenyl)-2,2′-pyridine (X = CN (a), F (b), H (c), OMe (d), and NMe2 (e)), in an attempt to explore the structure?activity relationships in their photophysical and electrochemical behavior and in their performance in dye-sensitized solar cells (DSSCs). When substituent X is changed from electron-donating NMe2 to electron-withdrawing CN, the absorption and emission maxima reveal systematic bathochromic shifts. The redox potentials of these dyes are also significantly influenced by X. The electronic properties of the dyes were theoretically analyzed using density functional theory calculations; the results show good correlations with the experimental results. The solar-cell performance of DSSCs based on dye-grafted nanocrystalline TiO2 using 3a?3e and standard N3 (bis[(4,4′-carboxy-2,2′-bipyridine)(thiocyanato)]ruthenium(II)) were compared, revealing substantial dependences on the dye structures, particularly on the remote substituent X. The 3d-based device showed the best performance: η = 8.30%, JSC = 16.0 mA?cm?2, VOC = 717 mV, and ff = 0.72. These values are better than N3-based device.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-200**

발표분야: 무기화학

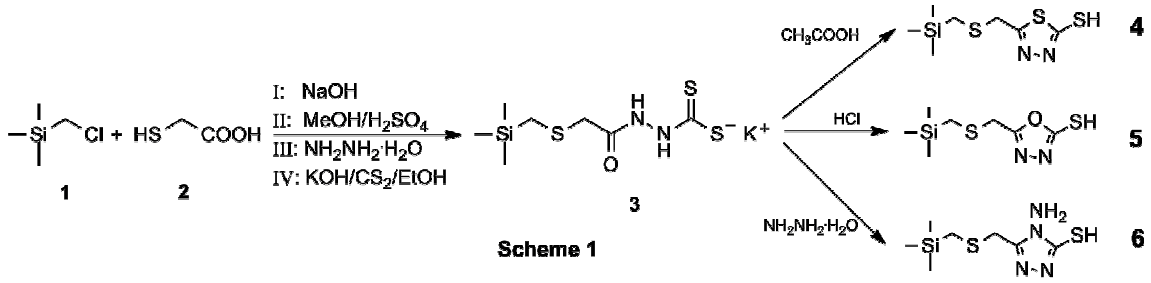
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Activity of a New Series of Sila-Substituted Azoles

Wang Tengjiao 조현모 이명의

연세대 화학 및 의화학과

Recently we reported the synthesis of a group of new sila-substituted 1,3,4-oxadiazoles and these compounds were evaluated for anti-allergic activity using RBL-2H3 as both of the in vitro model and the in vivo anaphylactic mouse model. With all experimental results, we believe that 2-(4-chlorophenyl)-5-(((trimethylsilyl)methylsulfonyl)methyl)-1,3,4-oxadiazole will be a useful clinical candidate for anti-allergic drugs.[1] In continuation of our research, a new series of azole derivatives containing silicon azoles drug[2] candidates were synthesized which were included different heterocyclic derivatives like: sila-substituted thio 1,3,4-thiadiazoles-2-thiol (**4**), sila-substituted thio 1,3,4-oxadiazoles-2-thiol (**5**) and sila-substituted thio 1,2,4-triazoles-2-thiol (**6**). In order to obtain these target compounds, the important intermediates potassium 2-(2-(((trimethylsilyl)methyl)thio/sulfonyl)acetyl)hydrazinecarbodithioate (**3**), were prepared in a multistep synthesis. In different conditions, the target compounds 4-6 were synthesized via the unstable salts **3 (Scheme 1)**.In this presentation, the biological activities will be discussed in detail.ReferenceG. D. Reddy; S. Park; H. M. Cho; T. Kim; M. E. Lee, J. Med. Chem., 2012, 55, 6438.Stephen Gately; Robert West, Durg Development Research, 2007, 68, 156.



Scheme 1

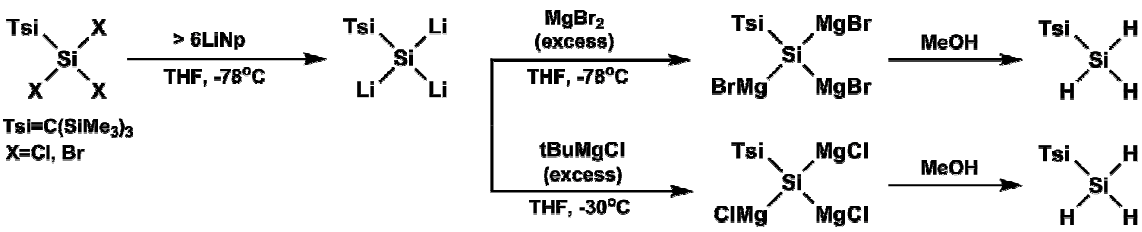
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **INOR.P-201**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Trilithiosilane and Its Transmetalation

송준현 조현모 이명의

연세대 화학 및 의화학과

The syntheses and structures of organosilicon lithium compounds have been the subject of much interest. Recently a few dilithiosilyl compounds including their synthetic applications and ab initio calculation, etc. were reported. However, trilithiosilane has not been reported yet. Last ten years we have synthesized stable halosilylenoids and dilithiohalosilanes formed from the reduction of trihalosilanes with strong reducing agents. These results prompted us to investigate a synthesis of trilithiosilanes.The reaction of trihalo[tris(trimethylsilyl)methyl]silane ($TsiSiX_3$, $Tsi=C(SiMe_3)_3$, X=Br, Cl) with more than 6 equivalents of lithium naphthalenide (LiNp) in THF at -78℃ gave trilithiosilane together with halodilithiosilane and halolithiosilane which are indirectly monitored by GC/MS after adding excess MeOH into reaction mixture. Transmetalation of lithiosilanes with $MgBr_2$, tBuMgCl and their thermal stability were also investigated. In this presentation, synthesis of trilithiosilane and its transmetalation will be discussed in detail.



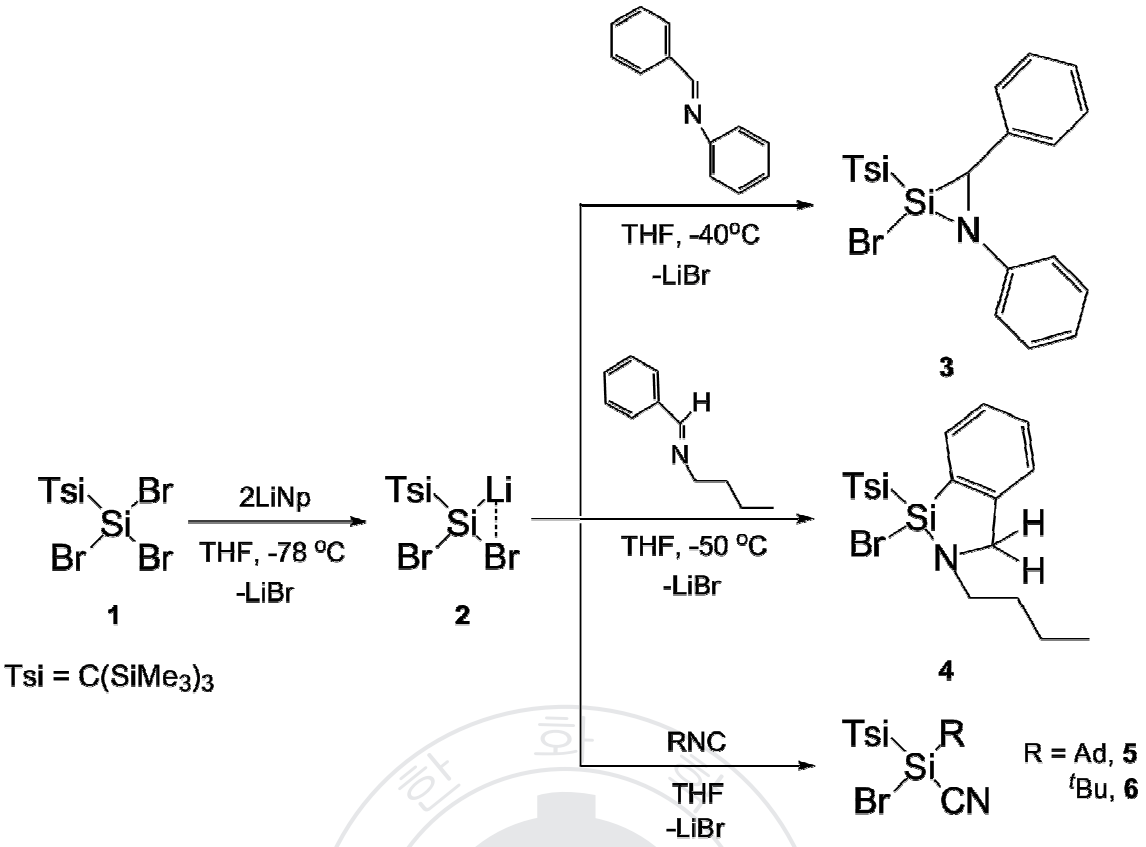
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **INOR.P-202**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reactions of Bromosilylenoid with Imines and Isocyanides

박서현 조현모 이명의

연세대 화학 및 의화학과

Silylenoids are species containing an alkali metal (M) and a leaving group (X, usually halogen) bound to the same silicon atom, which make them display amphiphilic properties. Reaction of a silylenoid with a compound containing CN multiple bonds has not been studied, whereas experimental studies of CN multiple bonds with silylenes have been reported by several groups, which can be shared with reaction characteristics of silylenoids. Herein, we report reactions of bromosilylenoid with imines and isocyanides.Bromosilylenoid, 2 was prepared from the reaction of tribromo[tris(trimethylsilyl)methyl]silane, 1 with two equivalents of lithium naphthalenide in THF at -78 ^{o}C. Then, compounds having CN multiple bonds, such as imines and isocyanides were added to resulting solution at same temperature. Interestingly, there were quite different results of reactions depending on imines. Silaaziridine, 3 was synthesized from the reaction of 2 with *N*,1-di(phenyl)methanimine, whereas with *N*-butylphenylimine, azaindane, 4 was formed. On the other hand, reactions of 2 with isocyanides such as 1-adamantane isocyanide and *tert*-butyl isocyanide afforded silacyanides 5 and 6 in good yields, respectively. In this presentation, we will discuss reactivities of bromosilylenoid with imines and isocyanides in detail.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-203**

발표분야: 무기화학

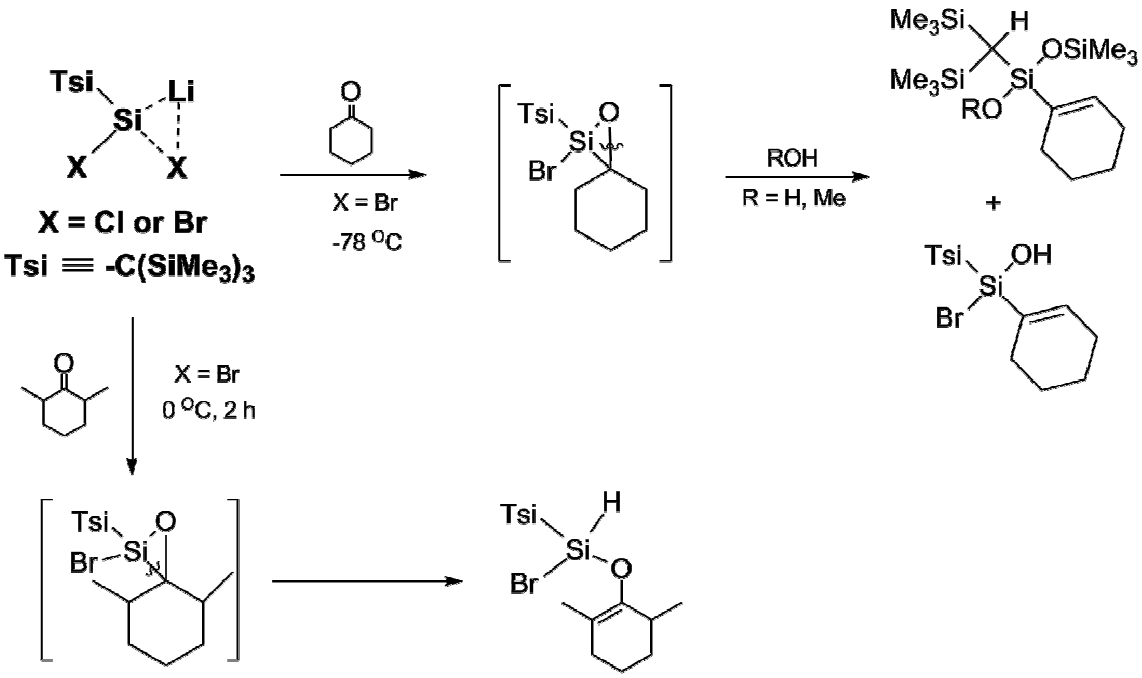
발표종류: 포스터, 발표일시: 수 16:00~19:00

Silylenoid Chemistry: Reactivities of Halosilylenoid with Carbonyl Compounds

김승한 이명의 조현모

연세대 화학 및 의화학과

Recently, we reported halosilylenoids stable at room temperature, which are bound to Li and halogen atoms on the same Si atom.[1-2] Halosilylenoids having the bulky substituent, Tsi (= trisyl, tris(trimethylsilyl)methyl), were synthesized by the reduction of trihalotrisylsilanes with 2 equiv of LiNp (lithium naphthalenide). We reported the reactivity of halosilylenoids with various carbonyls,[3-4] such as acetaldehyde, benzaldehyde, acetophenone and benzil.Now we report extended results of the reactivity of halosilylenoids toward ketones such as acetone, dimethylpentanone, tetramethylpentanone, cyclohexanone, and dimethylcyclohexanone. Interestingly, we obtained quite different products from the reactions of halosilylenoids with various ketones. In the reactions with acetone and cyclohexanone, C-O bond cleaved products were produced. Whereas with dimethylpentanone and dimethyl-cyclohexanone, Si-C bond cleaved products were obtained. With tetramethylpentanone, sterically hindered ketone, no reaction took place. In this presentation, we will discuss on plausible mechanisms for the reactivity of halosilylenoid with ketones in detail.



대한화학회
THE KOREAN CHEMICAL SOCIETY

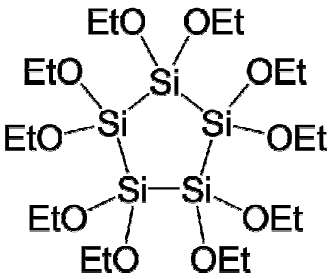
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **INOR.P-204**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

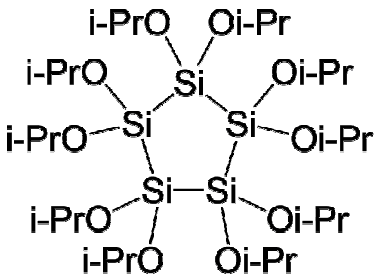
Syntheses of Alkoxycyclosilanes as New Precursors for Polysiloxane-polysilicon Hybrid Materials

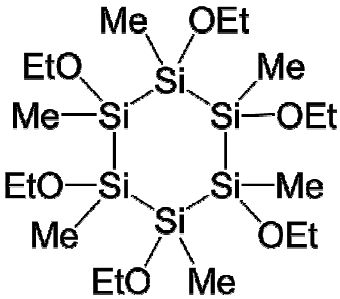
박성진 조현모 이명의

연세대 화학 및 의화학과

Cyclosilane is a silicon analogue of hydrocarbon ring compound. In contrast with cyclohydrocarbon compounds, general properties of cyclosilanes are similar with aromatic compounds, which come from delocalization of σ(Si-Si) electron. These compounds are attracting attention in application fields such as electronic materials. The cyclosilanes have been generally prepared by reductive coupling reactions of diorganodihalosilanes (R2SiCl2). The synthetic yields of cyclic silanes depend on the choice of reducing metals and substituent groups of diorganohalosilanes.We synthesized four, five and six membered ring silanes from the reactions of dichlorodiorganosilanes with reducing metals (Li and Mg) and then halogenated cyclosilanes were obtained by dephenylative chlorination. And nucleophilic substitution reactions of halogenated cyclosilanes with alcohols gave alkoxycyclosilanes which can be used as new precursors for polysiloxane-polysilicon hybrid materials.Using the new alkoxycyclosilanes with trimethoxymethylsilane, hybrids of polysiloxane and cyclosilane were prepared via hydrolysis and condensation. The materials which were soluble in organic solvent showed a high silicon content and optical property of deep UV absorption (193 nm). Thin films prepared with them via spin-coating and baking of the hybrids can be applied to etch selective process in semiconductor manufacturing since high silicon content materials show a high oxygen plasma resistance and a low CFx plasma resistance. And the deep UV absorption of thin films is key property to avoid unwanted reflections during patterning photoresists in ArF lithography process. We successfully prepared hybrid films and investigated their optical properties at 193 nm and etch selectivity toward O2 and CFx plasmas.







대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-205**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of CdTe/PbS core-shell nanostructure by simple sonochemical method

정원목 박종필 송미연 이원영 김항근 심일운 김영권

중앙대 화학과

Semiconducting nanocrystals are promising materials for various optoelectronic applications. Core-shell nanostructures such as CdTe/PbS, CuS/PbS, and PbTe/PbS are attractive for photovoltaic devices where the nanocrystals absorption could be tailored to allow maximum overlap with the solar spectrum. Here, CdTe/PbS core-shell structure which has broad light-absorption range is of great interest for photovoltaic devices. Firstly, CdTe nanoparticles were synthesized using $CdCl_2$ and Na_2Te in water. And then, CdTe/PbS core-shell nanocrytals were synthesized in ethylene glycol using CdTe NPs, $Pb(NO_3)_2$, and Thioacetoamide by sonochemical method. These core-shell nanocrytals were characterized by UV-vis spectrophotometer, near-infrared spectroscopy, X-ray diffraction, and high solution-transmission electron microscopy analyses.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-206**

발표분야: 무기화학

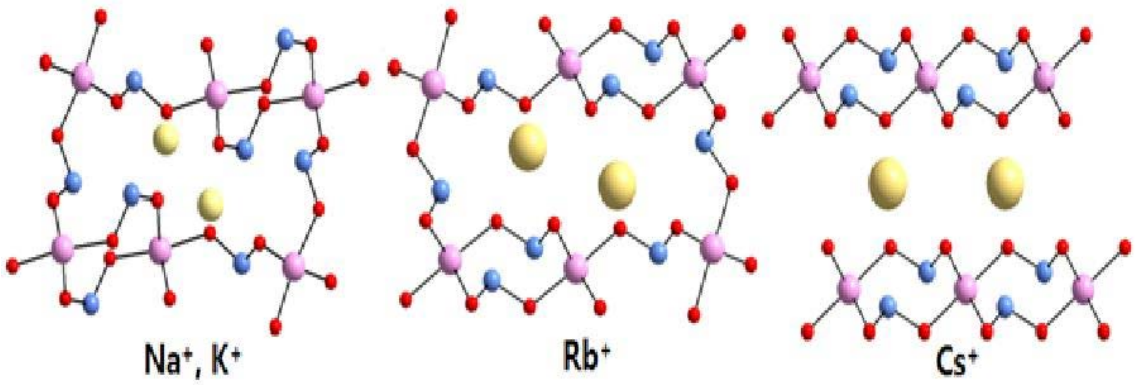
발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses, Structures, and Characterization of a Series of New Mixed Metal Selenites: $AIn(SeO_3)_2$ (A = Na, K, Rb, and Cs)

이동우 옥강민

중앙대 화학과

A series of new quaternary mixed-metal selenites materials, $AIn(SeO_3)_2$ (A = Na, K, Rb, and Cs), have been synthesized through hydrothermal and standard solid state reactions using A_2CO_3 (A = Na, K, Rb, Cs), $In(NO_3)_3?xH_2O$, In_2O_3, and SeO_2. The structures of the reported mixed metal selenites were determined by single-crystal X-ray diffraction. While the $AIn(SeO_3)_2$ (A = Na, K, and Rb) exhibit three-dimensional framework structures, $CsIn(SeO_3)_2$ reveals a layered structure. The cation size plays an important role in determining the framework structures of the materials. Complete characterizations including infrared spectroscopy, elemental analyses, and thermal analyses for the compounds are also presented, as are dipole moment calculations.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-207**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Cu_2SnSe_3 nanoparticles through a simple sonochemicalMethod

이원영 박종필 송미연 정원목 김항근 김영권 심일운

중앙대 화학과

Recently, cost of indium have increased because of its rarity. For this reason, Cu_2SnSe_3(CTSe) could be valuable material in photovoltaic applications to replace $CuInSe_2$. Synthesis of CTSe nanoparticles through a simple sonochemical method were performed under the multibubble sonoluminescence (MBSL) conditions. CuCl, $SnCl_2$, and Se powder were used for synthesis. Properties of Cu_2SnSe_3 nanoparticles were measured with XRD, SEM, UV-vis spectrophotometer, HR-TEM, and etc.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-208**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of SnS nanoparticles by simple sonochemical method

박종필 송미연 정원목 이원영 김영권 김항근 심일운

중앙대 화학과

IV-VI semiconductor nanoparticles such as PbS, and SnS that are optically active in visible light, near-infrared (NIR), and infrared (IR) are of great interest for their applications in photovoltaics and near-infrared detectors, and biomedical applications that is hyperthermia for absorption of strong IR in body. These applications have stimulated the development of proper synthetic method to make SnS NPs with narrow size distributions and well-defined optical properties. Here we synthesized SnS NPs of a few nanometers. SnS NPs nanoparticles were fabricated in ethylene glycol using $SnCl_2$ and thioacetoamide through sonochemical reaction. To control the SnS nanoparticle size, we used various ethanolamines such as ethanolamine, diethanolamine, and triethanolamine. These nanoparticles were characterized by UV-vis spectrophotometer, X-ray diffraction, and high solution-transmission electron microscopy analyses.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-209**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal Structures and Physical Properties of Eu(III) and Tb(III) Complexes with 6-hydroxypicolinic and 6-methylpicolinic acids

심용석 강성권

충남대 화학과

Metals in lanthanide series have different characteristics from transition metals because of their partially filled 4f orbitals. They emit lights in visible (strong: Sm3+, Eu3+, Tb3+, Dy3+, weak: Pr3+, Ho3+, Tm3+) and near infrared regions. Both metal organic compounds have been characterized by X-ray single crystal studies. Eu(III) and Tb(III) metals are coordinated to oxygen and nitrogen atom to form the distorted anti-square prism geometry. Tb(III) and Eu(III) complexes are investigated by the X-ray Single Crystal diffractometer, PL, IR, TGA, …etc.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-210**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Efficient Heterogeneous Catalysis by Hollow Mesoporous Aluminosilicate Nanospheres

김완석 노욱래 허성

한국외국어대 화학과

Recently, microporous crystalline aluminosilicates are widely used as a catalyst in the petrochemical and fine chemical industries due to their strong acidity, high stability, shape selectivity, and large ion exchange capacity. However, their usage is often limited to small substrates due to their small pore size. In order to overcome this fundamental hurdle, we prepared a series of new hollow mesoporous aluminosilicate nanospheres (HMAS) with controlled Si/Al ratio. The HMAS materials were fully characterized by transmission electron microscopy, scanning electron microscopy, powder X-ray diffraction, N_2 adsorption/desorption analysis, and solid-state NMR spectroscopy. The catalytic activities of HMAS materials were evaluated for several catalytic reactions such as the protection of benzaldehyde with pentaerythritol (PBP), condensation of benzaldehyde with 2'-hydroxyacetophenone (CBH), and esterification of benzyl alcohol with hexanoic acid (EBH). The HMAS materials exhibited superior activities for the model reactions compared with a commercial ZSM-5 zeolite.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-211**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

카드뮴이온에 의해서 유도된 배위고분자 젤의 제조 및 물성

이효희 정성호 정종화

경상대 화학과

피리딘기를 갖는 포단드형 리간드(I)를 합성하여 다양한 금속이온에 의한 배위고분자 젤을 제조하였다. 특히 카드뮴 이온과 리간드에 의해 제조된 배위고분자 젤의 다양한 물성을 AFM, UV-VIS, DSC 및 Rheometer 등으로 연구하였다.그 결과 리간드(I)의 배위고분자 젤은 π-π stacking 을 형성하지 않았으며, IR 연구에 의하면 리간드(I)은 분자간 수소결합을 형성하고 있었다. 또한 리간드(I)와 카드뮴이온 단결정의 단결정구조에 의하면 리간드와 피리딘과 카드뮴이온은 1:2 결합을 형성하고 있다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-212**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Redox-Inactive Metal Ion Effect on Iron(III)-Peroxo and -Hydroperoxo Complexes

김윤미 조재홍[1] 남원우[2]

이화여대 바이오융합과학과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과

Iron-oxygen species, iron(III)-peroxo, iron(III)-hydroperoxo and iron(IV)-oxo, are key intermediates in catalytic activation of dioxygen by iron-containing metalloenzymes. Recently, all three of these iron species have been spectroscopically characterized. Relative reactivity studies reveal that the iron(III)-hydroperoxo species are viable oxidants in both nucleophilic and electrophilic reactions by iron-containing enzymes.Unlike redox-active metals, such as iron and manganese, redox-inactive metal Ca^{2+} acts as an essential cofactor in the manganese-calcium (Mn_4Ca) active site of the oxygen-evolving complex (OEC) in photosystem II. However the exact functional role of Ca^{2+} remains unclear. Very recently, some of us reported the binding of the redox-inactive metal ion Sc^{3+} to a non-heme oxoiron(IV) complex, $[Fe(IV)(TMC)(O)]^{2+}$ (TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane). Interestingly, this interaction facilitates a two-electron reduction whereas only a one-electron reduction process occurs without the metal ions. To study metal ion effect on the iron(III)-peroxo and hydroperoxo intermediates, we employed Sc^{3+} and/or Y^{3+} as redox inactive metals. Here we are reporting new finding concerning the addition of Sc^{3+} and/or Y^{3+} to a mononuclear nonheme iron-peroxo complexes bearing a macrocyclic tetradentate N4 ligand, $[Fe(III)(TMC)(O_2)]^{+}$.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-213**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Unusual Catalytic Activity of a Copper Complex Containing Bromo-Substituted Pyridyl Schiff-Base Ligand in Oxidation of Phenolic Substrates

shuranjan sarkar 김유정 이홍인

경북대 화학과

Tyrosinase, which contains two copper ions in N-donor ligation, functions as a catalyst in the oxidation of phenolic substrate to catechols as well as in oxidation of catechols to corresponding quinones. Much effort has been spent on synthesizing mono and di-nuclear copper complexes as functional and structural models of tyrosinase. Here we report a new bioinspired monocopper complex containing Schiff-base ligand with bromo-substituted pyridyl side arms. The catalytic activities of the complex were tested by adding hydrogen peroxide or 3,5-di-tert-butylcatechol into the solution of the complex and monitored by EPR and UV-vis spectroscopy. The complexes indeed showed unusual catalytic activity for the oxidation of various phenols. This synthetic monocopper complex may both provide an insight on understanding the functional principles of the enzymatic action and lead the development of a novel bioinspired catalyst for oxidation and oxygenation chemistry. In this poster, we present the characteristics of the complex obtained by a combination of elemental analysis, UV-vis, IR, EPR and X-ray crystallography.

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발표분야: 무기화학

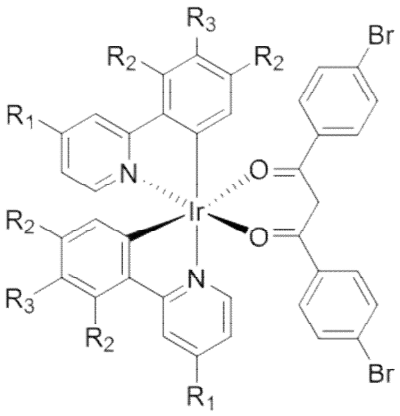
발표종류: 포스터, 발표일시: 수 16:00~19:00

Wide Bandwidth Emissive Heteroleptic Iridium(III) Complexes Bearing 1,3-Bis(*p*-bromophenyl)-1,3-propanedione

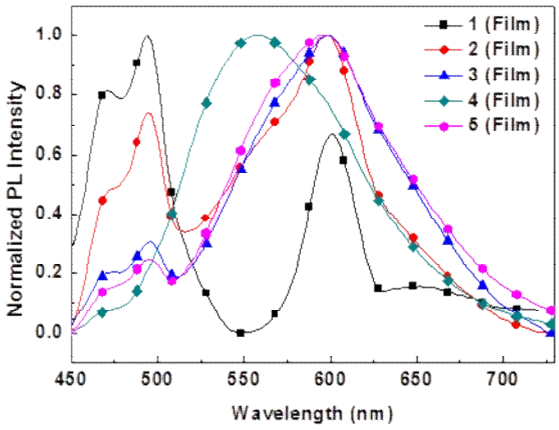
윤성재 김대영[1] 진성호[2] 강성권[3] 김영인[2]

부산대 첨단정보및디스플레이소재협동 [1]부산대 첨단정보 및 디스플레이소재협동과정 [2]부산대 화학교육과 [3]충남대 화학과

The heteroleptic iridium(III) complexes with extended π-conjugation system were designed and synthesized for organic light-emitting diodes (OLEDs); $(N^C)_2Ir(O^O)$, where N^C=2-phenylpyridine (ppy), 2-(2,4-difluorophenyl) pyridine (dfppy), 2-(2,4-difluorophenyl)-4-methylpyridine (dfpmpy), 2-(2,4-difluoro-3-trifluoromethylphenyl)-4-methylpyridine ($dfCF_3pmpy$), 2-(2,3,4-trifluorophenyl)-4-methylpyridine (tfpmpy) and O^O=1,3-bis(p-bromophenyl)-1,3-propanedione; $(ppy)_2Ir(dbacac)$ (1), $(dfppy)_2Ir(dbacac)$ (2), $(dfpmpy)_2Ir(dbacac)$ (3), $(dfCF_3pmpy)_2Ir(dbacac)$ (4) and $(tfpmpy)_2Ir(dbacac)$ (5). The complexes exhibited the wide bandwidth photoluminescence(PL) peak from blue to red region (450 ~ 700 nm). The performance of electroluminescence(EL) device based on complex 4 ($(dfCF_3pmpy)_2Ir(dbacac)$) was evaluated with the values of the CIE coordinate for device 1 at 10 mV/cm^2 of (0.484, 0.502), the maximum external quantum efficiency of 2.06 %, luminance efficiency of 5.18 cdA^{-1} and power efficiency of 1.80 lmW^{-1}.



1 = R_1 : H, R_2 : H, R_3 : H
2 = R_1 : H, R_2 : F, R_3 : H
3 = R_1 : CH_3, R_2 : F, R_3 : H
4 = R_1 : CH_3, R_2 : F, R_3 : CF_3
5 = R_1 : CH_3, R_2 : F, R_3 : F



대 한 화 학 회
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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-215**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of New Pd(II) Complexes for Potential Catalysts of MMA

김성훈 손유리 이하진[1] 이효선

경북대 자연과학대학 화학과 [1]한국기초과학지원연구원 전주센터

The development of well-defined palladium-based complexes capable of catalyzing MMA (Methyl methacrylate Polymerization), has been particularly focused due to their increased tolerance to functional group in the substrate. In this regard, the chemistry of palladium complexes with N-donor ligand have been extensively reported as this respect. Here, we report new palladium complexes $PdLnCl_2$ with their X-ray crystal structures, which was prepared by the starting material $Pd(CNCH_3)_2Cl_2$ ligated to Ln (L1~L3), where (L1 =N-((pyridin-2-yl)methyl)benzenamine), L2 = (4-fluoro-N-((pyridin-2-yl)methyl)benzenamine), L3 = (4-methoxy-N-((pyridin-2-yl)methyl)benzenamine). In addition, new Pd complexes were investigated for their catalytic polymerization ability toward MMA along with the effect of temperature control.

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발표코드: **INOR.P-216**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Characterization and Polymerization Study of Pd(II) Complexes with Mixed α-Diimine Ligands

김은희 김동일 김성훈 이하진[1] 이효선

경북대 자연과학대학 화학과 [1]한국기초과학지원연구원 전주센터

The reaction of $Pd(AN)_2Cl_2$ with α-diimine ligands, including N-cyclopentyl-pyridin-2-yl-imine (L_1), N-cyclohexyl-pyridin-2-yl-imine (L_2), N-1-piperidine-pyridin-2-yl-imine (L_3), in ethanol yielded (NN')$PdCl_2$ complexes, i.e., L_1PdCl_2, L_2PdCl_2 and L_3PdCl_2, respectively. The new synthesized Pd(II) complexes and their molecular structures were characterized by ^{1}H-NMR, ^{13}C-NMR and X-ray diffraction method. The X-ray crystallographic analysis revealed that the Pd atoms in the complexes have a distorted square plane geometry involving two nitrogen atoms and two chloro ligands. The catalytic activities of Pd(II) complexes for methyl methacylate (MMA) are also investigated in toluene at 0°C ~ 60°C.

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장소: 부산BEXCO

발표코드: **INOR.P-217**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effective enhancement of the performance of Z907 and TG-6 dyes based dye-sensitized solar cells by anchoring group modification

김점종 김보람[1] 성기현[1] 강만구 윤용진[1]

한국전자통신연구원 [1]경상대 화학과

Dye-sensitized solar cells (DSSCs) have been extensively studied as a novel sunlight to electricity conversion system. Polypyridyl ruthenium sensitizers such as N719 have shown to be excellent dyes in DSSCs and their photoconversion efficiency is more than 10 % under air mass 1.5 sunlight. The main drawback of the sensitizer is the low stability under prolonged heating at 80°C. In 2003, gratzel group have successfully developed more stablized Z907 dye with 7-8% efficiency by introducing nonyl alkyl group on the bipyridyl ligand. The low efficiency is because of the molar extinction coefficient of this sensitizer is lower than that of the standard N719 dye. Novel three ruthenium bipyridyl sensitizers with general formula $(Me_3PhN)_4[Ru(dcbpy)_2\text{-}(NCS)_2]$ (JJ-7), $(Me_3PhN)_2[Ru(dinonylbpy)(dcbpy)\text{-}(NCS)_2]$ (JJ-11) and $(Me_3PhN)_2[Ru(dihexylsulfanylphenyl)vinylbpy)(dcbpy)\text{-}(NCS)_2]$ (JJ-14) by anchoring group modification have been synthesized and demonstrated as efficient sensitizers in dye-sensitized solar cells. Under standard AM 1.5 sunlight, the solar cell of JJ-11 and JJ-14 using a liquid-based electrolyte exhibits an efficient conversion efficiency of 9.20 % and 9.68 %, respectively. The efficiencies of JJ-11 and JJ-14 are more hgher than those of couping dye, Z907 and TG-6.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fundamental Electron Transfer Properties of a Nonheme Mn(IV)(O) Complex

윤희정 이용민[1] Shunichi Fukuzumi[2] 남원우[3]

이화여대 바이오융합과학과 [1]이화여대 기초과학연구소 [2]Osaka University [3]이화여대 화학과

High-valent metal-oxo species have been taking center stage as key intermediates in the oxidation of organic substrates. Although manganese(IV)-oxo complexes have high prospect for providing valuable mechanistic insight into the catalytic activities, fundamental electron transfer (ET) properties of nonheme manganese(IV)-oxo complexes haven't been reported yet. In this presentation, we report for the first time the fundamental electron transfer properties of a nonheme manganese(IV)-oxo complex. Investigation of electron-transfer properties of a nonheme manganese(IV)-oxo complex, $[(Bn\text{-}TPEN)Mn(IV)(O)]^{2+}$, reveals that this manganese(IV)-oxo complex acts as a stronger one-electron oxidant than the iron(IV)-oxo analogue. As a result, an electron transfer process in *N*-dealkylation has been detected by the transient absorption spectrum of a radical cation intermediate, *para*-Me-DMA$^{?+}$, in the oxidation of *para*-Me-DMA by $[(Bn\text{-}TPEN)Mn(IV)(O)])]^{2+}$.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dioxygen Activation by a Nonheme Iron(II) Complexes in the Presence of Lewis Acid and NADH Analogue

방수희 이용민[1] 홍승우[2] Shunichi Fukuzumi[3] 남원우[4]

이화여대 바이오융합과학과 [1]이화여대 기초과학연구소 [2]이화여대 화학나노과학부 [3]Osaka University [4]이화여대 화학과

One primary goal in biomimetic research is to understand mechanisms of dioxygen activation, structures of reactive species, and reactivities of the intermediates involved in catalytic oxidation reactions by metalloenzymes, such as heme and nonheme iron oxygenases. In this presentation, we report the first example of using a biologically important electron donor, an NADH analogue, in the presence of redox-inactive metal ion, such as Sc^{3+}, Y^{3+}, Zn^{2+}, Mg^{2+} and Ca^{2+}, in generating nonheme iron intermediates by activating O_2. We have already demonstrated that high-spin nonheme iron(II) complexes with a low $Fe^{III/II}$ redox potential are able to bind and activate O_2 to generate the iron-oxygen intermediates and that the spin state and oxidation potential of iron(II) complexes can be tuned by varying supporting ligands and solvent systems. We demonstrate herein that a nonheme iron(II) complex activates O_2 and generates its corresponding Fe(IV)(O) complex in the presence of an NADH analogue and redox-inactive metal ion having stronger Lewis acidity, such as Sc^{3+}, Y^{3+} and Zn^{2+} ions, whereas a nonheme iron(II) complex generates its corresponding Fe(III)-O-O-M^{n+} (M^{n+} = Mg^{2+} and Ca^{2+}) in the presence of an NADH analogue and redox-inactive metal ion having weaker Lewis acidity.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Luminescent Li-based Metal-Organic Framework Tailored for Selective Detection of Explosive Nitroaromatic Compounds: Direct Observation of Sensing Mechanism

이재화 김태경 문희리

울산과학기술대 친환경에너지공학부

A luminescent lithium metal-organic framework is constructed from solvothermal reaction of Li^+ and a well-designed organic ligand, bis(4-carboxyphenyl)-*N*-methylamine (H_2CPMA). Li-based MOF can detect explosive aromatic compound containing nitro groups as an explosophore, by showing a dramatic color change with concurrent luminescence quenching in the solid state. The sensing mechanism is proved directly through single-crystal-to-single-crystal transformations, which show strong interactions between the aromatic rings of the electron-rich $CPMA^{2-}$ molecules and the electron-deficient nitrobenzene.

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발표코드: **INOR.P-221**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Molybdenum Disulfide Precursors

여소정 박보근[1] 유태수 김창균[1] 정택모[1] 전동주[1]

충북대 화학과 [1]한국화학연구원 화학소재연구본부

Stable 2D nanosheet molybdenum chalcogenides crystals have been widely studied for many applications such as solid lubricants, catalysts, lithium-battery cathodes, photovoltaic solar cells, and scanning tunneling microscopy (STM) tips due to their unique properties. Unlike no bandgap of pristine graphene, MoS_2 monolayer prepared from bulk crystal by scotch tape method shows semiconductor-like bandgap which is essential for the device applications. Atomic layer deposition (ALD) or chemical vapor deposition (CVD) method to prepare MoS_2 thin films usually requires suitable precursors. Herein, we report on the synthesis and characterization of novel monomeric molybdenum single precursor for MoS_2 thin film. The novel precursors were fully characterized by NMR, IR, mass spectroscopy, thermogravimetric analysis (TGA), and differential thermal analysis (DTA), as well as elemental analysis. MoS_2 thin film preparation using our novel precursors are under investigation.

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발표분야: 무기화학

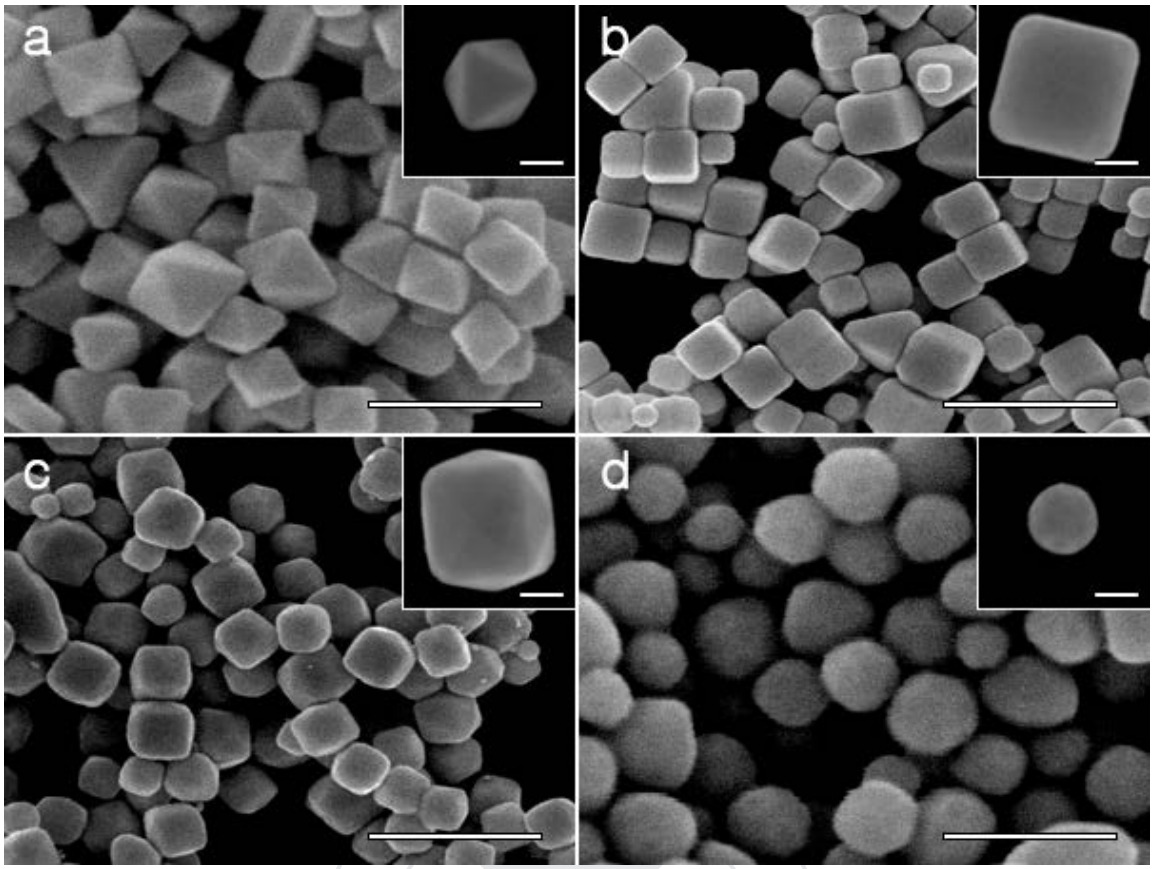
발표종류: 포스터, 발표일시: 수 16:00~19:00

Bovine Serum Albumin as an Effective Surface Regulating Biopolymer for Morphology Control of Gold Polyhedrons

이선주 송현준

KAIST 화학과

In the preceding work, we have synthesized gold polyhedral nanocrystals through the polyol process in the presence of poly(vinyl pyrrolidone) (PVP) and PVP analogues. 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. Bovine Serum Albumin (BSA) which is one of the most widely used proteins contains a structural motif of amides with bulky surroundings, so it is expected to strongly bind to the metal surface. We have used BSA as a surface regulating biopolymer for the synthesis of gold polyhedrons including octahedrons, cubes, tetrahexahedrons (THH), and higher polygons under the present polyol reaction conditions (Figure). BSA consists of various functional groups other than amide groups as compared to PVP, and it brings some differences in shape evolution and dispersity of the resulting gold nanocrystals. From FT-IR and SDS-PAGE analysis, we reveal that the secondary structure of BSA changes after the formation of gold nanocrystals. BSA is a promising surface regulating agent in the polyol synthesis so as to design biocompatible gold polyhedral nanocrystals for biological applications.



THE KOREAN CHEMICAL SOCIETY

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장소: 부산BEXCO

발표코드: **INOR.P-223**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Novel Germanium Precursors for Ge2Sb2Te5 (GST)

김효숙 박보근[1] 김창균[1] 정택모[2]

성균관대 화학과 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학소재연구단

Germanium complexes have been extensively studied due to potential application in germanium antimony telluride (GST) thin films for next generation nonvolatile phase-change random access memory (PRAM). Various routes to new molecular precursors for low temperature synthesis of germanium complexes were investigated. The germanium precursors newly synthesized for application in films are thermally stable and highly volatile and lessen incorporation of impurities. In this presentation, we will disclose the synthesis and characterization of novel germanium precursors on the basis of molecular design. Thermal decomposition of the germanium precursors was carried out to prepare germanium chalcogenide.

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장소: 부산BEXCO

발표코드: **INOR.P-224**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-resolution optical spectroscopy and modern ligand-field analysis of bis(ethylenediaminemonoacetato-N,N´,O)chromium(III) moiety

최종하 유건상[1] 홍용표[1]

안동대 화학과 [1]안동대 응용화학과

The sharp-line absorption spectrum of microcrystalline samples of $(H_2en)[Cr(edma)_2]_2Cl_4.2H_2O$ (edma=ethylenediaminemonoacetate) has been measured between 13000 cm^{-1} and 16000 cm^{-1} temperatures down to 5K. The emission, excitation, infrared and UV-visible absorption spectra have also been measured. The vibrational intervals of the electronic ground state are extracted from the far-infrared and emission spectra. The nine electronic bands due to spin-allowed and spin-forbidden transitions are assigned. Using the observed electronic transitions, a ligand field analysis was performed in the framework of the angular overlap model. The zero-phonon line in the sharp-line absorption spectrum splits into two components by 168 cm^{-1}, and the large ^2E_g splitting can be reproduced by the ligand field theory. It is confirmed that oxygen atoms of the edma ligand have strong σ- and π-donor properties toward chromium(III) ion.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Fluorene and Carbazole Dithienosilole Derivatives for Potential Applications in Organic Light Emitting Diodes

박형근 박정은 김진호 강영진[1]

강원대 화학과 [1]강원대 과학교육과

Several fluorene or carbazole-based dithienosiloles (DTSs) have been synthesized and their thermal, photophysical and electrochemical properties have been systematically investigated. These compounds show high thermal stability with glass transition temperature above 110 ℃ as well as decomposition temperatures at ~400 ℃. Intense green emission is observed in the of 500-510 nm spectral region for all compounds (ΦPL = 0.31 ~ 0.80), that is attributed to both the 5,5′-substituents of the DTS ring and DTS-based π-π* transition. Based on the emission spectra at 77K, the triplet energy for these compounds was calculated to be within 2.1~2.2 eV, indicating that they may be used as host materials for red emitters in organic light-emitting diodes (OLEDs). All compounds exhibit reversible oxidation and possess low-lying LUMO energies, owing to the conjugated fluorene/carbazole substituents on the DTS. This along with the high thermal/electrochemical stabilities and high fluorescent quantum efficiencies makes the new DTSs compounds promising candidates for use in OLEDs as emitters, host and electron-transporting materials.

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발표코드: **INOR.P-226**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bipyridine-based Ir (III) complexes emitting blue to yellow phosphorescence.

박정은 박형근 김진호 강영진[1]

강원대 화학과 [1]강원대 과학교육과

Cyclometalated Iridium(III) complexes are regarded as excellent phosphorescent materials and have been widely studied due to their ability to achieve a maximum internal quantum efficiency of nearly 100%, as well as high external quantum efficiency in organic light emitting diodes (OLEDs). Heteroleptic Ir(III) complexes, $(C^N)_2Ir(L^X)$, are considered to be promising phosphorescent metal compounds for application in OLEDs because they have both high thermal stability and phosphorescent efficiency. Particular attention has been emphasized on $Ir(ppy)_2(L^X)$ (ppy=2-phenylpyridine) complexes due to their HOMO-LUMO energy gap being easily adjustable by simple modification of either the ppy rings or L^X ligand. Our interest in the development of highly efficient phosphors for application in OLEDs has prompted us to synthesize and investigate the photophysical and electrochemical properties of $Ir(bpy)_2(L^X)$, (L^X, pic. = picolinate, prz. = pyrazinate, iq. = isoquinolinate, qnd = quinaldinate). Herein we describe the results of our investigation on the preparation, structural characterization, and photophysical properties of a series of heteroleptic Ir(III) complexes bearing alkoxy-functionalized bipyridine as a main ligand

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

자성 나노-다공성 실리카 껍질 구조체를 이용한 약물 및 유전자 전달 지지체로의 응용 연구

권용수 윤영일[1] 윤태종[2]

CHA의과학대 바이오공학과 [1]서울대 나노융합 [2]CHA 의과학대 바이오공학과

생체 적합성 나노 물질을 이용한 이미징, 약물 전달 지지체, 유전자 전달 지지체 등으로의 바이오 분야 응용 연구는 매우 활발히 진행되고 있다. 자기적 성질을 갖는 자성 나노 입자를 합성하고, 이의 표면으로 부터 졸-겔 방식으로 메조 다공성 구조체를 갖는 껍질을 쌓는데 성공 하였다. 결정성 또는 비결정성의 실리카 껍질이 쌓여진 자성 나노 입자보다 메조 다공성을 갖는 껍질이 자기적 성질 (이완율, r2)을 높이는데 기여 하였음을 확인 하였다. 합성된 자성 나노-메조 다공성 껍질 구조체를 세포내에 침투 시키고자 메조 실리카 껍질에 다양한 화학적 화합물을 처리 하였고, 세포가 성장하는 용액에서 안정성을 높일 수 있었다. 메조 다공성 실리카 껍질의 구조적 특징을 이용하여, 세포 성장을 억제하는 약물을 도입 할 수 있었으며, 이를 세포에 처리하여, 세포 사멸을 일으키는 과정을 밝혀냈다. 또한 약물을 이용한 세포 치료 뿐만 아니라, 유전자를 이용한 세포 치료의 가능성을 확인하기 위해서 합성된 나노 구조체에 양전하성을 갖는 화합물을 처리 하였고, 구조체와 유전자의 혼성체를 전기영동 분석법으로 확인 가능하였다. 이를 세포에 처리하여 세포질내에서 전달하고자 하는 유전자에 의한 단백질 발현이 성공적으로 이뤄졌음을 확인 하였다. 합성된 자성 나노-메조 다공성 실리카 나노 구조체는 세포내에 약물 및 유전자를 쉽게 전달 할 수 있는 가능성을 보였으며, 이에 대한 직접적인 세포 치료의 응용 연구를 진행 할 계획에 있다.

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발표코드: **INOR.P-228**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of New Tin Precursors

정은애 박보근 김창균 정택모

한국화학연구원 화학소재연구본부

Studies of metal oxide semiconductors have widely reported these types of semiconductors as candidates for optoelectronic device applications such as light-emitting diodes (LEDs) and thin film transistors (TFTs) over the last few years. Tin dioxide belongs to a class of materials that combines high electrical conductivity with optical transparency and thus constitutes an important component for optoelectronic applications.In this study, novel Sn precursors were synthesized and characterized by NMR, FT-IR, elemental analysis, and TGA/DTA. The structure of the compounds was studied by single crystal diffraction.

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Redox-Inactive Metal Ion Effect on the Epoxidation of Styrene Derivatives by Iron(IV)-Oxo Intermediate

권윤혜 이용민[1] Shunichi Fukuzumi[2] 남원우[3]

이화여대 [1]이화여대 기초과학연구소 [2]Osaka University [3]이화여대 화학과

Redox-inactive metal ions, such as Ca^{2+} and Mg^{2+}, play pivotal roles in biological redox systems, such as *photosynthesis and respirations*. Recently, we reported the first example of bind of metal ions such as Sc^{3+} and Ca^{2+} to Fe(IV)(O) complex. More importantly, the oxo-Sc^{3+} interaction facilitates a two-electron reduction by ferrocene, whereas only a one-electron reduction process occurs in the absence of the metal ions. In this presentation, we report remarkable acceleration effects of redox-inactive Sc^{3+} ion on the epoxidation of styrene derivatives by $[Fe(IV)(O)(N4Py)]^{2+}$ in CH_3CN at 298 K. The redox potential of $[Fe(IV)(O)(N4Py)]^{2+}$ in the presence of Sc^{3+} ion (10 mM), which was determined to be 1.19 V *vs.* SCE, exhibits a large positive shift as compared to the value in the absence of Sc^{3+} ion (0.51 V *vs.* SCE). The rate of reaction of *para*-MeO-styrene was remarkably accelerated as much as 10^3-fold in the presence of Sc^{3+} (10 mM) compared with that in the absence of Sc^{3+}. However, in other cases of *para*-X-styrene derivatives (X = Me, H and Br), the rates in the presence of Sc^{3+} were just 2 - 3 times faster than those in the absence of Sc^{3+}. We discussed herein the remarkable effects of Sc^{3+} ion in accelerating the reaction rate and changing the mechanism from direct oxygen transfer (DOT) to electron transfer followed by oxygen transfer (ETOT) in the epoxidation of styrene derivatives by a nonheme iron(IV)-oxo, $[Fe(IV)(O)(N4Py)]^{2+}$, and borderline between DOT and ETOT.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Ta Precursors Using ALD/CVD

신수정 정택모[1] 김창균[2] 박보근[2]

고려대 화학과 [1]한국화학연구원 화학소재연구단 [2]한국화학연구원 화학소재연구본부

Metal-organic complexes of early trasition metals, bearing nitrogen-containing ligands received increasing attention over the last decades. major application of these compounds is their use as precursors for thin films by MOCVD and ALD techniques. Tantalum nitride (TaN_x) films have been an attractive candidate as a diffusion barrier, gate electrode for CMOS (complementary metal oxide semiconductor), and electrodes for capacitors used in memory devices. Also tantalum carbo-nitride (TaC_xN_y) films have been studied as a gate electrode in the next generation nano-CMOS technology for its low resistivity, proper work function, and high reliability.We synthesized novel Ta precursors for TaN_x) and TaC_xN_y) thin film deposition using ALD/CVD process. All compounds have been characterized by means of NMR, FT-IR spectroscopy, elemental analysis, and TGA.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Novel Gallium Sulfide Complexes

박주현 김창균[1] 김종원 박보근[1] 정택모[1] 전동주[1]

충북대 화학과 [1]한국화학연구원 화학소재연구본부

Gallium sulfide (Ga_2S_3) is an important material for optoelectronic and photovoltaic applications due to its stability, wide band gap, and photoconductive behavior. Recently, high quality gallium sulfide thin films have been explored using ALD/CVD technique. Suitable precursors are needed to deposit thin films of inorganic materials. However, gallium sulfide precursors available for ALD/CVD process are very limited to gallium complexes with dithiocarbamate and alkanethiolate ligands. Therefore, it was essential to prepare novel gallium sulfide suitable for ALD/CVD precesses. Herein we report on the synthesis and characterization of new gallium sulfide complexes with designed aminothiolate ligand. The novel complexes have been characterized by means of ^{1}H-NMR, FT-IR, elemental analysis, and thermogravimetric analysis (TGA)

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Structures of Cu(Ⅰ)Cl(quinidine) and Cu(Ⅱ)$_2$ Cl$_2$ Cu(Ⅰ)$_2$ Cl$_2$ (quinidine)$_2$

강재은 도정환

건국대 화학과

Two new 1D noncentrosymmetric coordination compounds, Cu(Ⅰ)Cl(quinidine) and Cu(Ⅱ)$_2$ Cl$_2$ Cu(Ⅰ)$_2$ Cl$_2$ (quinidine)$_2$ have been synthesized and characterized by single-crystal X-ray diffraction techniques. A quinidine amino acid has two chiral centers, diastereomer, and enantiomer with quinine. This compound crystallize in the space group P2$_1$ 2$_1$ 2$_1$ of the orthorhombic system with in a cell dimensions : a=9.53194, b=19.13316, c=22.02555, α=90, β=90, γ=90. Cu(Ⅱ)$_2$ Cl$_2$ Cu(Ⅰ)$_2$ Cl$_2$ (quinidine)$_2$ crystallize in the space group P2$_1$ of the Monoclinic system in a cell dimensions : a=12.36807, b=15.62345, c=13.19995, α=90, β=115.44720, γ=90.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Robust photocatalytic water reduction with dendritic Ir(III) complexes: role of the arylsilyl-substituents

황동렬 박수영

서울대 재료공학부

Herein we report on a new series of novel cationic Ir(III) complexes comprising 4,4´-bis(4-(triphenylsilyl)phenyl)-2,2´-bipyridine as an ancillary ligand. Dendritic triphenylsilyl (TPS) moiety at the periphery prevents ligand exchange with solvents, such as water, thus renders the complex more stable and yields long-living photocatalytic water reduction system. Significant hydrogen evolution with maximum turnover numbers higher than 7000 were achieved applying the Ir(III) complexes as photosensitizers in combination with colloidal Pt as a water-reduction catalyst and triethylamine as a sacrificial reducing agent.

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Enhanced stability of photocatalytic water reduction system based on a supramolecularly-caged Ir(III) complex

유승찬 황동렬 박수영

서울대 재료공학부

A new cationic Ir(III) complex has been developed with 6-phenyl-2,2´-bipyridine as an ancillary ligand, which bears a pendant protective phenyl ring within the molecules. Supramolecular interactions between the phenyl group on the bipyridine and the phenyl ring on the cyclometalating ligand was found to enhance the stability of the Ir(III) complex from photodegradation study. Photocatalytical water reduction system employing the Ir(III) complex afforded higher turnover numbers (TONPS = 760) than the system employing the control photosensitizer without phenyl pendant (TONPS = 350).

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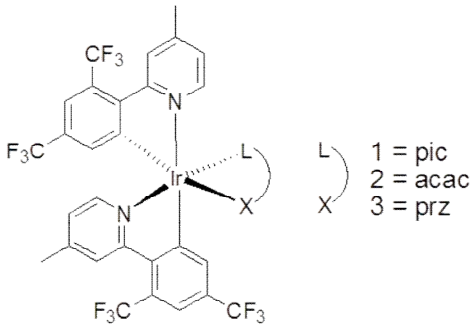
발표종류: 포스터, 발표일시: 수 16:00~19:00

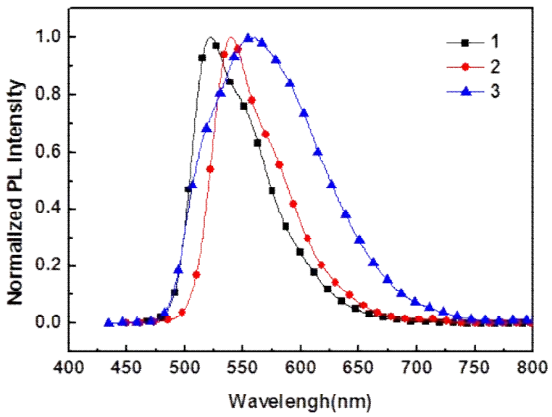
Phosphorescent Cyclometalated Iridium(III) Complexes Based on 2-(2,4-Ditrifluoromethylphenyl)-4-methylpyridine for Organic Light-Emitting Diodes : Tuning the Emission color by the Ancillary Ligand

황인혜 최혜경[1] 강성권[2] 김영인

부산대 화학교육과 [1]부산대 화학교육학과 [2]충남대 화학과

Recently, phosphorescent materials have been extensively studied and continue to be the focus of intense interest in material chemistry owing to their applications for organic light-emitting diodes with high performances. Herein three phosphorescent iridium(III) complexes, $(dCF_3pmpy)_2Ir(pic)$ 1, $(dCF_3pmpy)_2Ir(acac)$ 2 and $(dCF_3pmpy)_2Ir(prz)$ 3, where dCF_3pmpy = 2-(2,4-ditrifluoromethylphenyl)-4-methylpyridine, pic = picolinic acid, acac = acetylacetone and prz = pyrazine-2-carboxylic acid, were successfully prepared, and electrochemical, photophysical, and electroluminescent(EL) properties were investigated. The complexes 1, 2 and 3 exhibited the emission peaks at 522(550sh.) 539 and 560 nm showing a red-shift in the order of 1< 2 < 3. The electroluminescent properties of the complex 1 showed CIE coordinates of (0.36, 0.60), maximum external quantum efficiency of 6.66 % and luminance efficiency of 23.45 cd/A. We elucidated the color tuning of the studied complexes via relative energy level control using the chromophoric ancillary ligand. The structure of the complex 1 was additionally studied using X-ray analysis





대한화학회
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of two metal-organic coordination polymers,based on 4,4'-stilbenedicarboxylic acid with two different pillar ligands.

박경세 유수창 이동헌[1] 선호정[2] 심중표[3] 허다림

군산대 화학과 [1]전북대 화학과 [2]군산대 신소재공학과 [3]군산대 나노화학공학과

Two metal-organic coordination polymers, $[Zn_2(SDA)_2(bpe)(DMF)]$ (1) and [Zn(SDA)(bipy)]?2DMF (2), H_2SDA = 4,4'-stilbenedicarboxylic acid, bipy = 4,4 ’-bipyridine, bpe = 4,4’-(trans-bis(4-pyridyl)ethylene, and DMF = N,N’-dimethyl foramide, have been synthesized and their solid state structures have been determined and analyzed by X-ray crystallography. The solid state structure of (1) is a three fold interpenetrated two-dimensional network and, however, that of (2) is a five-fold interpenetrating three-dimensional diamond network. The coordination sphere of ZnO_5N in (1) is described as a distorted trigonal bipyramid, unusual for Zn(II) MOFs, with three equatorial positions occupied by one nitrogen atom from bpe and two oxygen atoms from two different SDA units and two axial positions occupied by an oxygen atom from DMF and an oxygen atom from a SDA unit. The coordination sphere of the complex (2) is described as a distorted octahedral. The Zn(II) centers are interconnected through the two SDA and two bipy to generate five-fold interpenetrating 3-D diamond network.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A dissymmetric building block for the construction of noble Metal Organic Framework.

조건형 김성민 허정석

충남대 화학과

Diverse shapes and sizes of molecular building blocks have been coined and used to make various topologies of network structures systematically. In most of cases, rigid and highly symmetric molecules are employed for empirical reasons. We prepared a new dissymmetric building block in which three carboxylic acid groups align making 120 degree and 90 degree of bent angles. This unusual combination resulted in a complex network structure when reacted with metal ions under solvothermal condition. In additions to that, all three binding sites takes different coordination geometries. Detailed structural aspects will be presented.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of vermiculite-TiNT/LDH filler composites

최현정 황성호 임상규

대구경북과학기술원(DGIST)

In this study, eco-friendly and non-flammable inorganic filler materials were prepared and then mixed with heat insulating materials, such as vermiculite, by simple wet-chemical mixing, in order to improve the heat resistant and flame retardant properties of heat insulating materials by forming higher porous structure. In this study, Titanate nanotube(TiNT) and Layered Double Hydroxide(LDH) nanoparticles as inorganic nano filler were prepared by hydrothermal method. And then, the well-dispersed vermiculite-TiNT/LDH composites were obtained by wet-chemically mixing with above inorganic nano fillers and vermiculites chemically expanded in H_2O_2 solution considering surface charges of two components. The transmission electron micrographs were obtained by using the high resolution transmission electron microscope. X-ray diffraction (XRD) patterns were obtained with an X-ray diffractometer using Cu-K_{a1}radiation. The Brunauer-Emmett-Teller (BET) surface areas were determined from nitrogen adsorption-desorption isotherms. The thermal characteristics such as thermal conductivity and diffusivity were measured by using the laser flash apparatus. Thermal conductivities were changed upon the type and amount of inorganic nano fillers. In special, the reduction in thermal conductivity was observed to be in proportion with the amount of inorganic nano fillers, which was thought to be closely related with the enhanced surface area and porosity of composites.

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New type of π - extented Porphyrins : Application in Single Crystalline Field Effect Transistors

채승현 최수정 이석중

고려대 화학과

In recent years, Organic Field-Effect Transistors (OFETs) are the most promising electronic devices fabricated using either well-defined single crystals (SCs) or thin films as the charge-transporting layers. Most of the organic semiconductors rely on the inherent structural uniqueness of building blocks such as planarity and π-conjugation, and their packing and interactions with adjoining building blocks. In this regard, porphyrins would be one of the best candidates for organic transistors because they could impart multiple inter- or intra-interactions. We obtained single -crystals of TTPH2, TTPZn, 2TBPH and 2TBPZ from slow diffusion of solvents and investigated their charge transport properties. The OFET devices based on these single-crystals show relatively high mobilities of 0.32 cm2V-1s-1 for TTPZn and 0.36 cm2V-1s-1 for 2TBPZ with high on-off current ratio of >104.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Size Modulation of Porous Coordination Polymer Particles and Their Applications in Heterogeneous Olefin Oxidation

김선돌 이경연 이다희 이석중

고려대 화학과

Nano- and micro-sized porous coordination polymers have received a great attention owing to their potential applications in catalysis, gas storage, optics, separation and recognition. They are often showed highly ordered crystalline features with well-defined porous networks that drive enormous fundamental structure and functional interests. Particularly, metalloporphyrins are excellent building blocks for the construction of these materials. They can be readily synthesized and modified with metal ions of different oxidation states and coordination preferences in their core, leading to incorporate various properties. Therefore, the preparation of porphyrin-based porous coordination polymers have been widely reported in latest years. However, the preparation of nano- and microscale porous coordination polymers with porphyrins is still quite rare. In here, we like to demonstrate the size modulation of nano and micro-crystalline porous coordination polymer particles based on Mn(III)-porphyrin and In(NO3)3 and their abilities toward heterogeneous catalysts.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

TFTs Based on Semiconducting Porphyrin Single Crystals and Its Anisotropic Carrier Transport Behavior

최수정 채승현 이석중

고려대 화학과

There has been a considerable interest in development of planar π-conjugated molecules for TFT (Thin Film Transistor) devices because π-conjugated systems provide more efficient π orbital overlapping and facilitate charge transport. In this regard, porphyrin is one of the best candidates for TFTs because it offers a variety of optical and electrochemical properties. Therefore, we have synthesized a series of novel π-extended Zn-porphyrin derivatives containing thiophene substituents. And their charge transport properties have been investigated. The TFT devices based on porphyrin single-crystals show excellent characteristics with high mobilities and on-off current ratios. In addition, we have obtained a single-crystalline microplate from slow diffusion method and its structure was characterized by single crystal X-ray diffraction. And unique anisotropic charge transport behavior with the position of single-crystalline microplate has been observed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

1-D polymeric and 2-D ladder structure of supramolecules from the reaction of hexaazamacrocyclic complexes of copper(II) with hexacyanoferrate(III)

곽지훈 이재명 Enkhzul Otgonbaatar

순천대 화학과

Ferricyanide is an important building block to get a multidimensional supramolecules because it has a various bridging pattern and its resulting product has a distinctive magnetic property. The heteronuclear complexes of $[CuL]\{[CuL][Fe(CN)_6]\}_2$ (1) and $[CuL']_3[Fe(CN)_6]_2$ (2), where L=3,10-dihydroxyethyl-1,3,6,8,10,12-hexaazacyclotetradecane,and L' = 3,10-bis(3-propylcarboxyl)-1,3,5,8,10,12-hexaazacyclotetradecane have been synthesized and structurally characterized by X-ray crystallography. Both copper(II) ions have a distorted octahedral geometry and linked via cyanide bridging to the iron(III) center and resulting supramolecular complexes of 1 shows 1-D polymeric anionic chain balanced charge with Cu(II) complexes by the coordination bonding, whereas 2 shows 2-D ladder structure cooperated by hydrogen bonding.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-243**

발표분야: 무기화학

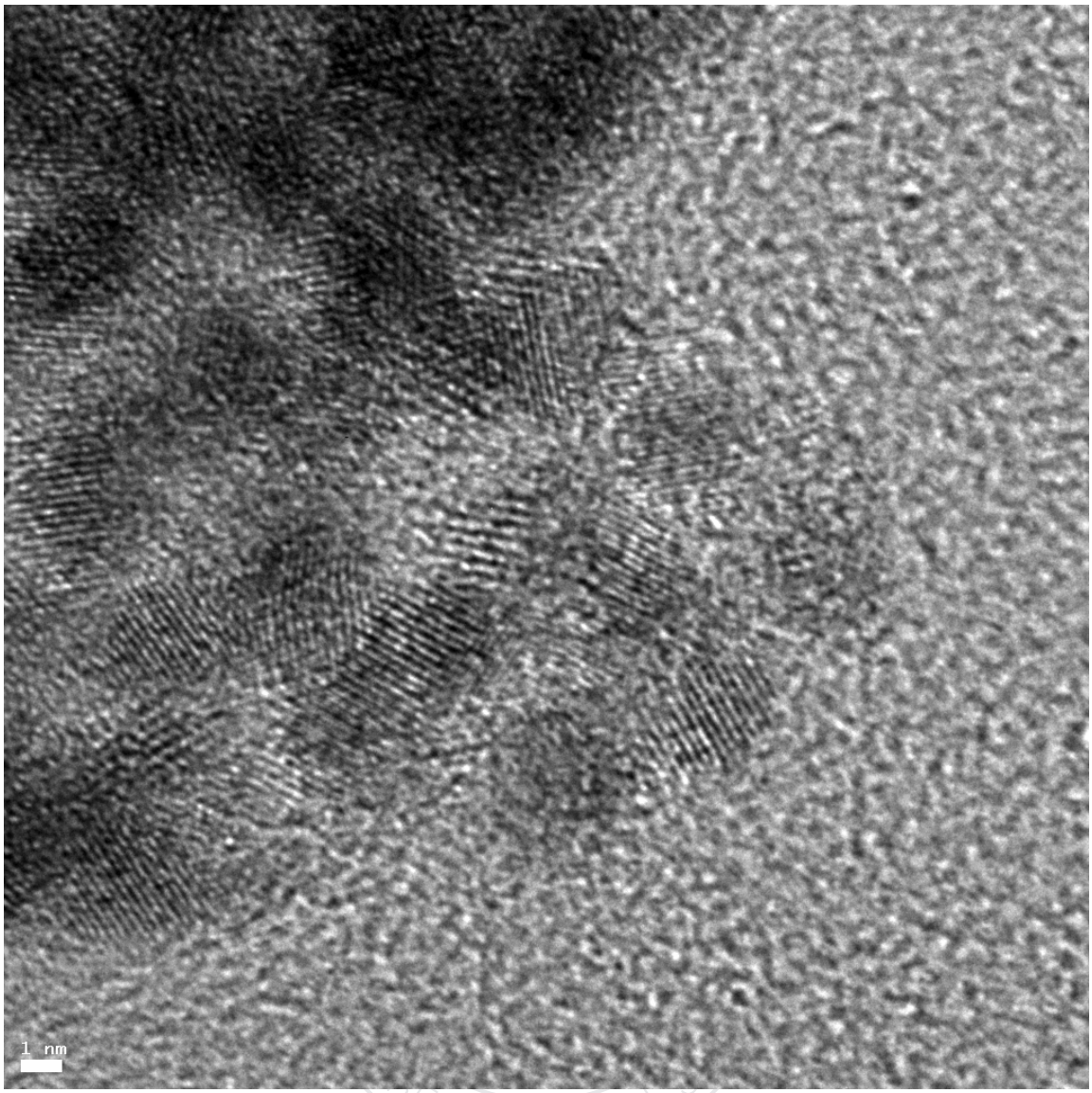
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pt-Sn 전구체로부터 Pt-Sn nanoparticle의 합성

박동국 윤성호[1]

국민대 화학과 [1]국민대 생명나노화학과

백 금(Platinum, 이하 Pt)과 같은 귀금속은 CO, NO_x 산화, 석유 가공(petroleum cracking), 연료 전지(fuel cell) 등에서 매우 효율적인 촉매로 알려져 있다. 특히 Pt 관련 촉매들은 사이즈, 모양, 구성원소, 구조에 따라 다양한 촉매 활성이 보고 되고 있다. 또한 Pt-이종 금속 촉매(bimetallic catalyst)는 물리적으로 두 금속을 섞은 물질보다 더 높은 효율을 보이고 있다. 최근들어, Pt/Sn 이종 금속 촉매는 methanol, ethanol 의 산화, alkane 의 dehydrogenation, aldehyde 의 선택적 hydrogenation(aldehyde to alcohol)에 대하여 매우 높은 활성을 가지고 있다고 보고된 이후, 많은 연구들이 이루어 지고 있다. 일반적으로 Pt/Sn 이종 금속 촉매의 상업적 응용은 실리카(silica), 알루미나(alumina) 등에 지지된 상태로 사용된다. 따라서 본 연구는 Pt-Sn 전구체를 통하여 Pt/Sn nanoparticle 의 합성 결과 및 합성된 nanoparticle 을 알루미나에 지지시키는 연구에 대하여 보고하고자 한다.



KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-244**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

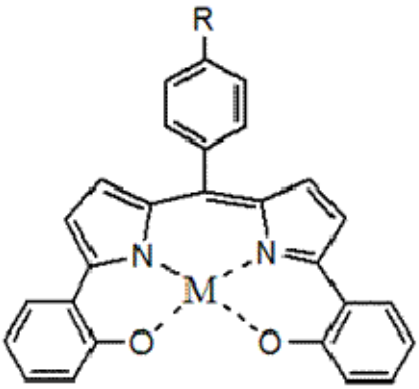
N_2O_2 주개 dipyrrin 리간드를 포함하는 전이금속 화합물의 합성과 분석

전여진 윤성호

국민대 생명나노화학과

Dipyrrin 기반의 전이금속 화합물은 배위되는 금속 이온의 종류와 또는 리간드의 전기화학적 준위를 조절 함으로써 HOMO 와 LUMO 의 간격을 조절 할 수 있다. 이러한 이유로 흡수 파장대와 인광 및 형광 특성을 변화시킬 수 있기 때문에 광범위한 응용 가능성을 가져 많은 연구가 추진되고 있다. 특히 dipyrrin-boron complex (BODIPY)는 뛰어난 형광성으로 인해 생물학적 센서, 페인트 및 잉크, 전자 발광 소재에 이용되고 있다. 더불어 가시광선 영역에서의 강한 흡광도를 가지기 때문에 현재 차세대 태양전지로 각광받고 있는 유기 태양전지와 DSSC 의 유기염료의 후보군으로 기대되고 있다. 본 연구에서는 2-hydroxyphenyl 그룹을 포함하는 N_2O_2 type 의 dippyrin 리간드를 사용하여 전이금속 화합물을 합성하고 이들의 물리 및 화학적 특성에 대하여 보고하고자 한다.

Acknowledgement : This work was supported by the Internatinal Collaborative R&D Program of the Korea Institue of Energy Technology Evaluation and Planning (KETEP) grant funded by Korea government Ministry of Knowledge Economy [20118520010020]



R = H, COOH, NO_2 and Me
M = Al^{3+}, B^{3+}, Fe^{3+}, $Mn^{3+}Co^{3+}$ and etc

대한화학회
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일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **INOR.P-245**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydroxide로 연결된 Cubane 형태의 망간 화합물의 합성 및 자성에 대한 연구

김남석 박규순[1] 윤성호

국민대 생명나노화학과 [1]국민대 화학과

최근 Photosystem II 의 Water Oxidation Center(WOC)의 활성화 자리에서 관찰되는 Mn 을포함하는 Cubane-type core 는 광합성 작용에서 매우 중요한 역할을 하는것으로 인식되어 많은 연구의 대상이 되고 있다. (1) 더불어 이러한 Cubane-type 전이금속 화합물은 독특한 자기적 성질을 나타내는 Single Molecule Magnet(SMM) 으로 작용할 가능성이 있어 무기화학의 주 연구 분야의 하나로 각광을 받고 있다. (2) 하지만 지금까지 보고된 manganese cubane 은 alkoxo bridged 19 종, oxo bridged cubane 12 종, hydroxo bridged 1 종으로 hydroxo bridged cubane 에 대한 연구가 매우 부족하기 때문에 앞으로 지속적인 연구가 필요하다.본 발표에서는 sterically hindered terphenyl-based carboxylate 리간드를 이용하여 그림에 나타낸 것과 같이 $[Mn_4(\mu_3\text{-}OH)_4(\mu\text{-}O_2CAr^{Ani})_2(\mu\text{-}OTf)_2(Py)_2]$의 합성과 결정구조 및 자성등의 특성 분석 결과에 대하여 보고하고자 한다.

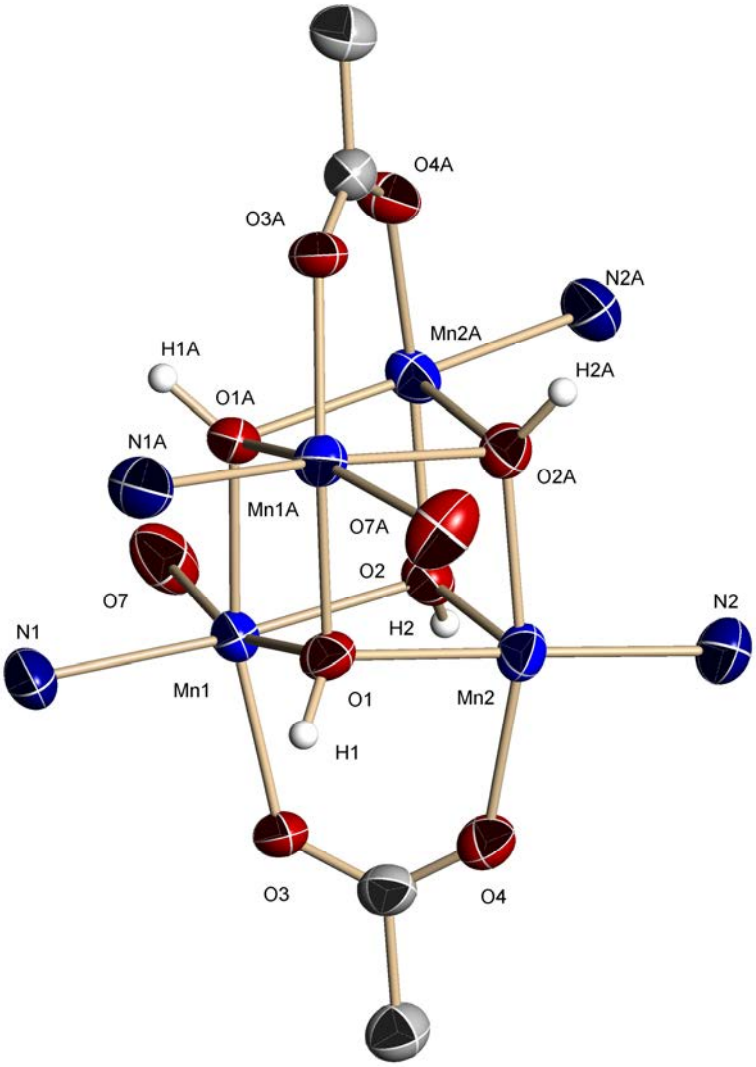
Acknowledgements: This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2010-0012349)

Reference

(1)Ferreira K. N., Iverson T. M., Maghlaoui K., Barber J., Iwata S. *Science* 2004, *303*, 1831.

(2)Galloway K. W., Whyte A. M., Wernsdorfer W., Sanchez-Benitez J., Kamenev K. V., Parkin A., Peacock R. D., Murrie M., *Inorg. Chem.* 2008, *47*, 7438

그림. 명확한 구조파악을 위하여 주변 그룹을 생략한 화합물중심부의 50% anisotropic ellipsoid 를 나타낸 ORTEP 그림.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-246**

발표분야: 무기화학

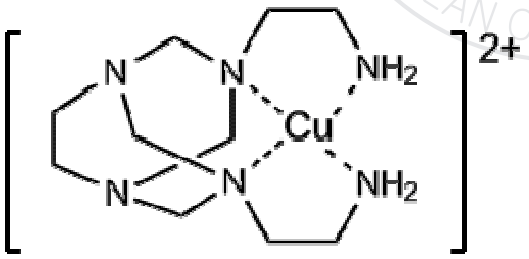
발표종류: 포스터, 발표일시: 수 16:00~19:00

Unusual luminescent complex prepared by polyazabicyclic complex of copper(II) with tetracyanoplatinate(II)

곽지훈 이재명 Enkhzul Otgonbaatar

순천대 화학과

Metal-metal electronic interactions in dimeric platinum(II) complex or in the stacked structure of it causes often intense color and luminescence whereas most mononuclear platinum(II) were known to be non-luminescent. However, unusually, [CuL][Pt(CN)$_4$] (1) prepared by the combination of [CuL]$^{2+}$and [Pt(CN)$_4$]$^{2-}$, in water shows intense blue color and luminescence property though it has no platinum-platinum interaction. We present the preparation and X-ray crystal structure of 1 as well as the photochemical property of it in detail.



1

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-247**

발표분야: 무기화학

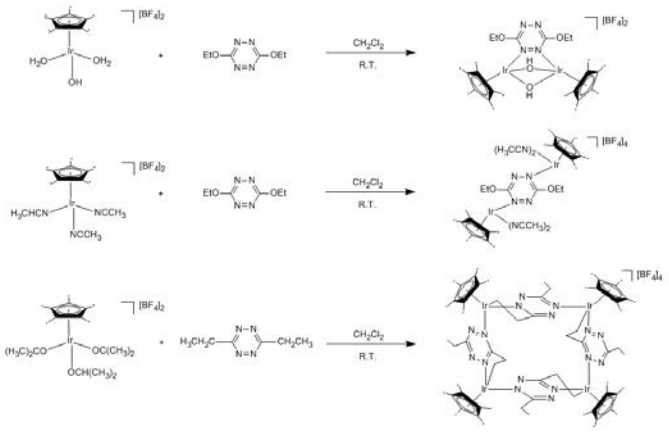
발표종류: 포스터, 발표일시: 수 16:00~19:00

1,2,4,5-Tetrazine Cp^*(Cp^*=C_5Me_5) Ir Complexes

이다해 강필재 최문근

연세대 화학과

The unique properties of 1,2,4,5-tetrazines, the most nitrogen-rich six-membered aromatic heterocycles originate in their extreme electron deficiency. The electron deficiency of the π-system was also a prerequisite for the ability of tetrazines to sustain efficient attraction with negatively polarized atoms or anions, a type of interaction that was only clearly recognized recently. In view of coordination chemistry, the very low energy of the π^* orbital localized at the four nitrogen atoms predetermines a strong interaction in tetrazine-coordinated-valent compounds. 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 coordination works with novel and unusual topologies and the influence of both tetrazine ligands and metal centers will be discussed. Especially taking into account the availability of Cp^*Ir complexes with multiple binding sites of tetrazine ligands generate various structures and unique reactivity as shown below.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-248**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Chemical Transformation of 2D Layered Transition Metal Chalcogenide Nanocrystals

이수정 천진우

연세대 화학과

Two dimensional(2D) transition metal chalcogenide(TMC) nanocrystals have a great potential for diverse applications in sensing, catalysis, electronic device and energy storage, possesing unique electronic, optical, electrochemical properties. Here, we present a colloidal synthesis of 2D-layered TMC nanodiscs of ZrS_2 and TiS_2 with controlled size. The anisotropy in surface energies of layered crystal structure was the key factor in the growth and the size control. For the assessment of their potential as energy storage material, we tested ZrS_2 discs as host material for Li+ intercalation and observed the discharge capacity enhanced by 230 % with great retention capability in comparison with bulk ZrS_2. Also, for constructing a new TMCs nanoderivatives, we used 2D layered TiS_2 nanodiscs as the templates and Cu ions as a chemical stimuli. Regio-selective nucleation of Cu_2S on the edges of TiS_2 nanodiscs leads to the structural transformation through TiS_2-Cu_2S intermediates and toroidal Cu_2S as final products. Moreover, the principles found in this study seem to be generalized as similar transformative behavior were observed with the presence of other cation stimuli.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-249**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic Properties of Oligonucleotide-Au Nanoparticle Complexes

김진홍 **Wu Qiong**[1] 강희경[2]

이화여대 화학과 [1]이화여대 화학나노과학과 [2]이화여대 화학·나노과학과

Single-stranded oligonucleotides (ssDNA) containing guanine bases in their sequences were adsorbed onto gold nanoparticles (AuNPs) by electrostatic interaction. Cyclic voltammetry of Ru(bpy)32+ in the presence of the ssDNA-AuNP complex resulted in an enhanced anodic current due to the oxidation of the guanine bases of DNA. The current obtained with ssDNA-AuNP appeared much smaller than the corresponding ssDNA alone. This current reduction was due to the decrease in solvent accessibility of the guanines in ssDNA immobilized to AuNPs. A progressive decrease in the current was observed in the titration of AuNPs to ssDNA, and a minimum current was eventually obtained, indicating complete binding of ssDNA. The size dependences of AuNPs on the interaction between ssDNA and AuNP were also studied, and the ssDNA adsorbed to 5nm AuNPs was more solvent-accessible for the Ru mediator than 13 and 30nm AuNPs.

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장소: 부산BEXCO

발표코드: **INOR.P-250**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photochemical Production of NADH Using Cobaloxime Catalysts and Carbon Dioxide Conversion

김진홍 김수진[1] 이정하[2]

이화여대 화학과 [1]이화여대 화학·나노과학과 [2]이화여대 화학나노학과

A visible light-driven photocatalytic system for the generation of NADH from aqueous protons was examined using cobaloxime as a catalyst, eosin as a photosensitizer, and triethanolamine as a sacrificial electron donor. Irradiation of a reaction solution containing cobaloxime, eosin, and TEOA converted NAD+ to NADH with a yield of 36 % in phosphate buffer. The reaction rates for the production of NADH were dependent on the concentrations of the catalyst, NAD+, and TEOA. 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. The rates obtained by the different substituents were linearly correlated with the Hammett coefficients of the introduced substituents. Lastly, the reduction of CO2 was carried out in the presence of formate dehydrogenase using the NADH photochemically generated using the cobaloxime/eosin/TEOA system.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-251**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, photoluminescence and magnetic properties of new dinuclear lanthanide metal complexes (Nd^{III}, Sm^{III}, Eu^{III}, Tb^{III}) using *N*-(2-pyridylmethyl)iminodiethanol (H_2pmide)

신종원 홍수경 안승현[1] 민길식[1]

경북대 화학과 [1]경북대 사범대학 화학교육과

We have prepared and characterized a series of dinuclear lanthanide metal complexes including *N*-(2-pyridylmethyl)iminodiethanolate, i.e. $[Nd(Hpmide)(NO_3)_2]_2$ (1), $[Sm(Hpmide)(NO_3)_2]_2$ (2), $[Eu(Hpmide)(NO_3)_2]_2$ (3) and $[Tb(Hpmide)(NO_3)_2]_2$ (4). These compounds have been investigated by single crystal X-ray diffractometry and magnetochemistry. In complexes 1 ~ 4, all lanthanide ions have same geometries and are coordinated with two N atoms and two O atoms from the Hpmide ligand and four O atoms of NO_3^- anions (η^2-NO_3^-). The distances between the lanthanide ions in dimer unit range from 3.753 ~ 3.807 Å. Compound 4 exhibited weak antiferromagnetic interactions between the Tb(III) ions, while 1 and 2 displayed strong antiferromagnetic interactions tithing the dimeric units, respectively. Compounds 2, 3 and 4 exhibited blue, red and green luminescence, respectively, under the UV/Vis lamp. In this poster, we will explain the detailed preparation, crystal structure, magnetic properties and photoluminescence as well as interesting coordination chemistry.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-252**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Spin crossover of iron(II) compounds with organic ligand including 4,4′-dipyridylamine units

신종원 홍수경 안승현[1] 민길식[1]

경북대 화학과 [1]경북대 사범대학 화학교육과

New Iron(II) supramolecular compounds, $[(tpmd)Fe_{0.5}(NCS)]_n$?$2CH_3OH$ (1), $[(tpmd)Fe_{0.5}(NCSe)]_n$?CH_3OH?H_2O (2) and $[(tpmd)Fe_{0.5}(NCBH_3)]_n$?$2CH_3OH$ (3), have been prepared by the self-assembly of Fe(II) species, various counterions, NCX (X=S, Se, BH_3) with *N*,*N*,*N*′,*N*′-tetra-4-pyridyl-methylenediamine (L, tpmd) in glovebox. Complexes 1, 2 and 3 have same space group and display two-dimensional brick-like coordination polymers due to the geometry of iron(II) ions with four N atoms in tpmd ligand and two N atoms of the NCX counter ions (X = S, Se, BH_3), respectively. Compound 1 exhibited weak antiferromagnetic interaction within the polymeric chain range from 300 K to 5 K. Compound 2 displayed two-step spin crossover behavior range from 200 K to 3 K, but no hysteresis observed in the temperature range. In this poster, we will present the detailed preparation of the ligand and metal compounds, crystal structure, magnetic properties as well as interesting coordination chemistry.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-253**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, catalytic and magnetic properties of dinuclear metal complexes (Fe^{III}, Cu^{II}) with H2pmide / Hpmide ligand (H_2pmide= *N*-(2-pyridylmethyl)iminodiethanol)

신종원 안승현[1] 정아림 홍수경 배정미[2] 김철[3] 민길식[1]

경북대 화학과 [1]경북대 사범대학 화학교육과 [2]서울과학기술대 정밀화학과 [3]서울과학기술대 정밀화학과 친환경소재제품센터

N-(2-pyridylmethyl)iminodiethanol (H_2pmide) ligand having an amine, two hydroxyl groups and a pyridine is considered to have the potential to form multinuclear metal complexes with transition or lanthanide metals. Recently, two dinuclear transition metal complexes, [(Hpmide)Cu(η^2-NO_3)Cu(H_2pmide)]$(NO_3)_2$ (1) and [(Hpmide)Fe$(NO_3)_2]_2(NO_3)_2$?2CH_3OH (2) have been synthesized using H_2pmide and $Cu(NO_3)_2$?3H_2O and $Fe(NO_3)_3$?9H_2O, respectively. In complex 1, one copper(II) ion is coordinated with two O atoms of hydroxyl group and hydroxo anion and two N atoms in Hpmide ligand and one O atom of bridging NO_3^- anion and has a distorted square pyramidal geometry. The other copper(II) ion is bonded with two O atoms of hydroxyl groups and two N atoms in H_2pmide ligand and two O atoms of bridging Hpmide ligand and NO_3^- anion and has a distorted octahedral geometry. In complex 2, each iron(III) ions adopts a six-coordinate distorted octahedral geometry with an N_2O_4 donor set from Hpmide ligand and NO_3^- anions. Compound 1 and 2 displayed antiferromagnetic interaction within dimeric units. Compound 2 showed efficient catalytic activities toward various olefin and alcohols with modest to excellent yield. In this poster, we will present the detailed preparation of the ligand and metal complexes, crystal structure, magnetic properties and catalytic activities.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-254**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Magnetically exchange-coupled nanoparticles for efficient heat induction

문승호 천진우

연세대 화학과

The conversion of electromagnetic energy into heat by nanoparticles has the potential to be a powerful, non-invasive technique for biotechnology applications, but poor conversion efficiencies have hindered practical applications so far. We demonstrate a significant increase in the efficiency of magnetic thermal induction by nanoparticles. We take advantage of the exchange coupling between a magnetically hard core and magnetically soft shell to tune the magnetic properties of the nanoparticle and maximize the specific loss power (SLP), which is a gauge of the conversion efficiency. We simulated SLP as a function of magnetocrystalline anisotropy K, diameter of the nanoparticle D, and magnetization M. The dependency on K chiefly results from the internal magnetic spin fluctuation (Neel relaxation), and the dependency on D is due to both Neel and Brownian relaxation. Our simulation indicates the optimal range of K and D for nanoparticles with high SLP values. High magnetization M is beneficial, too. The optimized core-shell magnetic nanoparticles have SLP values that are an order of magnitude larger than conventional iron-oxide nanoparticles. We also perform an antitumour study in mice, and find that the therapeutic efficacy of these nanoparticles is superior to that of a common anticancer drug.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-255**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of the magnetic Structure and spin orientations of clinopyroxene-type structure $LiFeM_2O_6$ (M=Ge and Si) by density functional theory approach

이창훈 심지훈 Myung-Hwan Whangbo[1] Erjun Kan[2]

포항공과대 화학과 [1]Notrh Carolina State University [2]Nanjing University of Science and Technology

The magnetic structure of the clinopyroxene compounds $LiFeSi_2O_6$ and $LiFeGe_2O_6$ have been investigated by extracting spin exchange interactions in terms of density functional theory study. The clinopyroxene compounds $LiFeSi_2O_6$ and $LiFeGe_2O_6$ compounds are crystallizing in a monoclinic space group P21/c. With the experimental frameworks, the magnetic structure of LiFeSi2O6 is described by a ferromagnetic coupling of Fe spins within the infinite zigzag chains of edge-sharing octahedral along the crystal c direction, while the coupling between these zigzag chains is antiferromagnetic and that of LiFeGe2O6 is different to the silicate: the magnetic unit cell doubled along the a-direction. Within the zigzag chains Fe spins along the crystal c direction are coupled antiferromagnetically, while the interchain coupling is antiferromagnetic when coupling goes via the Ge(B) tetrahedron and ferromagnetic when it goes via the Ge(A) tetrahedron1. From our DFT results, we reveal that the magnetic structures of both compounds are predicted the antiferromagnetic coupling within infinite zigzag chains of edge-sharing octahedra as well as interchain exchanges. The Curie-Weiss temperatures estimated from spin exchange interactions by performing energy-mapping analysis based on density functional theory calculations are in good agreement with experiment. The //c and //a orientations of the spins in the ordered magnetic structures of LiFeSi2O6 and LiFeGe2O6, respectively, were also examined by considering spin-orbit coupling and magnetic dipole-dipole interaction.(1) G. J. Redhammer, G. Roth, W. Treutmann, M. Hoelzel, W. Paulus, G. Andre, C. Pietzonka, G. Amthauer, J. Solid State Chem., 182, 2374-2384 (2009).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-256**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Superparamagnetic Metal-Carbon Nanocomposites with a Hollow Porous Sphere Structure

김다정 서원석

서강대 화학과

We have synthesized metal-carbon nanocomposites with a hollow porous sphere structure by a simple chemical vapor deposition (CVD) method. The Metal-carbon nanocomposites are composed of Metal/graphitic carbon (Metal/GC) nanocrystals, carbon nanotubes, and graphitic carbon. Solid core-mesoporous shell silica spheres with an average diameter of ~400 nm are used as templates for the synthesis of the metal-carbon nanocomposites. The carbon nanotubes in the nanocomposites were prepared from the catalytic function of oxidized Metal/GC nanocrystals. The prepared nanocomposites were characterized by X-ray diffraction (XRD), TEM, and Raman spectroscopy. We expect the superparamagnetic materials to be useful for biomedical applications including magnetic cell separation, bio-detection, drug delivery, and magnetic-resonance imaging.

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장소: 부산BEXCO

발표코드: **INOR.P-257**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photoactive NO-Releasing Ru(III) Nitrosyl Complexes with Tetradentate N4 bis-Pyridyl/bis-Carboxamide Ligands

조장훈 유영민[1] 남원우[2] 이홍인

경북대 화학과 [1]KIST 의공학연구소 [2]이화여대 화학과

Since the discovery of Nitric Oxide (NO) as one of the major signal-transduction molecules in cells, there have been many attempts to devise acute NO-delivering systems for the purpose of developing disease therapies as well as studying cell functions. Metal-nitrosyl complexes are often releasing NO by light activation. This ability can be adapted to killing cancer cells with high specificity because high concentration of NO in cells induces apoptosis. Ru-NO complexes have been studied for the usages of these photodynamic therapy (PDT) agents for a time. In this research, we have developed a new Ru-nitrosyl bis-pyridyl/biscarboxamide compound, [Ru(ebpp)(Cl)(NO)], where H_2ebpp= N,N'-(ethylene di-p-phenylene)bis(pyridine-2-carboxamide) to be tested as a model NO-releasing agent. The crystallographic analysis of the complex revealed that the ebpp ligand is tetradentately bound to Ru and the remaining two cis sites of the octahedral geometry are occupied by NO and Cl^-,Electronic absorption spectrum of the complex showed two absorption bands are 280 nm and 380 nm. Under the normal room light, 560 nm bands were growing. Simultaneous EPR (electron paramagnetic resonance) experiments at 110 K found that diamagnetic properties of the complex solution changed to a paramagnetic (S =1/2) species. These UV-VIS and EPR data can be interpreted as that the diamagnetic $[Ru\text{-}NO]^6$(Enemark-Feltham notation) electronic state of the complex becomes low-spin Ru(III) (d^5, S=1/2) state upon losing NO by photoactivation. In the present study, we explore the photosensitivity of a series of ruthenium nitrosyl complexes with tetradentate N4 bis-pyridyl/biscarboxamide ligands containing electron-donating methyl substituent group [Ru(R_2ebpp)(Cl)(NO)](R=CH_3)].

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장소: 부산BEXCO

발표코드: **INOR.P-258**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Uniform Porous Carbon Spheres Embedded with FeCo-Graphite Nanocrystals

이연 서원석[1]

서강대 바이오융합 [1]서강대 화학과

We have synthesized highly uniform and mesoporous carbon spheres embedded with FeCo-graphitic carbon shell nanocrystals (FeCo/GC@MCN) by a simple one-step CVD method. Mesoporous silica nanoparticles with diameter of ~140 nm were used as supports for the synthesis of the FeCo/GC@MCN. The FeCo/GC@MCN was characterized by XRD, TEM, BET, TGA, and Raman. The graphitic mesoporous carbon spheres exhibited high stability against HCl etching over a monitoring period of a week. By exploiting the chemical stability and superparamagntic properties, the FeCo/GC@MCN was expected to show the novel applications including drug delivery, catalytic supports and water treatments.

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발표코드: **INOR.P-259**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reactivity of High-Valent Ruthenium-Oxo Species

김진화 박혜진 서미숙 남원우[1] Antoni Llobet[2]

이화여대 바이오융합과학과 [1]이화여대 화학과 [2]Institute of Chemical Research of Catalonia (ICIQ), Campus Universitari de Tarragona

The high-valent metal oxo (M^{n+}=O) species have been implicated as active oxidising agent and are able to act as an efficient catalyst for chemical transformation of wide range of organic substrates. They have also been invoked as key intermediates in the oxygen-evolving complex (OEC) in photosystem II. Many ruthenium-oxo species act as an efficient water oxidation catalyst in model complex. In the presentation, generation of high-valent ruthenium-oxo species and their reactivity aspects towards externally added substrates will be presented.

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발표코드: **INOR.P-260**

발표분야: 무기화학

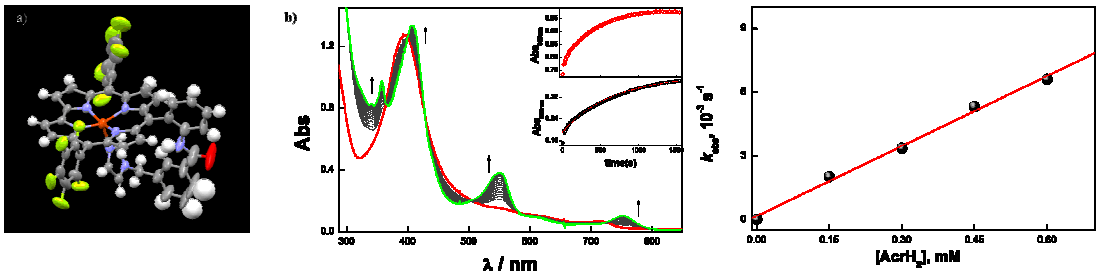
발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization and Reactivity of Iron-Oxo(corrole) Complex

김은정 서미숙 남원우[1]

이화여대 바이오융합과학과 [1]이화여대 화학과

High-valent metal-oxo complexes have been implicated as reactive intermediates in a range of biological transformations and in many catalytic oxidation processes. Iron is one of the most common metals in the catalysts, especially the catalysts in nature, where it is found in the form of porphyrin-iron, mononuclear non-heme iron, and diiron assemblies. In this presentation, the oxidation of the Fe(corrole) complex, such as Fe^{III}(PFC-Im)with various oxidants give the reactive high-valent iron-oxo corrole complex. The characterization of Fe(O)(PFC-Im) with various specctroscopics method, such as UV-Vis, ESI-MS, EPR and EXAFS. This complex is competent to oxidize substrates in several reactions, such as hydride-transfer, electron-transfer, alcohol oxidation and oxygen-atom transfer reactions. FeV(O)(PFC-Im) will be discussed.Fig 1. a) X-ray structure of Fe(PFC-Im) complex. b) UV-Vis spectral change of Fe(O)(PFC-Im) with $AcrH_2$ in CH_3CN: CH_3OH= 1:1 at -40° C



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-261**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure and Reactivity of Fe(IV)-Peroxo complex

권은지 홍승우[1] 서미숙 이용민[2] 남원우[3]

이화여대 바이오융합과학과 [1]이화여대 화학나노과학부 [2]이화여대 기초과학연구소 [3]이화여대 화학과

Oxygen-containing mononuclear iron species such as iron-peroxo, iron-hydroperoxo and iron-oxo are key intermediates in the catalytic activation of dioxygen by iron-containing metalloenzymes. TAML (tetraamidomacrocyclic ligand) is a tetraanionic ligand capable of stabilizing Fe(V)-oxo intermediate for the first time. Herein, we attempted to synthesize a novel Fe(IV)-peroxo intermediate by using $[Fe^{III}(TAML)]^-$ as a starting complex. Upon addition of excess amount of solid potassium superoxide in the presence of cryptand, we were able to generate fairly stable $[Fe^{IV}(O_2)(TAML)]^{2-}$ intermediate. The comparison of X-ray crystal structures between $[Fe^{III}(O_2)(TMC)]^+$ and $[Fe^{IV}(O_2)(TAML)]^{2-}$ gave detailed structural insight into iron-peroxo species. This intermediate showed nucleophilic reactivity in the aldehyde deformylation reaction.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of starshape Donor-Acceptor-Donor Based Organic Semiconductors Containing Fused-amine for Solution-Processed Small Molecule Organic Solar Cells

백상현 조나라 김철우 고재중

고려대 소재화학과

The synthesis and photovoltaic characteristics of new organic semiconductors, Fused-amine-BT-HxTh3 (1), and Triph-amine-BT-HxTh3 (2), are reported. These semiconductors have an unsymmetrical donor A-acceptor-donor B (DA-A-DB) framework composed of a benzothiadiazole acceptor between two different donors, Fused-amine (or triphenyl amine) and terthiophene. This motif was introduced as donor B in the unsymmetrical DA-A-DB structure to increase solubility in organic solvents and extend the conjugation length to be similar to the DTS(PTTh2)2 small molecule. In case of Fused-amine, they have good interaction with PCBM as well as absorb red shift compare with triphenyl amine unit. Consequentially, they have higher performance than triphenyl amine. The fused-amine compound gave high efficiency of 4.16% with a short circuit photocurrent density (Jsc) of 11.34, an open circuit voltage (Voc) of 0.74, a fill factor 0.49.

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발표코드: **INOR.P-263**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and charactrize Small Molecule Bulk-Heterojunction Solar Cells based on a diversity of donors and acceptors conjugated.

임남우 김철우 백상현 조나라 고재중

고려대 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. Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. In this study, We have introduced a structure of Acceptor-Donor-Acceptor molecular structure in a field of OPVs. As a Donor, benzodithiophene was adopted due to the fact that has given a high charge carrier mobility. Furthermore, avoiding edge to face interactions and improving a solubility, we introduced substituted alkyl group(Triisopropyl acetylene) at Benzo[1,2-b:4,5-b']dithiophene-4,8-dione. By adopting such the A-D-A structure with conjugated donor with Silole, bezothiadiazole, derivative thiophene with hexyl cyanoacetate as the eletron-withdrawing terminal, all of the various units has recently been used in OPVs have been analyzed the properties.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-264**

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 김철우 임남우 고재중

고려대 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 Flu-IT-PhF and Flu-ITT-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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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Substituent Effect on 5,6-Substituted Benzothiadiazole Based Organic Semiconductors for Solution Processed Organic Solar Cell

조나라 백상현 고재중

고려대 소재화학과

Solution processed organic solar cells fabricated by means of versatile printing techniques can provide the most attractive advantages of device such as low cost, light weight, solution processability. Most of high efficiencies have been reported in organic solar cells fabricated with bulk- heterojunction materials comprising of low-bandgap semiconducting polymers and [6,6]-phenyl-C61 (or 71)-butyric acid methyl ester (PCBM). Very recently, the fluorine-substituted benzothiadiazole motifs were reported as an effective electron accepting unit to give the low-bandgap semiconducting polymer, showing polymer solar cell of 5-7% efficiency. In this poster, we studied substituent effect on benzothiadiazole on 5,6-position related to the efficiency for organic solar cells. Because 5,6-substituted benzothiadiazole play an important role in donor-acceptor organic semiconductor. The substituents often used to control absorption wavelength and electron accepting properties.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Suitable Organic Sensitizers for Cobalt (II/III)?Based Redox Electrolyte

임기민 송주만 최혜주 고재중

고려대 소재화학과

We already synthesized and announced sensitizers based on Indenothiophene derivative. In this paper, we modify suitable structures for cobalt (II/III)?based redox electrolyte. The photovoltaic performance of JK-303 and JK-304 are increased about 10% relatively JK-302. We report here on the synthesis and electrochemical properties of a series of indenothiophene-based organic dyes, which have O-alkylatied fluorene derivative as donating group, cyanoacrylic acid as withdrawing group and indenothiophene derivative as bridging group. Consequently we synthesize and develop efficacious sensitizers based on indenothiophene derivative, and try to discover the reason of high performance through in this study.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic Sensitizers Containing Planar Bridging Group for Dye Sensitized Solar Cells

최혜주 조나라 백상현 도광석 임남우 임기민 고재중

고려대 소재화학과

Dye sensitized solar cells(DSSCs) are currently attracting wide-spread interest as low-cost alternatives to conventional solid-state photovoltaic devices. Controlling the light harvesting in DSSCs is very important due to the scientific and industrial interest to enhance the photoenergy conversion efficiency. Molecular engineering to obtain red-shift absorption spectra has been suggested for the extension of π-conjugation of spacers. For enhancing π-electron delocalization, we introduce structural modifications of planar bridging group. Dye 1 and 2 gave increase of Jsc value compared with reference dye.

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발표분야: 무기화학

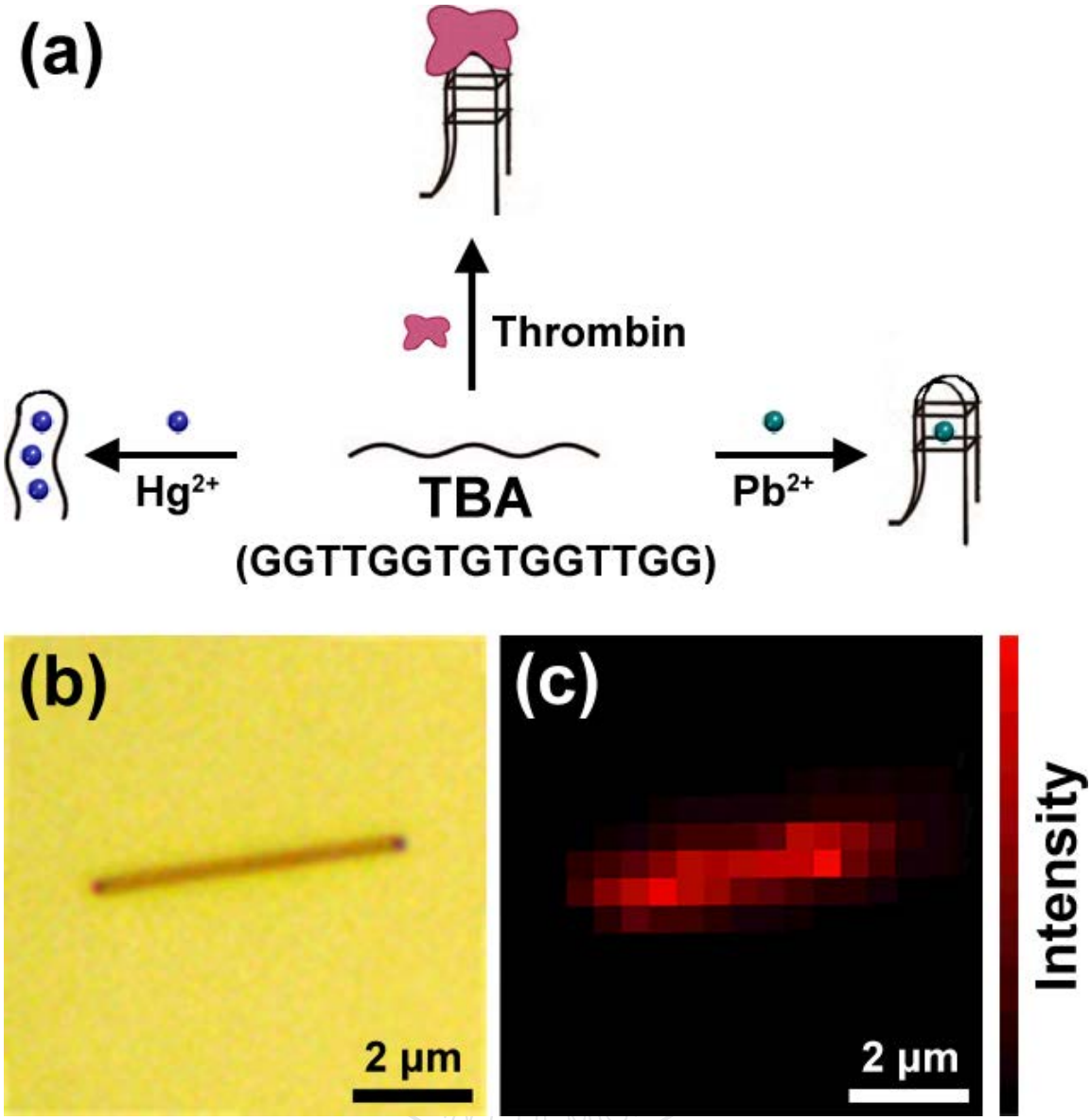
발표종류: 포스터, 발표일시: 수 16:00~19:00

Aptameric Nanowire SERS Sensor for Molecular Detection

이효반 김홍기[1] 김봉수

KAIST 화학과 [1]KAIST(KAIST) 화학

Single nanomaterial based molecular sensor has been great demand for biological, chemical and medical studies, because it can potentially be employed as practical nanosensor with improved sensitivity and resolution. We report an aptameric single Au nanowire (NW) surface-enhanced Raman scattering (SERS) sensor that has sensing capability of human α-thrombin, lead, and mercury ions. This sensor can be fabricated simply by laying aptamer-modified NW onto a Au film. Upon the target molecules binding with aptamer, SERS signals of single NW are changed, enabling to detect thrombin, Pb2+, and Hg2+ at concentrations as low as 10 pM, 50 pM, and 10 nM, respectively. Single Au NW SERS sensor is easy to fabricate and stable over considerable amount of time, which might be applicable to practical sensor for environmental monitoring and biomedical assay.


(a)
Thrombin
Hg2+
TBA
(GGTTGGTGTGGTTGG)
Pb2+
(b)
2 μm
(c)
2 μm
Intensity

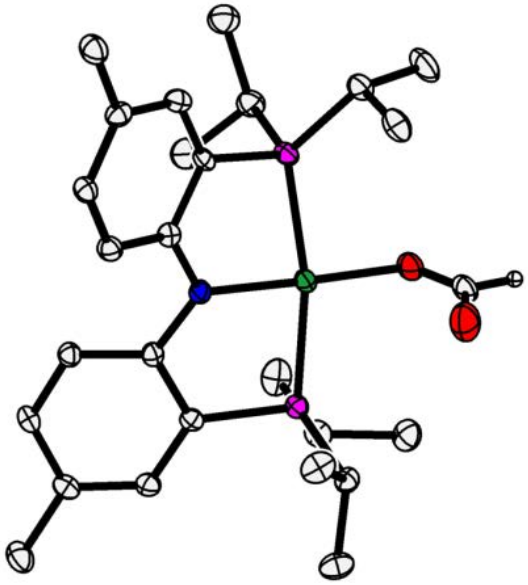
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **INOR.P-269**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

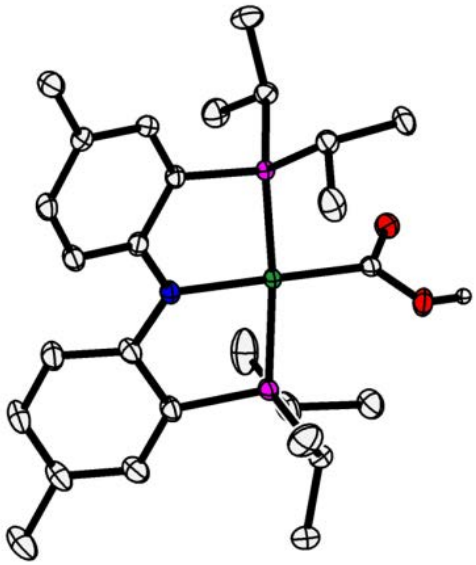
Two binding modes of CO_2 on a nickel center; Ni-OCHO vs. Ni-COOH

유창호 김진 이윤호

KAIST 화학과

Activation of carbon dioxide is receiving great attention in terms of reducing greenhouse effect and utilizing carbon dioxide as a cheap and abundant C1 source for useful chemicals and fuel. Reducing carbon dioxide is challenging due to its high activation barrier. However, the nature already shows the methodology to utilize carbon dioxide as a carbon source and an energy carrier. Especially, some microbes such as Rhodospillum Rubrum manipulate CO_2 to produce CO catalyzed by CODH; Carbon monoxide dehydeogenase. The recent X-ray crystallographic data revealed the structural information of the active site of CODH, where CO_2 is bound on a nickel center in square planar environment. It also shows the binding mode of CO_2 on a nickel center via a Ni-C bond. Thus, studying Ni-CO_2 species possessing a Ni-C bond can be a fine strategy for activating CO_2. We will present two binding modes of CO_2 on a nickel center in a square planar geometry; a nickel formate (Ni-OCHO) and a nickel carboxylic acid (Ni-COOH) according to our recent progress with a pincer-type ligand, PNP (PNP = N[2-PiPr$_2$-4-Me-C_6H_3]$_2$). A formate complex (PNP)NiOCHO was obtained from the reaction of (PNP)NiH with CO_2, while (PNP)NiCOOH was produced from the carbonlylation of a corresponding hydroxyl complex with CO. This is the first structural example of a nickel carboxylic acid complex revealing a Ni-$^1\eta$-COOH binding mode in a square planar environment. The reactivity study of (PNP)NiCOOH will be also demonstrated, particularly toward a protonation which gives a nickel carbonyl complex, {(PNP)NiCO}{BF_4}. Detailed structural data, spectroscopic analysis, and further reactivity studies will be discussed.





대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-270**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Structural Characterization of$(Org)_2[Fe(Se_4)_2]$ (Org = Ph_4P, Et_4N, PPN)

김재명 김강우

인천대 화학과

In the field of the metal polychalcogenide chemistry, the bis(tetrachalcogenido)metallate, $[M(Q_4)_2]^{2-}$ (Q = S, Se, Te) anions are among the most well known molecular complexes. It has been known that the structures of metal polychalcogenide anions are often dependent on the size of organic counter-cations. $[Fe(Se_4)_2]^{2-}$ is a new member of the $[M(Q_4)_2]^{2-}$ family and features as the first metal octachalcogenide incorporating the metal of a Fe triad. We employed relatively large organic cations such as $(Ph_4P)^+$, $(Et_4N)^+$ and $(PPN)^+$ to stabilize the $[Fe(Se_4)_2]^{2-}$ anion.Here we report the synthesis and structural characterization of new compounds, α- and β-$(Ph_4P)_2[Fe(Se_4)_2]$, $(Et_4N)_2[Fe(Se_4)_2]$ and $(PPN)_2[Fe(Se_4)_2]$.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of MBiS2 (M = Na, K) under Hydrothermal and Solvothermal Condition

강수민 전영진

건국대 응용화학과

Ternary compounds such as MBiS2 (M = Na, K) have been known to show interesting thermoelectric properties. Especially, even though they are known for 100 year, detailed approaches to theses compounds have been scarce because easy synthetic method is not well established. Synthesis of MBiS2 (M = Na, K) under hydrothermal and solvothermal conditions, respectivley, and the characterization of them using various methods such as PXRD, SEM, EDX, Diffuse-Reflectance UV-vis spectroscopy will be presented.

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Reactivity and Structural Characteristics of Vanadium Complexes Supported by Tri- and Tetradentate Phosphine Ligands

김진 유창호 이윤호

KAIST 화학과

Activation of small molecules utilizing earth-abundant 1st row transition metals is one of the important issues for resolving the global energy problem. Especially we are interested in developing an energy efficient molecular catalyst for the industrial processes such as Haber-Bosch and Fischer-Tropsch process. In nature, dinitrogen can be fixed and reduced to ammonia catalyzed by a series of nitrogenase enzymes found in nitrogen-fixing bacteria. According to the recent reports, the vanadium containing nitrogenase can catalytically reduce carbon monoxide to hydrocarbons. This finding motivated us to synthesize a series of vanadium complexes mimicking the active site of nitrogenase for developing small molecule activation catalysts. Here, we will report the synthesis and characterizations of vanadium complexes supported by an anionic triphosphino ligand [PPP]. The reactivity of the [PPP]V complexes towards N_2 and CO will be discussed. Utilizing a tetradentate triphosphinoamido ligand, [PNP_2] we also prepared 5-, 6-coordinate vanadium complexes for investigating effects of amido moiety and geometric variation in their reactivity. Detailed characterizations, and further reactivity studies will be presented.

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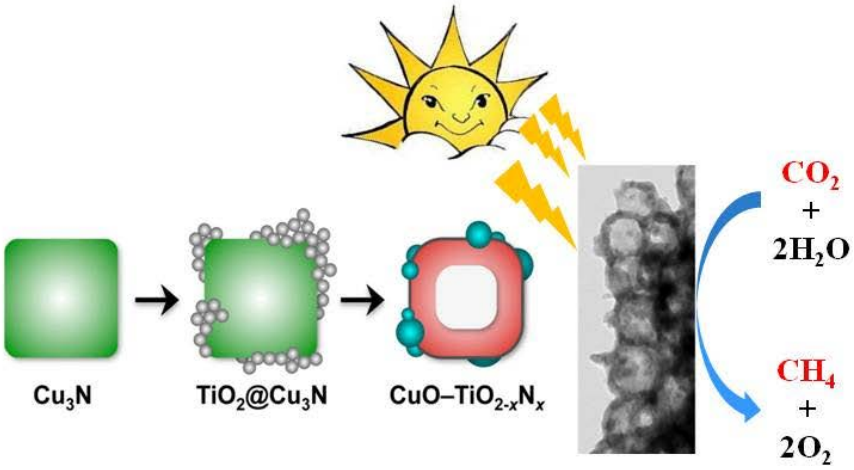
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic Conversion of CO2 into Methane under Solar Irradiation

인수일 Dimitri D. Vaughn II[1] Raymond E. Schaak[1]

대구경북과학기술원(DGIST) 에너지 시스템 공학과 [1]Department of Chemistry, The Pennsylvania State University

Carbon dioxide is a greenhouse gas of growing concern, and its atmospheric concentration continues to rise from the ongoing burning of fossil fuels. Catalysts that use sunlight to convert CO2 into hydrocarbon fuels are attractive to help mitigate this problem, because they are able to simultaneously consume waste CO2 and generate useful sources of energy in a sustainable and carbon-neutral manner. Here, we describe a multi-template strategy for synthesizing hollow nanocubes of CuO-TiO2-xNx, a new hybrid material that photocatalytically converts CO2 into methane under solar irradiation. The synthetic strategy uses uniform Cu3N nanocubes as both a morphological and compositional template for subsequent deposition of a partial TiO2 shell, oxidation of the Cu3N core to form hollow CuO nanocubes, and low-temperature (450 °C) incorporation of the expelled nitrogen into the TiO2 framework to form crystalline TiO2-xNx. The synthetic method is well suited to scale up for the production of large quantities of material at an economic cost. The catalytic performance of the CuO-TiO2-xNx hollow nanocubes (41.3 ppm g-1h-1 of methane) is comparable to other reported photocatalysts that convert CO2 into methane using solar irradiation and without using noble metal co-catalysts. This work has been chosen as a "Hot Paper" by the Editors for its importance in a rapidly evolving field of high current interest (Angew. Chem. Int. Ed., 2012, 51, 3915-3918).



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Novel Graphene π-conjugated Pd catalysts for the Emulsion Copolymerization of functionalized norbornene with bulky olefins

이웅준 이익모

인하대 화학과

Polynorbornene has been a good candidate for the optical devices working in the short wavelength but brittleness prevented this material from further applications. Copolymerization of functional norbornenes with norbornene or dicyclopentadiene(DCPD) would be a possible method for the improvement of properties of norbornenes. Many Pd or Ni complexes are known to polymerize norbornene but they are sensitive to the polar groups of functional norbornenes. In our search for the active catalytic systems for the polymerization of functional norbornenes, we found that Graphene π-conjugated Pd complexes with β-diketiminates were quite soluble in common organic solvents but highly stable in water. Emulsion copolymerization of functional norbornenes with bulky olefins has been achieved in the presence of Graphene π-conjugated Pd complexes with β-diketiminates and the effects of various reaction parameters have been investigated.In this presentation, preparation and copolymerization behaviors of an efficient Graphene π-conjugated Pd catalytic system will be discussed.

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synthesis of zinc complexes containig symmetric alkyl-substituted β-diketiminato ligand

이병기 이익모

인하대 화학과

A novel preparative method of symetric β-diketimines with alkyl substituents from 1,3-diketones has been developed. 1,3-Diketone was reacted by alkyl amine to produce β?ketoimine, which reacts further with alkyl amines in the presence of dimethylsulfate which is known as an O-alkylating reagent. This method can be applied without solvent with easy scale-up and good yield. Dimethylsulfate proves high reproducibility, low cost and potentially safer than conventional agent such as triethyloxonium tetrafluoroborate (Meerwein's salt). Microwave proves Instantaneous local superheating, Efficient energy transfer, Rapid processing of materials with cost reduction, High yields, green reactions, employment of milder and simple experimental procedure. Successful synthesis of β-diketimines with alkyl substituentsand we synthesised several zinc complexes containig symmetric alkyl-substituted β-diketiminato ligands.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Shape Controlled Synthesis of Tubular Microporous Organic Networks

천지슬 손성욱

성균관대 화학과

During the last half decade, amorphous and microporous organic networks (A-MON) have been extensively prepared via diverse organic reactions among the building blocks. Usually, the related studies have focused on the inner porosity of materials and the resultant high surface area. In addition, by screening the geometry of building blocks, the pore size and surface area of A-MON could be controlled. Recently, several building blocks with tetrahedral geometry have been used as connector for obtaining A-MON with 3D inner network structure. However, the studies on the outer shape evolution of A-MON having 3D inner networking are quite rare, possibly due to the following two reasons. First, because the outer shape of A-MON can be expected to be amorphous, the control of the outer shape was not seriously considered. Second, an isotropic shape such as spherical materials can be expected when the tetrahedral building blocks were used to induce 3D inner network structure. Thus, the mechanism of outer shape evolution of A-MON was not seriously considered yet. This work suggests the optimized synthetic method for tubular shape evolution of amorphous and microporous organic networks. Under conventional Sonogashira coupling conditions, the gradual addition of dihalo-building block to its mixture with tetra(4-ethynylphenyl)methane resulted in the formation of tubular materials

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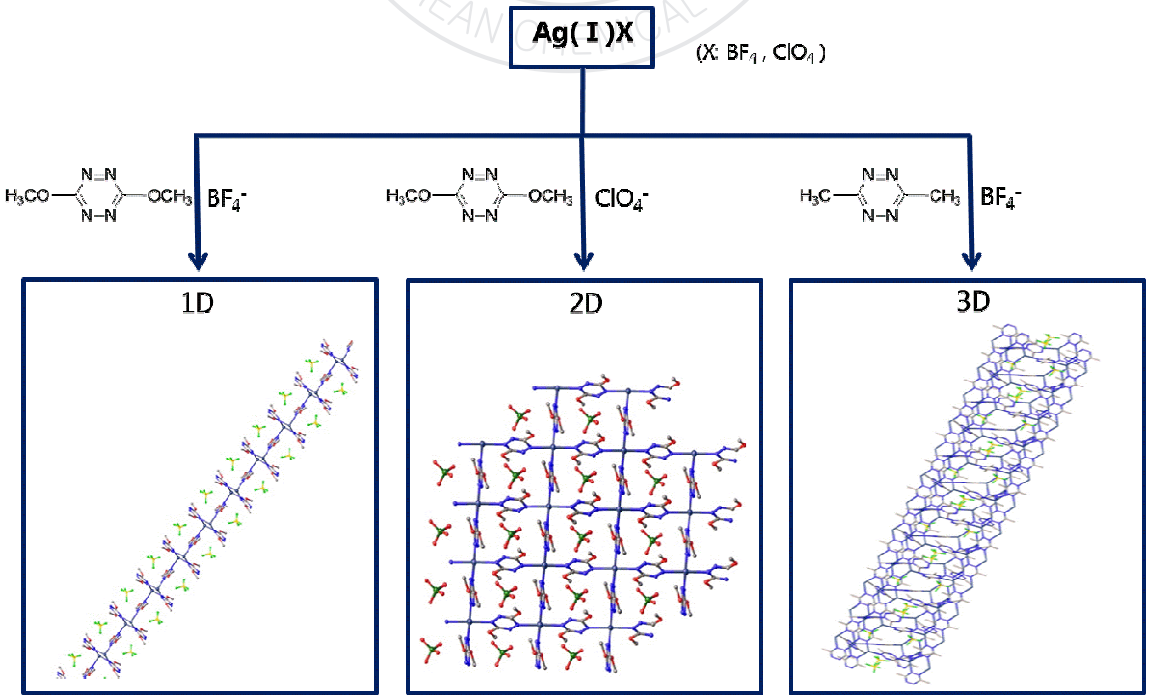
발표종류: 포스터, 발표일시: 수 16:00~19:00

Supramolecular Architecture of Ag^+ Coordination with 1,2,4,5-Tetrazines

이혜희 강필재 최문근

연세대 화학과

The interesting feature of tetrazines is that since they have the multiple metal binding sites, they make Ag^+ complexes easily with one- and two- and three dimentional coordination frame works. In context of coordination polymers, the combination of coordinative and weaker secondary interactions such as hydrogen bonds, anion-pi interaction of ring, has been employed in the construction of a variety of supramolecular architectures. In this study we investigate the influence of the supramolecular structures using the different anions and tetrazines.



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Ultrasensitive Detection of miRNA by force-based AFM

구현서 박준원

포항공과대 화학과

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 such as cell differentiation, proliferation, and apoptosis. Additionally, the expression level of miRNAs is associated with various human diseases. Thus, miRNA detection has become an important emerging topic in biomedical fields. Various analytical approaches have been developed for detection of miRNA. However, conventional tools have several disadvantages for sensitive detection. For example, Northern blotting requires the large amounts of samples and is time-consuming. In RT-PCR, the use of complimentary short primer can introduce signal bias due to the low melting temperature of duplex with miRNA. Therefore, here we report another approach to detect miRNA at the single-molecule level using force-based AFM. We generated specific force maps to visualize the detection of DNA-RNA duplex onto the surface by AFM mapping. For this study, complementary DNA probe was spotted to capture synthetic miRNA on the dendron-coated surface and then, hybridization of synthetic miRNA was performed. Hybrid binding domain (HBD) was expected to improve the sensitivity of AFM tip because of the selective binding to DNA-RNA duplex. Therefore, We attatched HBD onto the denron-coated AFM tip to increase recognition of DNA-RNA duplex onto surface. The non-linear force-distance curves and mapping showed specific interaction between DNA-RNA duplex onto the surface and HBD-immobilized AFM tip. However, this specific force curves were not detected between the only complementary DNA probe spotted onto surface and HBD-immobilized AFM tip. We expect this study will lead us to development of an ultrasensitive miRNA detection tool.

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기능성 실버 나노와이어의 제조 및 특성 분석

이상경 김수정[1] 구상만[2]

한양대 수소연료전지 공학과 [1]한양대 수소연료전지공학과 [2]한양대 화학공학

최근 들어 제어된 크기와 형상을 갖는 금속 나노와이어의 제조에 대하여 많은 연구가 진행되고 있다. 이들 금속 나노와이어들은 bulk 물질들이 가지고 있지 않는 양자크기 효과와 더불어, interconnects 및 nanodevice 를 구성하는 능동형 소자로서 높은 응용가능성을 보여주는 바, 특히 금속 중 가장 높은 열적, 전기적 전도성 및 낮은 광흡수율을 나타내는 실버 의 특성으로 인하여 실버 나노와이어의 경우 상대적으로 많은 관심의 대상이 되고 있다. 향상된 물리적인 특성을 발현하기 위하여서는 균일한 orientation 과 높은 aspect ratio 를 갖는 나노와이어의 제조가 필요한 바, 실버 나노 와이어를 제조한 방법으로는 carbon nanotube, anodized aluminum oxide 등과 같은 hard template 를 사용하는 방법, DNA, rod 형태의 micelle 등의 soft template 를 사용하는 방법 등이 주로 사용되어 왔으나, 최근 들어 불순물 혼입 방지를 위한 template 제거와 같은 추가공정을 피하기 위하여 surface-capping reagent 등을 이용한 직접 용액 합성법에 대한 연구가 활발히 진행되고 있다. 이들 직접 용액 합성법에는 protein 이나 기능성 고분자 및 계면 활성제 등을 capping agent 로 사용한 후 화학적 환원제를 첨가하는 방법, citrate 를 capping agent 및 환원제로 사용하는 방법 및 polyol 을 용매 및 환원제로 사용하는 방법 등이 있는데, 이들 template 를 사용하지 않는 방법들의 경우 상대적으로 낮은 수율 및 높은 반응 온도가 단점으로 알려져 있다.본 연구에서는, polyol process 이용하여 high aspect ratio 및 균일한 orientation 을 갖는 실버 나노와이어를 제조하였다. Polyol process 는 전구체로서 실버염을 사용하고, ethylene glycol 을 용매 및 환원제로, poly(vinylpyrrolidone)을 capping reagent 로 사용하여 실버 나노 와이어를 제조하는 방법으로 최근 들어 가장 많이 사용되고 있는 방법이다. 본 연구에서는 polyol process 의 공정 변수 조절 및 첨가제 변화를 통하여 상대적으로 작은 반경을 갖는 실버

나노 와이어를 제조하고, 분광학적인 방법을 통하여 이들에 대한 물리적, 화학적 특성에 대하여 조사하였다.

대한화학회
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Guest molecule-triggered magnetic variation in an expanded MOF-74 type material Co_2(dobpdc)

유대원 이우람 임광수 홍창섭

고려대 화학과

Magnetic MOFs have become one of current subjects because they carry magnetic and sorptive properties at the same time. In MOFs, magnetic properties can vary depending on the guest molecules adsorbed in the pores. We have prepared 3D porous framework, Co_2(dobpdc) (dobpdc = 4,4'-dioxido-3,3'-biphenyldicarboxylate) by microwave methods, which adopts an expanded MOF-74 structure type. Several samples with various solvent molecules were synthesized and the solvent molecules within the pore were easily removed. We will present the detailed sorption and magnetic properties in the presentation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

High carbon dioxide adsorptions in mesoporous MOFs with acidic or basic sites

이우람

고려대 화학과

We prepared a magnesium compound $[Mg_2(dotpdc)(DMF)_2](DMF)_x(H_2O)_y$ ($Mg_2dotpdc$; 1) with a three dimensional network structure, adopting an expanded Mg-MOF-74 structure type, using a microwave reactor. The solvent molecules in the pores were removed upon evacuation to generate open metal sites. Notably, the high-density open metal sites are located at each corner of a hexagon, which propagate along the 1D channels. These materials exhibit exceptional CO_2 adsorption capacities associated with the presence of the unsaturated metal centers. And coordinatively unsaturated Mg^{2+} cations lining the 28.8-?-diameter channels of 1 were functionalized with polyamine (X=diamine or triamine) to afford X-Mg_2(dotpdc). This compound displays a great capacity for CO_2 adsorption at low pressures. The structures and sorption properties of these compounds will be presented in detail.

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A Mononuclear Dysprosium Complex Exhibiting Field-Induced Single-Ion Magnet Behavior

임광수 유대원 홍창섭

고려대 화학과

We prepared a 6-coordinate disprosium(Ⅲ) complex, $[Dy{\cdot}L(OiP)_2]{\cdot}PF_6$ (1), where L(OiP) = (diisopropyl phosphito-P)cobaltate. Compound 1 was characterized by elemental analysis, IR, PXRD, and single crystal X-ray diffraction. In compound 1, Dy^{3+} is coordinated by six oxygen atoms from the L(OiP) ligand. The coordination sphere of DyⅢ ion is close to D_{3d} symmetry. In the absence of dc field, the compound 1 shows no out-of-phase signals of ac magnetic susceptibilities. This is due to the fast relaxation of the magnetization through a quantum tunneling process. The fast quantum tunneling pathways at zero dc field can be prevented by applying an external magnetic field, which results in slow relaxation of magnetization. Detailed structural and magnetic studies will be given in the presentation.

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기능성 유-무기 복합 실리카 입자의 제조 및 특성 분석

김수정 이상경[1] 구상만[2]

한양대 수소연료전지공학과 [1]한양대 수소연료전지 공학과 [2]한양대 화학공학

마이크로 이하의 크기를 갖는 기능성 hybrid 실리카 입자 (혹은 ORMOSIL 입자)들은 촉매, 안료 및 전자재료 등과 같은 전통적인 산업분야뿐만 아니라, bio-labeling, medical diagnostics 및 drug delivery 등과 같이 최근 첨단 산업으로 대두되고 있는 바이오산업분야로의 응용 가능성에 대하여 많은 관심의 대상이 되고 있다. 이들 기능성 실리카 입자들은 생체물질과 유사한 크기를 갖고 있을 뿐만 아니라 독성이 없기 때문에 biomedical 분야에 특히 적합한 물질로 인식이 되어 multicolor imaging 은 물론 site-selective binding, detection 및 separation 등과 같은 multiplex tasking 에 적합한 구조를 갖는 입자의 제조 및 변형에 대한 많은 연구가 진행되고 있다. 현재까지 기능성 실리카 입자들은 대부분의 경우 tetraethylorthosilicate (TEOS)를 사용하여 얻어진 실리카 입자의 표면 개질 반응을 통하여 제조되고 있는 바, 이러한 표면 개질을 이용한 기능성 실리카 입자의 제조는 긴 시간 및 여러 단계의 반응을 필요로 한다는 것 및 개질된 관능기들의 불균일한 분포 가능성 등과 같은 단점 등을 보여주는 바, 기능성 실리카 입자들의 보다 경제적이고 폭 넓은 산업적 응용을 위하여, 간단하면서도 효율적인 제조 방법의 개발이 절실히 요구되고 있다.본 연구에서는, St?ber process 와 차별화된 self-emulsion process 를 이용하여 크기 및 형상이 제어되고, 입자의 내/외부에 균일하게 분포된 유기 관능기를 갖는 기능성 실리카 입자를 제조하였다. 본 연구에서 사용된 self-emulsion process 는 물을 용매로 사용하고 원료로 사용하는 phenyltrialkoxysilane monomer 의 소수성을 이용하여 self-emulsion droplet 을 형성 한 후, 이들 droplet 들 내부에서의 hydrolysis 및 condensation 을 통하여 기능성 실리카 입자를 제조하는 방법으로 기존의 St?ber process 에 비하여 입자의 크기 및 형상제어가 용이하다는 점 이외에도 입자의 내부 구조 제어도 가능하다는 장점을 보여주고 있다. 또한 외부 유기

관능기들의 추가 표면 반응을 통하여 새로운 유기 관능기의 도입 가능성도 확인 할 수 있었다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Improvement of Visible Light Photocatalyic Activity of Silver Phosphate upon Hybridization with Layered Titanate Nanosheets

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Novel porous nanocomposites of Ag_3PO_4—layered titanate with improved photocatalytic activity are synthesized by an electrostatically-derived self-assembly reaction between negatively-charged titanate nanosheets and $Ag(NH_3)_n^+$ complex cations, which is followed by the reaction with ammonium dihydrogen phosphate. Upon the reaction with dihydrogen phosphate ions, the $Ag(NH_3)_n^+$ complex hybridized with layered titanate is transformed into spherical silver phosphate nanocrystals with the average size of ~15 nm, leading to the formation of the Ag_3PO_4—layered titanate nanocomposites. The homogeneous hybridization of layered titanate and silver phosphate is confirmed by powder X-ray diffraction, high-resolution transmission electron microscopy, and elemental mapping analysis. Field emission-scanning electron microscopy and N_2 adsorption-desorption isotherm analyses clearly demonstrate the creation of porous structure with expanded surface area via the house-of-cards-type stacking structure of titanate nanosheets. The present nanocomposites display an intense absorption of visible light, a result of the hybridization of layered titanate with narrow bandgap semiconducting silver phosphate. The obtained Ag_3PO_4—layered titanate nanocomposites are fairly active as photocatalyst under the irradiation of visible light (λ>420 nm), highlighting the usefulness of the present self assembly-phase transition route in synthesizing efficient visible light active photocatalysts.

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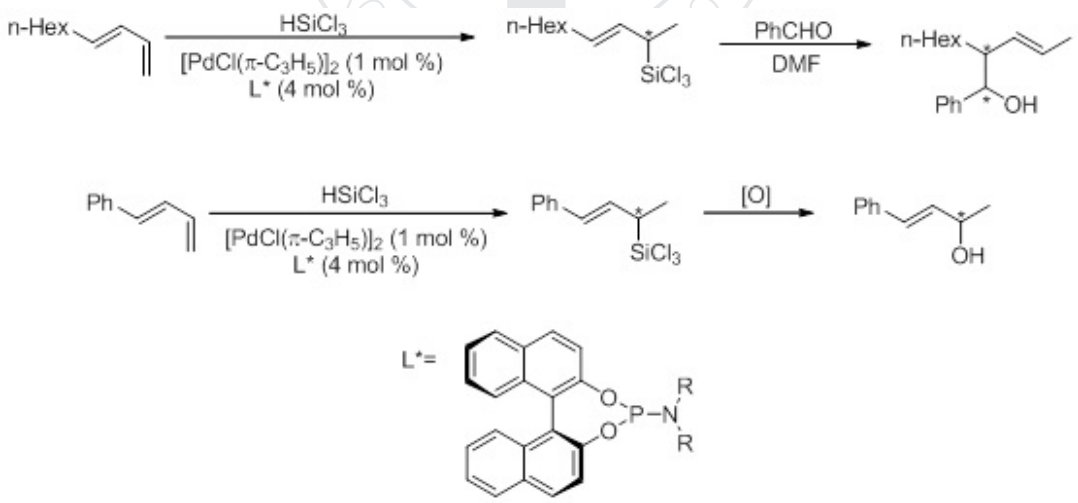
Palladium-catalyzed asymmetric hydrosilylation of linear 1,3-dienes with chiral phosphoramidite ligands

신혜미 남궁숙 한진욱

한양대 화학과

Pd-catalyzed asymmetric hydrosilylation of alkenes with trichlorosilane is important example of hydrometallation reactions that display excellent regioselectivities and enantioselectivities for a variety of olefins. The optically active hydrosilylation products are versatile intermediates in organic synthesis via some efficient transformations like homoallyl alcohols or allyl alcohols. Regioselectivity and enantioselectivity are dependent on chiral phosphoramidite ligands used.



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A 3D Co(Ⅱ) metal-organic framework with a triazine derivative ligand

정은아 홍창섭

고려대 화학과

Triazine-based ligands have been used to construct MOFs with permanent porosity and charming topologies. Hence, we attempted to use a new triazine derivative to construct a large-pore MOF with specific topology. We have synthesized a new 3D metal-organic framework from cobalt bromide and H_3L (H_3L =2,4,6-tris(4-hydroxy-3-carboxyphenylamino)-1,3,5-triazine) under a solvothermal condition. The structure of the complex was determined using single-crystal X-ray diffraction. A secondary building unit consists of one Co(Ⅱ) ion and four L^{3-} ligands. Co(Ⅱ) is coordinated by five O-donors from carboxylates and one nitrogen atom from triazine ring. In this presentation, detailed structure, thermal stability and other related properties of the crystal will be demonstrated.

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A 2-D layered MOF exhibiting proton conductivity and CO_2 preferential adsorption

방원주 홍창섭

고려대 화학과

A new bi-functional 2D layered metal organic framework based on a tripodal flexible ligand, 1,3,5-Tri(4-carboxyphenoxy)benzene (H_3TCPB) as a linker and zinc nitrate as a metal source has been synthesized. Three zinc centers in a secondary building unit are linked by two $TCPB^{3-}$ ligands and water molecules are axially coordinated to two zincs, which forms an infinite 2D layer. The 2D sheets are piled up as AB stacking mode along the c axis. $Zn_3(TCPB)_2(H_2O)_2]?4DMF?3H_2O$ (1?4DMF?$3H_2O$) underwent solvent exchange with $CHCl_3$ and then was heated at 50 ℃ for 4 h to remove free DMFs. We have measured proton conductivity and gas sorption with the above activated sample. Compound 1 shows proton conductivity under room temperature, 98 % RH condition. Water mediated proton conductivity is attributed to the hydrophilic environment formed by axially coordinated water molecules, and aryl ether oxygens. The complex exhibits preferential CO_2 adsorption as well.

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은 나노와이어의 직경과 길이에 따른 표면저항 및 광학적 특성

오수연 이상훈 최원종 이효정 오문비

(주)나노픽시스 기술연구소

은 나노와이어는 우수한 전기 전도성 및 유연성을 지니고 있어 투명전극인 ITO 를 대체함과 동시에 플렉서블 디스플레이에 적합한 재료로 최근 연구가 활발히 진행되고 있다. 본 연구는 은 나노와이어의 직경과 길이에 따른투명전극의 표면 저항 및 광학특성을 연구하였다. 은 나노와이어의 평균 직경은 각각 30 nm, 42 nm 및 53 nm 인 와이어를 사용하였고, 길이에 따른 영향을 비교하기 위한 은 나노와이어는 직경 30nm, 길이는 각각 5, 10 및 25 ㎛였다. 4-probe 로 면저항을 측정하였으며, Uv-vis spectrophotometer 를 이용하여 광투과도를 측정하였다. 은나노 와이어의 직경이 작을수록 면저항은 낮아지는 것을 확인하였다. 이는 은 나노와이어의 직경이 작을수록 은 나노와이어의 질량대비 와이어의 수 평균 밀도가 증가하여 균일한 전기 전도성 네트워크 형성에 따른 것이며, 또한 와이어의 길이가 길어질수록 와이어간 접촉수 감소에 따른 접촉저항이 감소하여 표면 저항이 감소하고 광 투과도가 증가됨을 확인하였다.

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Silver Nanowire(AgNW)의 정제에 따른 투명전극의 표면저항 및 광학특성 연구

오문비 이상훈 이효정 오수연 최원종

(주)나노픽시스 기술연구소

ITO 를 대체하여 투명전극으로 이용할 수 있는 물질 중 가장 우수한 성능을 지닌 AgNW 는 Polyol 용매내에서 합성되며, 합성 후 반응용매 내에는 촉매, 은입자 및 capping agent 인 Poly(vinylpyrrolidone)[PVP]을 함유하고 있다. AgNW 기반 투명전극 형성 시 촉매 및 은입자들은 AgNW 전도성 네크워크 사이에 위치하여 접촉 저항 및 Haze 를 증가 시키며, 절연체인 PVP 는 수십 nm 두께로 AgNW 표면에 코팅되어있어 표면전기저항을 증가시키게 된다. 이에 용해도차 침강법에 의해 정제 후 AgNW 를 사용한다. 정제횟수 및 정제도에 따라 촉매 및 은입자의 내포율을 광학현미경 및 FE-SEM 으로 확인하였고, TEM 을 통하여 AgNW 표면의 PVP 제거율을 확인하였다. 또한 정제에 따른 AgNW 기반 투명전극 형성 후 UV-visible Spectrometer 및 4-probe 를 이용하여 투과도 및 표면 전기저항을 측정하였다. AgNW 기반 투명전극의 표면 저항은 1 차 정제 시 140 Ω/□, 2 차 정제시 110 Ω/□, 3 차 정제 시 100 Ω/□, 그리고 4 차 정제 시 80Ω/□이였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Incorporation of Cationic Tin(IV) Porphyrin on Surface of TiO_2 for Visible Light-Induced H_2 Production

김성현 김희준

금오공과대 응용화학과

A photocatalyst that is active under visible light is of paramount importance as an essential element of solar energy utilization. A variety of approaches are being made in search of visible light-induced photocatalysts. We have studied visible light-induced photocatalysts based on porphyrins. We have been interested in an approach to incorporate tin(IV) porphyrins as visible light absorbing sensitizers at the TiO_2/H_2O interface. The surface of TiO_2 particles coated with perfluorosulfonate polymer (Nafion?) can bind water-soluble cationic tin(IV) porphyrins within the Nafion layer through electrostatic attraction. Incorporation of cationic tin(IV) porphyrin into the layer of Nafion on TiO_2 and the visible light-induced production of H_2 by this hybrid photocatalyst will be presented in detail.

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제조 변수에 따른 Silver Nanowire의 형상 제어

이효정 이상훈 최원종

(주)나노픽시스 기술연구소

Silver Nanowire(AgNW)는 전기 전도도가 우수하고 가시광선영역에서 투과도가 매우 높은 소재로써 투명전극 및 플렉시블 디스플레이 등에 적용할 수 있다. 투명전극에 적용 되기 위해서는 낮은 표면 전기저항 및 높은 광 투과도는 필수요소이다. 이에 종횡비 700 이상의 직경 40nm 이하, 길이 25~30um 의 AgNW 제조가 선행 되어야 한다. 이에 본 연구에서는 Polyol process 를 이용하여 AgNW 를 제조 하였고 변수에 따른 길이 및 직경의 변화를 관찰 하였다. 제조 변수로는 Cappping agent 와 silver salt 의 몰비율, 촉매의 량, 그리고 주입 속도의 변화를 주었다. 그 결과 평균 길이 25 ㎛, 직경 35~40nm 수준의 Silver nanowire 를 합성 할 수 있었다. 제조된 AgNW 는 FE-SEM 과 TEM 을 이용하여 분석을 하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Control of Intramolecular Photoinduced Electron Transfer in Cyclometalated Ir(III) Complexes Tethering a Di(2-picolyl)amino Moiety and Implications for Phosphorescence Zinc Sensing

우하나 유영민[1] 남원우[2]

이화여대 대학원 바이오융합과학과 [1]KIST 의공학연구소 [2]이화여대 화학과

Photoinduced electron transfer (PeT) has been successful for the creation of a variety of molecular sensors for the detection of diamagnetic metal ions, such as labile zinc. We previously reported the development of the phosphorescent zinc sensor based on a cyclometalated Ir(III) complex scaffold, and revealed that zinc-induced modulation of PeT was responsible for its phosphorescence response. This finding promoted us to investigate structural effects in PeT between the Ir(III) cyclometalates and a zinc-chelating di(2-picolyl)amino group. Photophysical and electrochemical properties of a series of cationic Ir(III) complexes with various cyclometalating ligands were investigated. The studies established that phosphorescence modulation by the excited-state PeT, thus zinc response, was governed by the classical Rehm-Weller theory. Furthermore, a Coulombic barrier located in the cyclometalating ligand had negligible influence in PeT. It is envisioned that these conclusions will provide important guidance to the future development of

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Phosphorescence Zinc Biosensing with Molecular Probes based on Iridium(III) Cyclometalates

조소민 유영민[1] 남원우[2]

이화여대 바이오융합과학과 [1]KIST 의공학연구소 [2]이화여대 화학과

A series of iridium(III) complexes bearing cyclometalating ligands with various bandgap and electron density have been prepared and evaluated for the detection of biological zinc ions. A metal-chelating di(2-picolyl)amino group was tethered to a neutral 1,10-phenanthroline ligand, which constituted the cationic iridium(III) complexes. The structural variations in the cyclometalating ligands produced phosphorescence zinc responses with color-tuned emission profiles from blue (498 nm) to red (675 nm). The zinc sensing properties of the complexes were assessed in acetonitrile and physiologically simulated buffer solutions, and the studies revealed that the zinc responses depended strongly on the nature of the cyclometalating ligands. Finally, zinc biosensing utility has been demonstrated by phosphorescent visualization of exogenously supplied zinc ions in live HeLa cells.

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Performance enhancement of Sb2S3-sensitized photoelectrochemical solar cell using TiO2 nanorods as photoanode

허진혁 임상혁[1] 석상일[1]

고려대 화학과 [1]한국화학연구원 화학소재연구단

One-dimensional (1D) nanostructured materials have received a great deal of attention because they can have unique properties that are not seen in bulk or three-dimensional materials. To exploit the structural advantage inherent in 1D photoelectrodes such as an efficient charge transport and well-developed macroporosity, we used them as photoelectrode in Sb2S3-sensitized photoelectrochemical solar cells using cobalt redox electrolyte. The TiO2 nanorods were prepared by sacrificial templating of ZnO nanorods grown on a dense TiO2 layer/FTO film. By simply replacing the conventional mesoscopic TiO2 electrode with the TiO2 nanorod electrodes, we could greatly reduce the nonlinear behavior of power conversion efficiency of Sb2S3-sensitized photoelectrochemical solar cells with illuminated sun intensity. This can be ascribed that TiO2 1D photoelectrodes provide sufficient pore-space to relieve the mass transport problem at vicinity of Sb2S3 and cobalt electrolyte.

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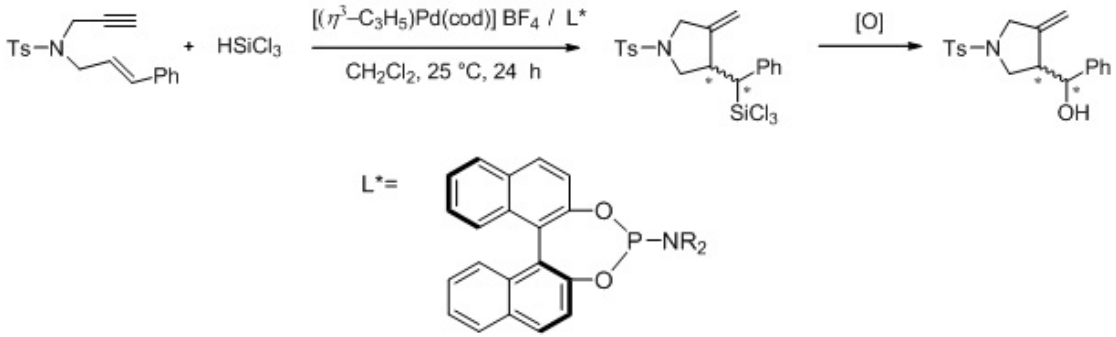
Cationic palladium-catalyzed asymmetric hydrosilylation/cross-coupling of 1,6-enyne with chiral phosphoramidite ligands

기세훈 박희건 한진욱

한양대 화학과

Cationic palladium-catalyzed asymmetric hydrosilylation/cross-coupling of 1,6-enyne provides one of the most efficient routes to optically active allylsilanes, which are able to be further derivatized to useful synthetic intermediates such as homoallyl alcohols having a cyclic moiety. Chiral phosphoramidite ligands, containing an axially chiral monophosphine, were applied to palladium-catalyzed asymmetric hydrosilylation/cross-coupling of 1.6-enyne. Enantioselectivities were varied dramatically according to the chiral phosphoramidite ligands used.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-296**

발표분야: 무기화학

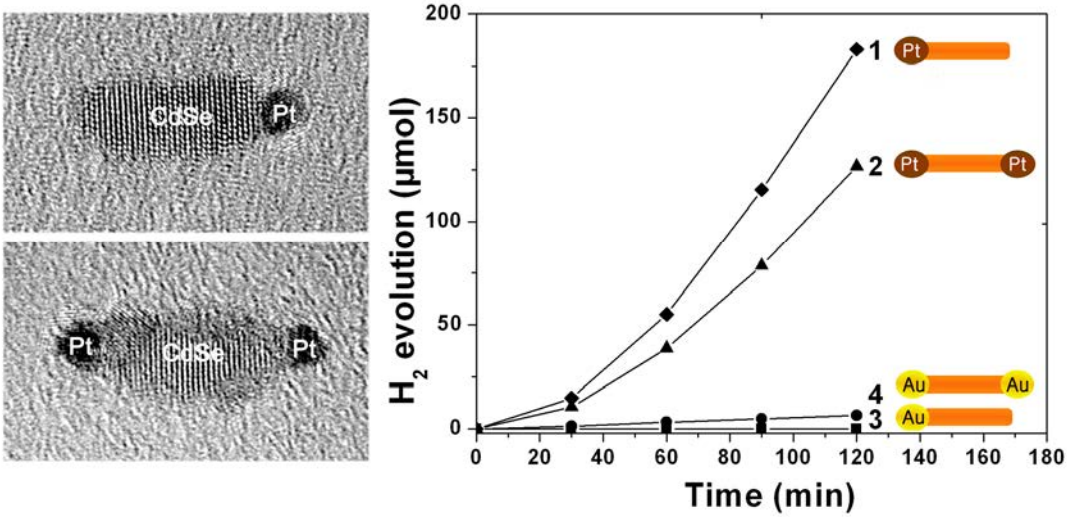
발표종류: 포스터, 발표일시: 수 16:00~19:00

Geometric effect of single or double metal-tipped CdSe nanorods on photocatalytic hydrogen generation

방정엽

KAIST 화학과

Photocatalytic hydrogen generation is one of the potential reactions for the production of environmentally clean and renewable energy resources from sun light. Although TiO_2 has been studied as a highly effective photocatalysts for decades, the wide band gap of TiO_2 in the ultraviolet region moved the research interest into semiconductors absorbing visible light, such as complex metal oxides, nitrides, and sulfides. Among these materials, cadmium chalcogenides have mostly been used as essential elements of the photocatalysts due to their narrow band gaps and band energies at relatively low potentials. Recently, several hybrid nanostructures of CdS and CdSe with metals have been synthesized and employed for the photosplitting of water. Different from the previous catalytic studies, well-defined morphology and components of the hybrid nanocatalysts provided valuable information of photo-induced charge separation and transfer processes during the reaction. In the present work, we focused on geometrical (single or double tipped) and compositional (Pt or Au) variations of active metal components on the CdSe nanorods. These colloidal nanostructures were employed for photocatalytic hydrogen generation from water under the identical reaction conditions with visible light irradiation (Wavelength $\geq$ 420 nm). The catalysts exhibited a significant dependency of the catalytic activity both on the catalyst geometry and the choice of the metal tips, which could be elucidated by the energetic consideration of hole transfer to the sacrificial reagents and electron transfer to the metal tips on the CdSe nanorod.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-297**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual-Tridentate Fe(III) Complexes Containing Bidentate Tetrazole Ligand For Selective binding with Alkali Metal

박가현 고민정 이휘현 이준승

전남대 화학과

The syntheses, characterizations and alkali metal recognition studies of iron complexes containing tetrazole ligands, which form high dimensional coordination polymers in the solid status, are investigated. From the reaction of iron(III) perchlorate, {5-(2-hydroxy) phenyl}tetrazole (LH2) and 2,2'-bipyrimidine(bpym) in H2O, high dimensional mixed metal coordination polymers, [Li3(bpym)1.5FeL3(H2O)6]n (1a), [Na3(bpym)1.5FeL3(H2O)7] n (2a), [K3(bpym)FeL3(H2O)7]n (3a) were synthesized with high yield and their solid structure were determined from X-ray diffraction studies. In all three structure, dual-tridentate iron anion fragment (FeL33-) was observed. As the ion sizes of alkali metals increased, more strong binding between alkali metal ion and iron fragment were observed. Because iron fragment has outstanding coordination ability, extremely short Fe - K distance, which is most short distance among reported in literature, was observed in complex 3a. When bpym was excluded in the reaction, 0-D [Li3FeL3(H2O)3] (1b), 2-D [Na3FeL3(H2O)7] (2b) and [K3FeL3(H2O)7] (3b) were synthesized and coordination between alkali metal ion and iron fragment (FeL33-) was stronger than bpym contained species. In particular, due to lack of binding sites, potassium binds to TzOH ligands with σ and π character in complex 3b.

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

액상법을 이용한 graphene의 제조 및 표면 개질

박종웅 이종서 구상만

한양대 화학공학과

Graphene 은 sp2 혼성화된 궤도함수를 갖는 탄소원자들로 이루어진 연속된 벤젠 모양의 이차원 구조를 갖는 single layer 형태의 물질로 우수한 열적, 전기적, 광학적 및 기계적 특성들로 인하여 최근 들어 microelectronics 및 복합재료 분야에서 높은 관심의 대상이 되고 있다. 이들은 기존의 고분자 물질과 적절히 복합화 할 경우 적은 양으로도 최종 복합물질의 전기적, 물리적 성질을 획기적으로 향상시킬 수 있다. 일반적으로 고분자/graphene 복합소재의 특성은 고분자 기재에 대한 첨가된 graphene 의 분산성에 많은 영향을 받는바, 복합소재의 가공성 및 성능 향상을 위하여 graphene 표면의 개질에 대한 많은 연구가 진행되고 있다. 화학적으로 개질되거나 기능화된 graphene 은 주로 graphene oxide 를 이용하여 얻어진 graphene 을 사용하여 제조하는데, 전구체인 graphene oxide 의 경우 주로 Hummers 법과 같은 다단계 공정을 이용하여 graphite 로부터 chemical oxidation 을 통한 exfoliation 으로 얻어진다. 화학적 개질 또는 기능화된 graphene 은 안정성이 높아질 뿐만 아니라 THF, toluene 등과 같은 다양한 종류의 유기용매에 매우 뛰어난 분산성을 보여주는데, 최근 들어 이러한 graphene 의 표면 개선을 위하여 다양한 방법들이 개발되고 있다.본 연구에서는 modified Hummers 법을 이용하여 graphite 로부터 graphene oxide 를 합성한 후, graphene oxide 와 다양한 종류의 유기실란들과의 반응을 통하여 화학적 기능화를 유도하였다. 또한 이들 유기실란으로 기능화 된 graphene oxide 를 이용하여 용액상에서의 화학적인 환원 반응을 통하여 표면이 개선된 reduced graphene sheet 를 제조한 후, 개질에 사용된 유기실란의 관능기(hydrophilic/hydrophobic, aliphatic/aromatic 등)의 변화가 표면 개선된 graphene oxide 및 reduced graphene 의 분산성에 미치는 영향에 대하여 분광학적인 방법을 이용하여 조사하였다. 또한 환원제의 종류에 따른 reduced graphene sheet 의 분산성 및 물리적, 화학적 특성의 변화에 대해서도 조사하였다.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

BSA-Mediated Cucurbit[6]uril and Spermine Interaction Measured by Force-Based Atomic Force Microscopy

배영인 백강균 김기문 박준원

포항공과대 화학과

Atomic force microscopy (AFM) has been generally used to study specific interaction between host-guest complexes as well as biomolecule pairs. We measured the single unbinding force of a host-guest complex, cucurbit[6]uril (CB[6]) and spermine. To observe unbinding event of the complex at a single molecule level, a dendron was immobilized on both an AFM tip and a substrate. Subsequently, a dendron-coated tip was functionalized with spermine. And bovine serum albumin (BSA) was introduced on the dendron-coated substrate before the immobilization of CB[6]. Under the condition, we observed characteristic stretching in the force-distance (f-d) curve showing single unbinding force due to the elasticity of the protein. For bridging CB[6] and BSA, we introduced homo-bifunctional linker. In case of this reaction, some of the linkers connect amine parts of BSA. And we also observed distinguishable stretching depending on the reaction solvent of the linker. Organic solvent led us to obtain relatively more stable and short stretching f-d curve than buffer solvent. With these approaches, unambiguous sorting the specific unbinding event and distinguishing different behavior of stretching depending on the solvent were possible.

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발표코드: **INOR.P-300**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single Nanoparticle Attached with edge of AFM tip for Tip Enhanced Raman Spectroscopy

박익범 김웅[1] 박준원[1]

포항공과대 융합생명공학부 [1]포항공과대 화학과

Tip enhanced Raman spectroscopy (TERS) has been proposed as a method to detect a variety of chemical bond, biological and material sample. The one of the best challenge to TERS technique is how to make novel TERS tips. In this study, a single gold nanoparticle is attached with edge of AFM tip for TERS.1,2 Various silver staining conditions were examined to grow a silver shell thickness (10nm~50nm) of gold attached with edge of AFM tip. As the last step, a gold coating is placed as the protective silver layer. It is expected that the single Au-Ag-Au layered nanoparticle at the edge of an AFM tip will show its efficacy for TERS.

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발표코드: **INOR.P-301**

발표분야: 무기화학

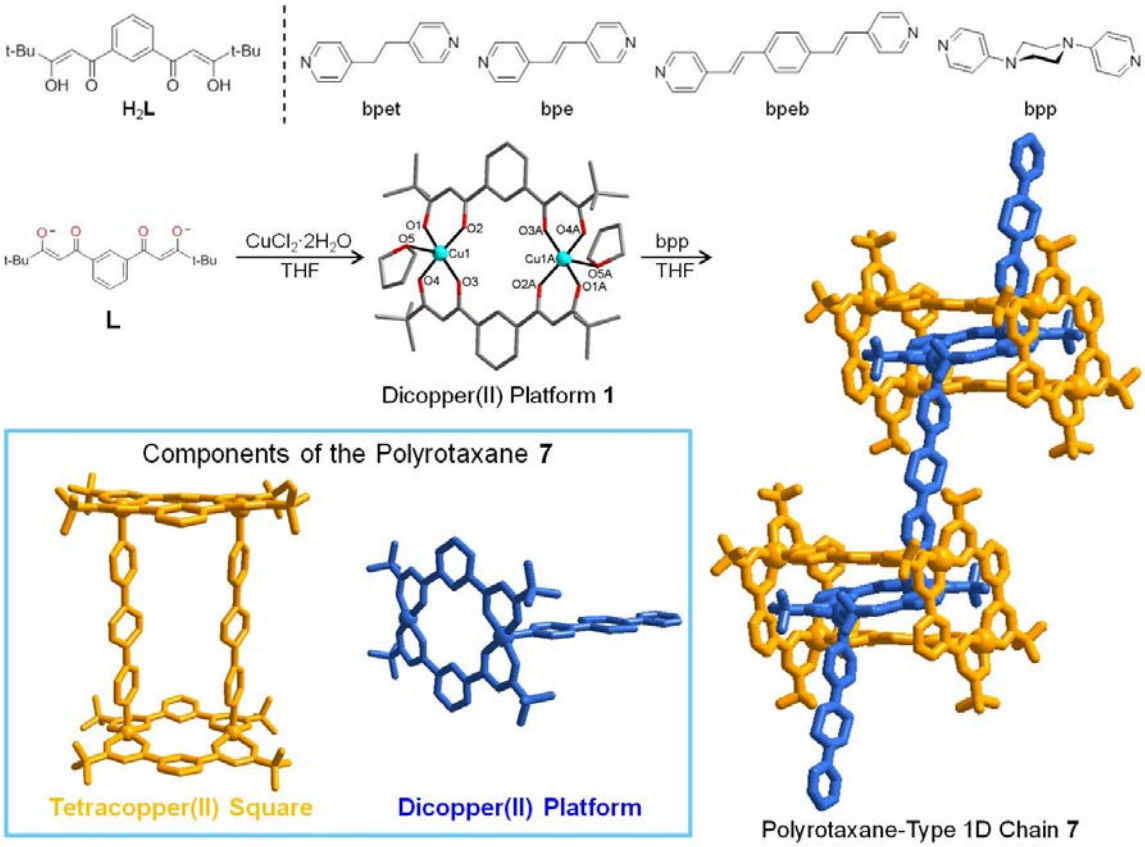
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembly of Extended Metallo-Supramolecules incorporating Bis-β-Diketonato Ligand

주희영 박기민 이심성

경상대 화학과

The assembly reactions of bis-β-diketonato ligand (H_2L) with $CuCl_2 2H_2O$ and $Ni(NO_3)_2 6H_2O$ afforded a planar 'platform-like' complexes $[Cu_2(L)_2(THF)_2]$ (1) and $[Ni_2(L)_2(THF)_2(H_2O)_2]$ (2), respectively. Uncharged complexes 3-7 between the dicopper(II) platform complex 1 and dipyridyl derivatives (L': bpet, bpe, bpeb, and bpp) have been synthesized. X-ray structure determinations show that the dipyridyl coligands L' coordinate in a bridging fashion via both their heterocyclic nitrogen atoms on alternate sides of 1 to produce isostructural stairway-type 1D chains such as $[Cu_2(L)_2(bpet)]_n(2THF)_n$ (3), $[Cu_2(L)_2(bpe)](bpe)(THF)\}_n$ (4), and $[Cu_2(L)_2(bpeb)]_n(4THF)_n$ (5). Interestingly, the reaction of 1 with bpp gave a mixture of $[Cu_2(L)_2(bpp)]_n(2THF)_n$ (6) and $\{[(Cu_2L_2)_2(\mu^2\text{-bpp})_2][(Cu_2L_2)(\mu^2\text{-bpp})](bpp)\}_n$ (7), which show stairway-type 1D polymer and polyrotaxane-type structures, respectively.



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장소: 부산BEXCO

발표코드: **INOR.P-302**

발표분야: 무기화학

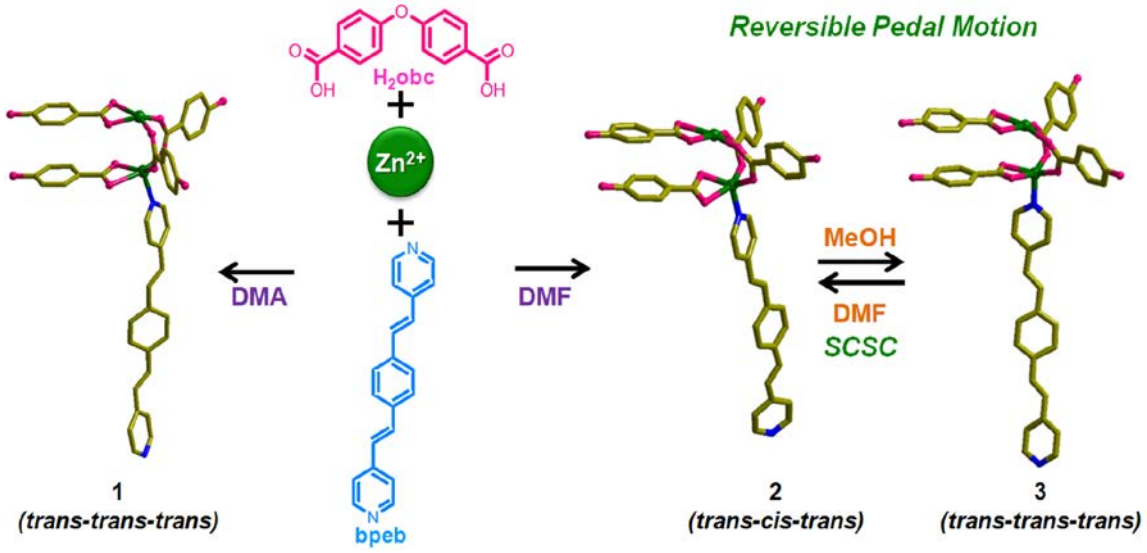
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-Induced Supramolecular Isomerism Exhibiting A Reversible Pedal Motion-Type Single-Crystal to Single-Crystal Transformation

박인혁 이심성 Jagadese J. Vittal[1]

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

The assembly reaction of a dipyridyl derivative (bpeb) with dicarboxylic acids (H_2obc) and zinc(II) nitrate in the presence of DMA, DMSO, H_2O, and NaOH solution enabled the isolation of a 3-fold interpenetrated pillared-layer porous coordination polymer $[Zn_2(obc)_2(bpeb)]\cdot 5H_2O$ (1) with the *trans-trans-trans* isomer of bpeb pillar ligand. When DMF was used instead of DMA, a supramolecular isomer $[Zn_2(obc)_2(bpeb)]\cdot 2DMF\cdot H_2O$ (2) with the *trans-cis-trans* isomer of bpeb ligand was isolated. In MeOH, 2 was transformed via the solvent exchange in a single-crystal to single-crystal (SCSC) manner to afford $[Zn_2(obc)_2(bpeb)]\cdot 2H_2O$ (3) with the trans-trans-trans isomer of bpeb, a polymorph of 1. Conversion of 3 to 2 was achieved by immersing 3 in DMF. The reversible conformational changes in bpeb induced by solvents were demonstrated. This is also accompanied by the subtle changes in the unusual isomer of the paddle-wheel structure. Compounds 1 and 2 as well as 2 and 3 are supramolecular isomers.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **INOR.P-303**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

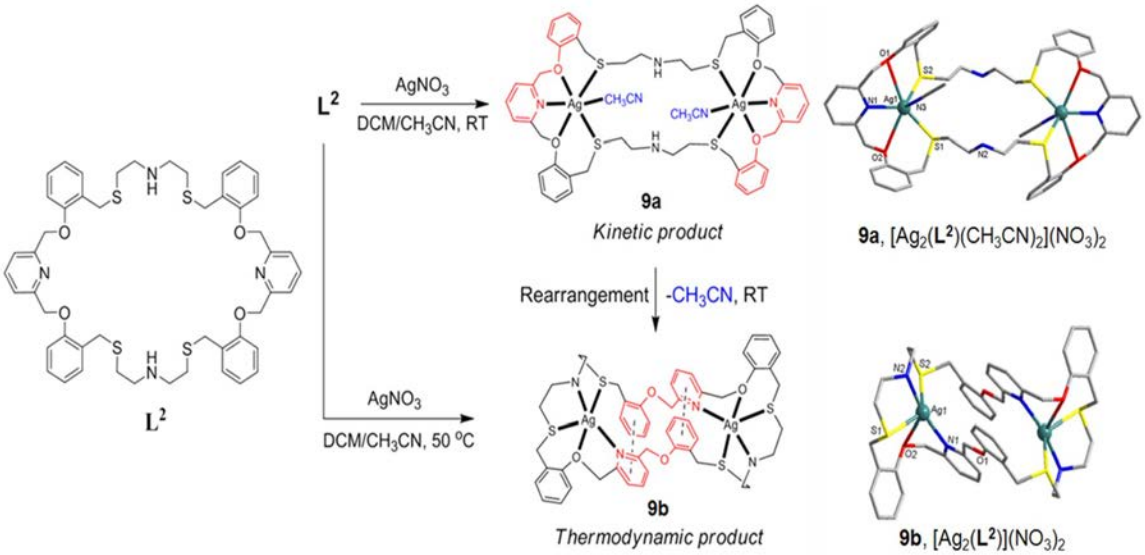
Two Dinuclear Silver(I) Complexes of a Large Macrocycle Exhibiting Different Coordination Environments

이슬기

경상대 화학과

Recently, we have reported a 40-membered $N_4O_4S_4$ macrocycle L^2 though a 2:2 cyclization of the corresponding dithiol and dichloride as a minor product during the preparation of a 20-membered $N_2O_2S_2$ macrocycle L^1.[1] In extension of our previous work, some new complexes of L^1 and L^2 are reported. Interestingly, the complexation of L^2 with silver(I) nitrate afforded two kinds of endocyclic dinuclear complexes. One is a dumbbell-like disilver(I) complex with a formula $[Ag_2(L^2)(CH_3CN)_2](NO_3)_2$ (1a), in which two silver(I) ions occupy two NO_2S_2 binding sites in the extra-large cavity of L^2 and each silver(I) is coordinated by one acetonitrile. Another one is a disilver(I) complex $[Ag_2(L^2)](NO_3)_2$ (1b), in which two silver(I) occupy only two N_2OS_2 binding sites of L^2 and the intramolecular π-π stacking between two benzene-OCH_2-pyridine moieties located at opposite site of L^2 is exist. Time-dependent crystallization experiments unambiguously show that 1a is a kinetic product and transforms into a thermodynamically more stable 1b. In addition, the complexation of L^2 with mercury(II) perchlorate and 1,4-diazabicyclo[2,2,2]octane (dabco) obtained an endocyclic dinuclear complex linked with dabco. All complexes were structurally characterized by the single crystal X-ray analysis.

Referance1. Jung, D.; Chamura, R.; Habata, Y.; Lee, S. S. *Inorg. Chem*. 2011, *50*, 8392.



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THE KOREAN CHEMICAL SOCIETY

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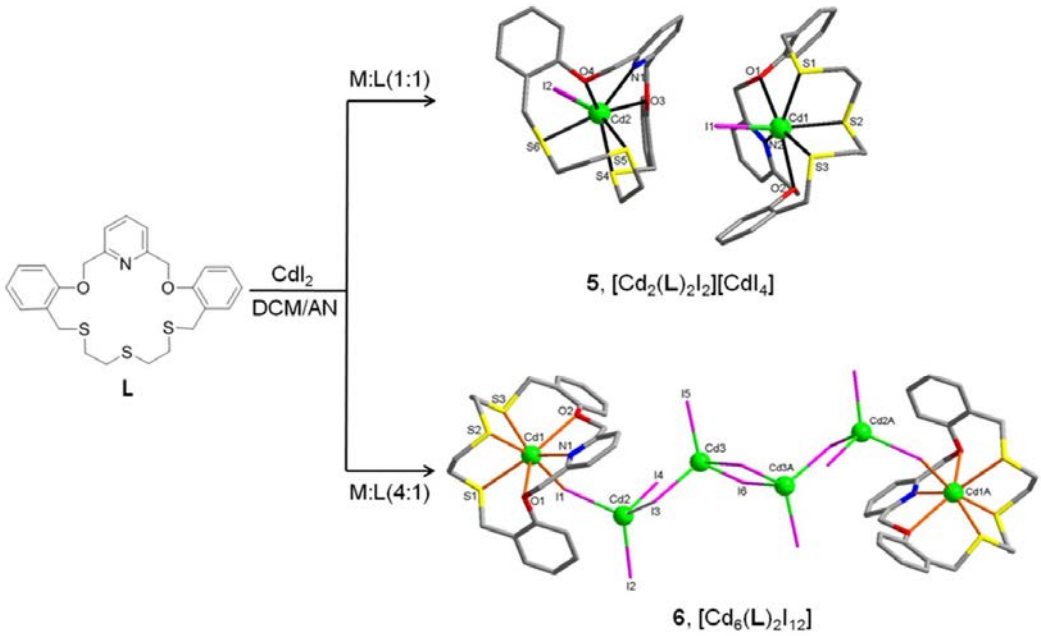
발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural Variety of Supramolecular Soft Metal Complexes of Thiaoxaaza-Macrocycles

이형환

경상대 화학과

The pyridine-containing thiaoxaaza-macrocycle L was synthesized by dithiol-dichloride coupling reactions using Cs_2CO_3 in DMF under high dilution condition. A comparative investigation of the coordination behavior of L with Ag(I), Cu(I), Hg(II), and Cd(II) is reported. The X-ray structures of six complexes (1-6) 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 $AgNO_3$, L forms a rare example of a 1D coordination polymer $\{[Ag_2(L)(NO_3)_2]?CH_3CN\}_n$ (1) incorporating endo/exocyclic metal ion coordination. The reaction of L with mercury(II) perchlorate gave an endocyclic complex $[Hg(L)](ClO_4)_2$ (3), while with mercury(II) bromide an exocyclic complex $[Hg(L)Br_2]$ (2) is obtained. In the reaction with CuI, again, L forms an exocyclic 1D coordination polymer $[Cu_2I_2(L)]_n$ (4) linked by Cu_2I_2-rhomboid giving a zigzag chain. The reaction of L with cadmium(I) iodide gave two kinds of complexes 5 and 6 depending on the variation of the metal-to-ligand ratio (see below).



Reference

1. Kang , E. J.; Lee, S. Y.; Lee, H.; Lee, S. S. *Inorg. Chem.* **2010**, *49*, 7510.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 수 16:00~19:00

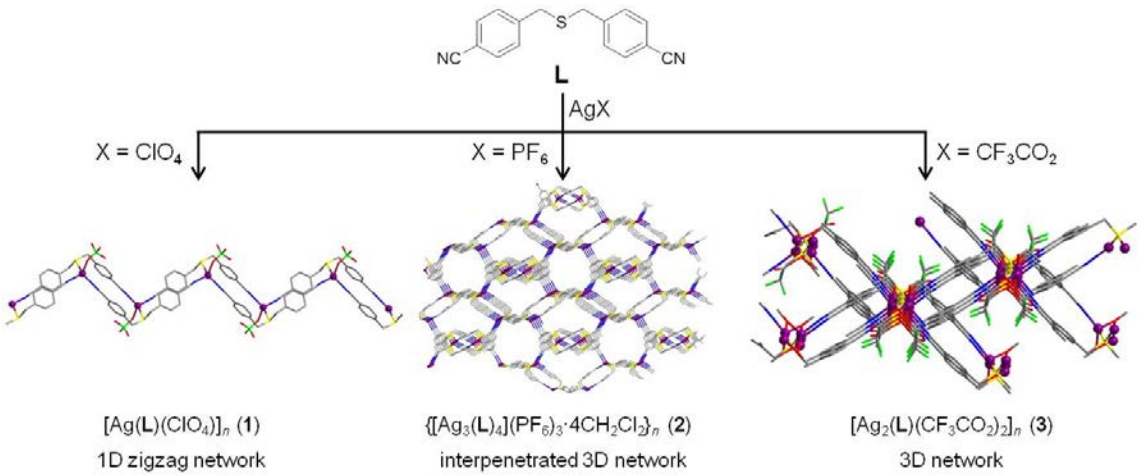
Anion Effects on Supramolecular Silver(I) Complexes of Bis(4-cyanobenzyl)sulfide

이은지 박기민 이심성

경상대 화학과

A bis(4-cyanobenzyl)sulfide (L)[1] was employed as a building block and its supramolecular silver(I) complexes are reported. The reactions of L with silver(I) salts (X = ClO_4^-, PF_6^-, or $CF_3CO_2^-$) afforded the respective anion-dependent complexes 1-3 with different topologies. $AgClO_4$ afforded a double-stranded 1D polymeric array of formula $[Ag(L)(ClO_4)]_n$ (1). Meanwhile, treatment of $AgPF_6$ afforded a 2-fold interpenetrated 3D polymeric array of formula $\{[Ag_3(L)_4](PF_6)_3?4CH_2Cl_2\}_n$ (2). The reaction of $AgCF_3CO_2$ also gave a 3D polymeric array of formula $[Ag_2(L)(CF_3CO_2)_2]_n$ (3), in which the 3D network is made up of the double-stranded (Ag-L)n backbones and further bridged by anion. The formations of such discrete, 1-D, and 3-D supramolecular complexes are discussed in terms of anion effect. In addition, the reaction of L with a mixture of CuI and HgI_2 afforded a typical pillared layered 3D heteronuclear complex of formula $[Cu^{I}_2Hg^{II}_1(L)I_4]_n$ (4), in which its 2D layer is formed by the networking of Cu^{I} and Hg^{II} iodides.

Ref. C. Barkenbus, E. B. Friedman, R. K. Flege, *J. Am. Chem. Soc.* 1927, *49*, 2549.



대한화학회
THE KOREAN CHEMICAL SOCIETY

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장소: 부산BEXCO
발표코드: **INOR.P-306**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

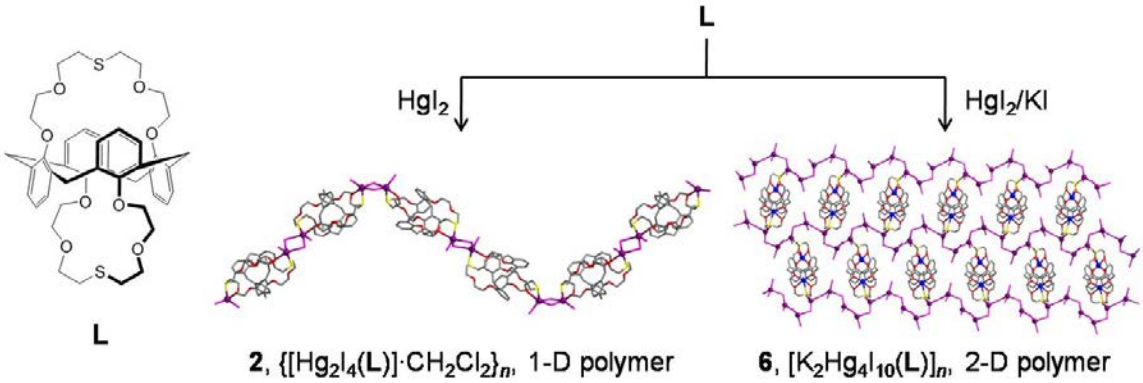
Networking of Calix[4]-*bis*-monothiacrown with Soft Metal Ions and Potassium(I) by Endo/Exocyclic Complexation

김자연 이재영[1] 이심성

경상대 화학과 [1]건양대 나노바이오화학과

In the extension of our previous work on the exocyclic coordination polymers of calix[4]-*bis*-monothiacrown (L) exhibiting a photoluminescence switching behavior,[1] its new networking patterns via homo- and heteronuclear system are reported. In the reactions of L with $Hg(SCN)_2$ and HgI_2 gave commonly 1D coordination polymers 1, $[Hg_2(SCN)_4(L)]_n$ and 2, $\{[Hg_2I_4(L)]\cdot CH_2Cl_2\}_n$ with a similar network pattern, in which Ls are linked by -X-Hg-X_2-Hg-X- (X=SCN for 1, X=I for 2, see below). CdI_2 also gave a 1D coordination polymer 3, $[Cd_2I_4(L)]_n$ showing a similar pattern. Interestingly, the reaction of CdI_2 in the presence of HgI_2 obtained a 1D coordination polymer 4, $[Cd_3Hg(L_2)I_8]_n$ linked with -I-Cd-I_2-Cd-I- and -Hg(I_2-Cd-I_2)-, alternatively. Treatment of L with KI in the presence of CdI_2 afforded a discrete endocyclic dipotassium(I) complex 5, $[K_2(L)][Cd_2I_6]\cdot CH_2Cl_2$, in which the square-type dicadmium(II) hexaiodide cluster $[Cd_2I_6]^{2-}$ exists in a separated form. The reaction of L with KI in the presence of HgI_2 afforded a 2D brick-wall type coordination polymer 6, $[K_2Hg_4I_{10}(L)]_n$ with the endocyclic dipotassium(I) complex linked by exocyclic mercury(II) iodide cluster backbone (see below). On the other hand, the stepwise reaction of 7, $[(Cu_4I_4)(L)(CH_3CN)_2]_n$ with KI gave a kinetic product 8, $[K_2(Cu_2I_4)(L)]_n$ and a thermodynamic product 9, $[K_2(Cu_2I_4)(L)]_n$, which show 1D and 2D structures linked with rhomboidal Cu_2I_2 clusters, respectively, encapsulating two potassium(I) ions inside the cavity in each case.

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



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **INOR.P-307**

발표분야: 무기화학

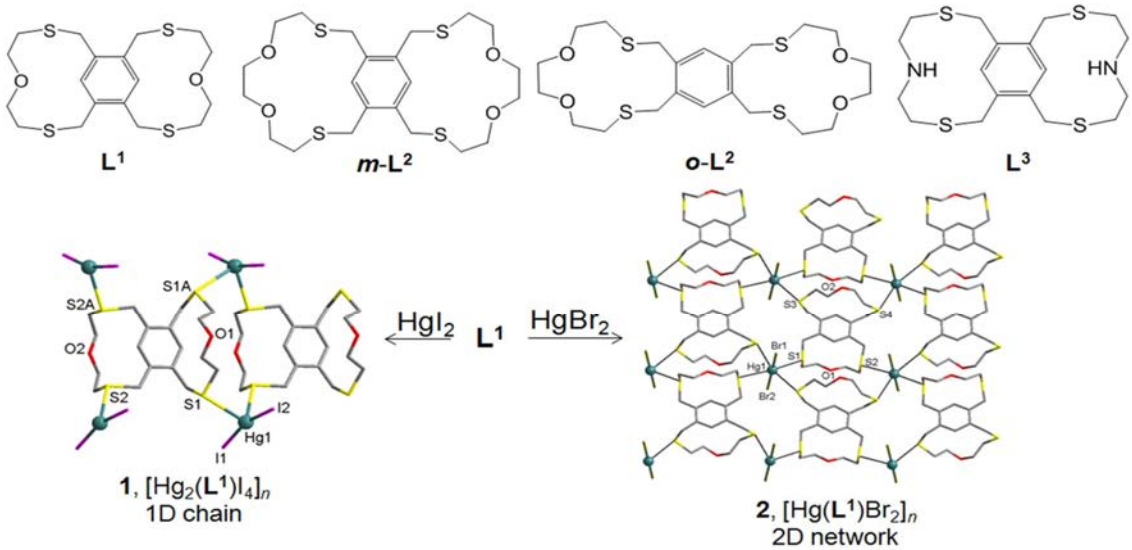
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Supramolecular Complexation of *Bis*-Thiamacrocycles

DEUKAM SIEWE ARLETTE

경상대 화학과

Since the *bis*-thiamacrocycle L^1 was reported by Loeb[1], a limited amount of works have been done concerning the related complexation behaviors so far. In the present work, we report the synthesis of a series of novel *bis*-thiamacrocycles L^2 and L^3, and their complexes with supramolecular structure. Basically, the novel *bis*-thiamacrocycles were obtained by 1,3-*bis*-cyclization between tetra(bromomethyl)benzene and corresponding dithiol in the presence of Cs_2CO_3 under high dilution condition. In preparing L^2, however, a mixture of *bis*-thiamacrocycle isomers (*o*-L^2 and *m*-L^2) was obtained. From the reactions of thiaphilic metals with these *bis*-thiamacrocycles, some supramolecular complexes were isolated. The reaction of L^1 with mercury(II) iodide afforded a 1D chain complex $[Hg_2I_4(L^1)]_n$ (1) (see below). When reacting with mercury(II) bromide, L^1 gave a 2D network complex $[HgBr_2(L^1)]_n$ (2). In the reactions of the regio-isomers *o*-L^2 and *m*-L^2 with lead(II) perchlorate afforded a 1D polymer $\{[Pb_2(o\text{-}L^2)(?_2\text{-}ClO_4)_2(ClO_4)_{2]}\}_n$ linked by anion and a discrete 2:1 complex, $[Pb_2(m\text{-}L^2)(CH_3CN)_2(H_2O)_2(ClO_4)_2](ClO_4)_2$, respectively.



Reference

1. Loeb, S. J.; Shimizu, G. K. H. *Can. J. Chem.* **1994**, *72*, 1728.

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Synthesis of Nanoparticulate Iron Oxide Tubes from Microporous Organic Nanotubes as Stable Anode Materials for Lithium Ion Batteries

강나래 손성욱[1]

성균관대 에너지과학과 [1]성균관대 화학과

Diverse porous materials have been in the spotlight for several decades due to their wide range of applications as adsorbents, gas storage materials, solid support for catalytic materials and etc. According to their components, these materials can be classified into three groups; inorganic materials, metal-organic composites and purely organic systems. Among these porous materials, organic porous materials have attracted special attention due to the low densities and robustness. Transition metals have widely been applied as part of electronic devices such as solar cells, fuel cells and batteries. To bring out the best in each of them, we introduced transition metal to porous organic materials to use as an anode materials for lithium ion batteries. In this presentation, we will announce the recent results in development of microporous organic materials. Through Sonogashira coupling between the tetrakis(4-ethynylphenyl)methane and N,N'-di(4-iodophenyl)-4,4'-bypyridinium dichlorides, microporous organic nanotubes were prepared. The resultants were used as a template for secondary inorganic materials, Fe2O3 nanotubes with a high surface area. The electrochemical studies on the Fe2O3 nanotubes were conducted, which showed the high discharge capacities and excellent stabilities for anode materials in lithium ion batteries. This study shows that the synthetic chemistry for microporous organic networks can be applied in development of inorganic energy storage materials.

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Prussian Blue Nanoparticles on Transparent Graphene Film: The first Graphene-based Electrochromic Systems

고주홍 손성욱

성균관대 화학과

Electrochromism is a reversible color change of materials through an applied voltage. One example of an electrochromic material is Prussian Blue FeIII4[FeII(CN)6]3 which is an interesting material in terms of its electrochemical and magnetic propertiesIn this presentation, we report the electrochromic performance of the electrochemically deposited Prussian Blue nanoparticles on transparent graphene film. Considering the slow electron transfer behavior of high-quality graphene, the response times of graphene film were compared with of the commercial indium tin oxide (ITO) electrode. To control the size and thickness of the Prussian Blue, we adjusted the scan cycle number in cyclic voltammetry.The response times of the Prussion Blue nanoparticleson transparent graphene film were 4.2-38.0 s for bleaching and 3.3-28.6 s for coloring (half as fast as those on ITO electrode).

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Synthesis of a redox-active porous coordination network

구진영 **Yakiyama Yumi Masaki Kawano**

포항공과대 첨단재료과학부

Phenalenyl derivatives have drawn much attention in view of molecule-based magnets, and organic metal and conducting materials. In this study, we have newly designed and synthesized nitrogen-modified phenalenyl-based ligand, 2,5,8-tripyridyl-1,3-diazaphenalene (DAP). This molecule can work well for preparing various porous coordination networks because of its highly symmetrical structure. The negative charge of DAP anion delocalizes in the central azaphenalenyl skeleton which will afford unique physical properties. The resulting network will be the first example of a ligand-based redox-active coordination network. Here, we will report preparation and characterization of DAP and a porous coordination network consisting of DAP and metal ions.

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전구체 분해반응으로 유도된 2차 구조를 갖는 SnO2-염료감응 태양전지

박경완

가톨릭대 화학과

고체반응으로 합성된 Li2SnO3 를 전구체로 이용하여 2 차구조를 갖는 염료감응 태양전지의 전극물질을 합성하였다. 전구체 Li2SnO3 는 용융염 KCl 또는 KNO3 와 섞은 후 파이렉스 튜브에 넣고 진공 밀봉한 후 7-14 일간 573K 에서 가열하였다. 반응 후 수용염을 세척하여 제거한 후 2 차구조를 갖는 SnO2 를 성공적으로 회수하였다. 합성된 SnO2 는 SEM, BET, XRD 등을 이용하여 분석하였으며, 염료감응 태양전지 광전극에 적용하였다. 합성된 SnO2 는 유사한 크기의 전구체인 Li2SnO3 보다 7 배나 넓은 BET 표면적을 나타내었고, 미세한 나노막대의 일차구조물이 촘촘하게 쌓인 2 차구조를 보여주었다. 염료감응 태양전지에 적용해보았더니 1.7%의 에너지 변환 효율을 나타내어 일반적인 SnO2 나노입자 태양전지에 비해 향상된 광전환 특성을 보여주었다.

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Design of multi-interactive molecules

이길령 Yakiyama Yumi Masaki Kawano

포항공과대 첨단재료과학부

In the biological system, multi-point weak intermolecular interaction plays a crucial role for stabilizing metastable states. Introduction of multi interactivity into molecules can induce various kinds of unique properties such as trapping of metastable phases.Hexaazaphenalenyl (HAP) skeleton is three fold fused ring system with six nitrogen atoms which can provide effective coordination and hydrogen bonding sites. Recently, we have newly designed and synthesized HAP-based highly symmetrical ligand having three pyridyl or carboxyl groups. They showed unique properties such as surface mediated structure transformation and building various porous networks. Moreover, in order to extend the potential of HAP-based system, we designed new ligands and synthesized intermolecular interaction molecules. Here, we report the molecular designs and syntheses of the hexaazaphenalenyl-based molecules with structure information.

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Structures and Photoluminescence Properties of Copper(I)-Halide Coordination Polymers Based on N/S Mixed Donor Ligands

천상훈 전영은 김태호 김진은

경상대 화학과

Recently, we have focused on the development of luminescence copper(I) coordination polymers with dithioether ligands. During our investigation on copper(I) coordination polymers, the structures and photoluminescence properties for CuI coordination polymers with dithioether ligands have been reported. Herein, we report structures, thermal behaviors and photophysical properties of two coordination polymers based on N/S mixed donor ligands. The N/S mixed donor ligands (L^1 and L^2) were synthesized by the reaction of nicotinic acid and $RSCH_2CH_2CH_2NH_2$ (R=benzyl and cyclohexyl, respectively). Cu(I) coordination polymers $[CuIL^1_x]_n$ (1) and $[CuIL^2_y]_n$ (2) were prepared by the reaction of CuI and ligands.

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Synthesis and Structures of Photoluminescent Cu(Ⅰ) Coordination Polymers Based on Pyrazine Ligands with Thioether Substituents

전영은 천상훈 김태호 김진은

경상대 화학과

Recently, we have focused on the development of luminescence copper(I) coordination polymers with dithioether ligands. During our investigation on copper(I) coordination polymers, the structures and photoluminescence properties for CuI coordination polymers with dithioether ligands have been reported. Herein, we report structures, thermal behaviors and photophysical properties of two coordination polymers based on N/S mixed donor ligands. The N/S mixed donor ligands (L^1, L^2 and L^3) were synthesized by the reaction of 2-pyrazinecarbonyl chloride and $RSCH_2CH_2CH_2NH_2$ (R=benzyl, cyclohexyl and *t*-butyl, respectively). Cu(I) coordination polymers $[CuIL^1_x]_n$ (1), $[CuIL^2_y]_n$ (2) and $[CuIL^3_z]_n$ (3) were prepared by the reaction of CuI and ligands.

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Selective Encapsulation and Structural Transformation of Meta-Stable Sulfur Trapped by Porous Coordination Network

Hiroyoshi Ohtsu **최완욱** **Masaki Kawano**

포항공과대 첨단재료과학부

Porous coordination network has been applied to gas sorption/separation/storage, guest sorption, catalytic reactions, etc. Recently, we demonstrated that a pore of a porous coordination network can be used as a crystalline molecular flask in which chemical reaction can occur. The robust networks maintain crystallinity and enable direct observation of unstable species by X-ray diffraction. In this talk, we report trapping reactive sulfur into a pore of a porous coordination network. We succeeded in trapping a small reactive sulfur in the porous coordination network of $[(ZnI_2)_2(TPT)_3]_n$ by gas phase diffusion at 260℃ for 6 hours. Ab initio powder structural analysis indicates that a smaller reactive sulfur species were encapsulated in the pore of the network. This network was transformed to S_6 encapsulated network when it was heated with NH_4Cl that indicates catalytic structural transformation.

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Organization of polystyrene beads with various sizes on substrates

박이슬 윤서영 이진석

숙명여대 화학과

The organization of colloidal particles on various substrates is important to use as a building blocks in modern science and technology. It is necessary to develop methods for organizing them into large scale for many precise applications. There are two methods to achieve organization of colloidal particles such as “wet self-assembly” and “dry manual assembly”. It is used to biotechnology and nanotechnology. Recently, many studies have proven to employ these platforms into biological application which are related to development of cells. In this work, we synthesized polystyrene beads with various sizes using dispersion polymerization method. We used AIBN (2,2-Azobis(isobutyronitrile)) as initiator to make styrene radicals which need styrene polymerization. We controlled polystyrene bead size by changing the experimental parameters such as reaction temperature and injection rate of styrene mixed AIBN. And then, we organized polystyrene beads with various sizes using Langmuir-Blodgett method which deposited from the surface of a liquid onto a solid by immersing the solid substrate into the liquid to obtain monolayer arrays on the substrate in large-scale. We will employ these substrates which are consisting of hexagonal close-packing monolayers into biological field.

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Synthesis of graphene flakes with different size and shape using chemical vapor deposition method

정다희 이진석

숙명여대 화학과

Graphene is a two-dimensional carbon material that has attracted great scientific and technological interest due to its intriguing physical properties and enormous potential for various applications. Although mechanical peel is known to produce high quality graphene flakes, practical applications require continuous graphene layers over a large area. However, graphene synthesized by CVD on Cu substrates has shown great promise owing to its large size, high quality, and transferability to arbitrary substrates. In general, the electric properties and device performance are strongly dependent on the size, shape, crystallinity, layer numbers, and edge structures of pristine graphene. Controlling these parameters of graphene in synthesis or post-synthesis manipulation is thus critical to achieve tunable properties and optimized device performance. In this research, we present an advanced CVD method to enable controlled size and shape by changing experimental parameters such as annealing condition, flow rates and cooling environment. In order to control the shape, we varied pre-reaction conditions, ramping speed and reaction time at low pressure and CH_4 to H_2 ratio at atmospheric pressure. Using this technique, various shaped graphene flakes were synthesized in a different pressure chemical vapor deposition process.

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Various Porous Network Formations Composed of CuI and Td-symmetry Ligand and Element Phosphorus Encapsulation

Hakuba Kitagawa Hiroyoshi Ohtsu Masaki Kawano

포항공과대 첨단재료과학부

We succeeded in obtaining various CuI network crystals selectively utilizing labile structural nature of CuI and Td-symmetry tetradentate ligands by using kinetic and thermodynamic control. These crystals have different CuI units (infinite chain, dimer, and tetramer), each of which has different void space. Also, we succeeded in encapsulating element phosphorus into the infinite chain type CuI unit network crystal. In this poster presentation, we will report on the detail of the syntheses, the reaction mechanism, and the structures of these network crystals.

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NIR-Emitting $CdTe_xSe_yS_{1-x-y}$ Core/Shell Structured Quantum Dots with Chemical Composition Gradient

신재호 이진규

서울대 화학부

The development of materials with optical properties in near-infrared (NIR) range has been arising for its various applications; optical imaging of biological system, sensitizer for solar cell, NIR telecommunication, etc. The most prevalent QDs which optical window ranges 600 ? 900 nm in wavelength are CdTe/CdSe core/shell structured QDs with type-II heterojunction. However, core/shell structured type-II QDs have inherent problems in general such as lattice strain, less confinement of charge carriers, many defect sites due to few monolayers of shell, delicate synthetic procedure such as SILAR (Successive Ionic Layer Adsorption and Reaction) or ALE (Atomic Layer Epitaxy). To overcome these issues, we synthesized $CdTe_xSe_yS_{1-x-y}$ core/shell1/shell2 structured quantum dots with chemical composition gradient based on the kinetic control of each precursor. The size of the QDs was approximately 6 nm despite of the composition, but their optical property varied with strong luminescence in the range of 600 ? 750 nm. The emission wavelength was mainly governed by the composition of CdTe and CdSe, and the incorporation of CdS as a protection layer enhanced PL intensity.

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In Situ Observation of Retinal Photoisomerization in a Coordination Network by X-ray Crystallography

Kojima Tatsuhiro Yakiyama Yumi Masaki Kawano

포항공과대 첨단재료과학부

A pore of porous coordination network can be used as a crystalline molecular flask for reactions. The robust as well as flexible nature of coordination networks enables maintaining crystallinity to directly observe molecular structure changes by single crystal X-ray diffraction. Recently, we succeeded in synthesizing a hexaazaphenalene-based highly symmetrical ligand, TPHAP. In this talk, we report encapsulation and photoisomerization of retinal in a porous coordination network composed of TPHAP and Zn ions. We prepared a crystal of [(ZnI)(TPHAP)?x(retinal)]n (1a), which encapsulates retinal in 3D-intercalated biporous network, and collected single-crystal X-ray diffraction data of 1a at 85 K. The crystal 1a was irradiated with a UV-LED light source (wavelength = 365 nm) at 85 K for 15 min. After irradiation, data collection (1b) was carried out again. X-ray crystallographic analysis of crystals 1a and 1b revealed that an asymmetric unit of each crystal contains three kinds of retinal molecules (retinal A, B, and C). Interestingly, we found that only retinal C showed phtoisomerization on irradiation though retinal A and B showed a little change. This result indicates that the biporous network can provide several different sites for guest encapsulation and induce unique photoisomerization depending on the site atmosphere. We will report the detailed crystallographic analysis of photoreaction including spectroscopic results.

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Synthesis of metal-organic frameworks using alkaline earth metal ions and tripodal aromatic carboxlic acids

심재웅 최상범 유래경 김자헌

숭실대 화학과

Two isostructural MOFs (MgTATB and CaTATB) have been synthesized by solvothermal reactions between tripodal aromatic carboxylic acid (H_3TATB) and Mg and Ca ions, respectively. They were stable up to 450 ^{o}C based on TGA analyses. While the evacuated MgTATB was porous with a moderate BET surface area of 950 m^2/g, CaTATB did not show a permanent porosity. MgTATB produced too weak X-ray reflections to be usable for crystal structure determination. Fortunately, we could solve the crystal structure of CaTATB of which simulated pattern is well-matched to that of MgTATB. We will discuss the syntheses, porosity, and structural aspects of MgTATB and CaTATB.

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Structure and porosity of a metal-organic framework built from calcium ions and tripodal organic ligands

노경규 오유진 김자헌

숭실대 화학과

A new metal-organic framework, CaBTB was synthesized by the reaction of calcium hydroxide and benzene-1,3,5-tribenzoic acid (H_3BTB). The crystal structure shows that calcium ions form an infinite chains bridged by the carboxylates of the organic linkers and water molecules or hydroxide ions. The non-interpenetrating framework provides microporous channels containing many THF molecules. The evacuated CaBTB was stable under vacuum, and could adsorb nitrogen gas.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation, characterization and application of CoS thin films using chemical bath deposition for supercapacitors

임이슬

한양대 화학과

Cobalt sulfide thin films were prepared by a simple chemical bath deposition method. We studied the effect of PH on film formation and its effect on capacitive properties. The structure and morphology of CoS thin films is examined by X-ray diffraction analysis, scanning electron microscopy and UV-Vis spectroscopy. The results show that the films are composed of uniformly sized grains having sizes around 20 nm at a pH of 11. At a PH value of 10 the film is composed of disordered grains and at pH 12 the grain size is increased up to 50 nm. The electrochemical capacitive performance of the films was investigated by cyclic voltammetry and charge-discharge measurements. The CoS thin film fabricated at pH=11 exhibit a specific capacitance of about 131 F/g in 1M KOH electrolyte. The amounts of inner and outer charges are calculated to investigate the contribution of mesoporous structure on charge storage where relatively higher contribution of inner charge infers good ion diffusion into matrix of cobalt sulfide.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Growth and characterization of SnO2-ZnO hybrid nanostructures for Photovoltaic devices

김은경 한성환

한양대 화학과

We report here on fabrication of SnO2 nanoplate- ZnO nanorod hybrid nanostructures for semiconductor sensitized solar cells. Upright standing nanoplates were grown on FTO substrates at low temperature followed by growth of ZnO nanorods. This hybrid architecture showed higher light scattering effect confirmed from diffuse reflectance measurements, which resulted in remarkable improvement photocurrent density attributed to high light harvesting efficiency and better charge transport in a photoelctrochemical cell.

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Metal Ion Metathesis in Metal Organic Frameworks: Framework Constituting Metal Substitution by Direct Ion Exchange

김용휘 Sunirban Das[1] Saurav Bhattacharyya[2] 홍순상[3] Srinivasan Natarajan[2] 김기문

포항공과대 화학과 [1]School of Chemistry, University of Hyderabad [2]Indian Institute of Science, Bangalore [3]포항공과대 지능초분자연구단, 화학과

With growing interests on metal-organic frameworks (MOFs), post-synthetic modification receives considerable attention to get more control over the materials, as a pre-synthesized highly porous and desirable framework can be chosen for further modification to fine tune the pore environment without disrupting the framework topology. However, substitution or replacement of framework-constituting components from a pre-assembled framework without changing the framework topology or structure has not been explored. We recently reported the complete exchange of framework-constituting metal ions from robust microporous frameworks keeping the original framework topology intact. Extending this work, we have demonstrated the synthesis of a new Mn(II) framework and metal ion exchanges of Mn(II) framework to produce Fe(III), Co(II), Ni(II), Cu(II) frameworks, which were difficult to achieve through direct synthesis. We observed a facile metal ion exchange without altering the framework structure or structural integrity. Although, the process involves the simultaneous breaking and making several dative bonds between the ligands and leaving and incoming metal ions, the ion exchange processes occurred via single crystal to single crystal transformation manner. The resulting five MOFs showed similar porosities but different hydrogen sorption capacities for Fe framework, which are attributed to the different degrees of interaction between the gas molecules and the open metal species.

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Q-band Pulsed EPR Study of Cu-amyloid-β peptide Complexes

김동훈 김선희

한국기초과학지원연구원 물성과학연구부

Alzheimer's disease (AD) is a neurodegenerative disorder characterized by deposition of extracellular amyloid plaques, the major component being the amyloide-β peptide(Aβ). Metal ions such as copper are found in high concentrations within plaques in the AD brain. The mechanisms that lead to plaque formation are not fully understood, although metal-induced Aβ oligomerization is believed to play a key role, possibly via an oxidative stress pathway. Furthermore, determination of the binding coordination of Cu^{II} to Aβ is crucial to understood Aβ aggregation behavior. We used Q-band pulsed EPR spectroscopy to elucidate the structure of Cu- Aβ. Pulsed ENDOR spectroscopy has the advantage of detecting couplings of atom directly bound to the Cu^{II} ion. We will present the coordination of the Cu^{II} site revealed by ^{1}H, ^{2}H, ^{17}O, ^{14}N ENDOR studies.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An EPR and Spin-trap study on Metal-Aβ ; Comparison of hAβ vs mAβ

김남희 김선희

한국기초과학지원연구원 물성과학연구부

Amyloid β (Aβ) is a central characteristic of Alzheimer's disease (AD). Neurodegeneration observed in Alzheimer disease (AD) is believed to be related to the toxicity from reactive oxygen species (ROS) produced in the brain. Unlike human Aβ peptide(hAβ), murine Aβ peptide(mAβ) whose peptide differs from the human Aβ peptide by three point mutations, does not show amyloid deposition.Thus, it is important to investigate the difference between hAβ and mAβ to better understand the AD mechanisms. For this purpose, we studied using CW-EPR the coordination of metal ions to hAβ (1-16) and mAβ (1-16). ROS such as hydrogen peroxide and deleterious OH radicals were proposed to trigger neurotoxicity in AD. To detect such as species, we employed 5,5′-dimethyl-1-pyrroline-oxide (DMPO) as a spin trap. This result will deepen our knowledge of ROS production by metal amyloid peptides.

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Reactions of Reactive Sulfur Trapped in a Porous Coordination Network

최완욱 Hiroyoshi Ohtsu Masaki Kawano

포항공과대 첨단재료과학부

Porous coordination network is 3-dimensional crystalline porous material that has been used for gas sorption/separation, catalytic reaction and guest encapsulation, etc. Recently, we succeeded in trapping unstable sulfur allotropes in a thermally stable porous coordination network, $[(ZnI_2)_2(TPT)_3]$ (TPT: 2,4,6-tris(4-pyridyl)triazine) by gas phase diffusion. Ab initio powder structural analysis and elemental analysis revealed that S_3 was trapped in a pore of the network.Herein I report unique reactions of S_3 in the pore with benzonitrile and benzyl alcohol. The S_3 trapped network powder reacted with benzonitrile to give a single crystal which is the same network as the starting material for the thermally stable porous network. Noteworthy is that this reaction did not occur without presence of S_3 in a pore, indicating that S_3 induces structural transformation from powder to single crystal. Benzylalcohol also induced structural transformation for the S_3 trapped powder network.

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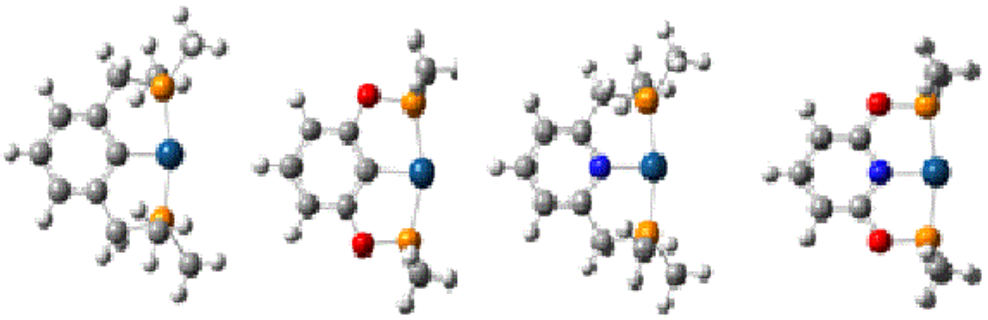
Ligand effects on C-H bond activation of alkanes catalyzed by Ir(Pincers) complexes: DFT/ECP study

곽옥금 Shubin Liu[1] Maurice Brookhart[2] 김봉곤

경상대 화학교육과 [1]Renaissance Computing Institute, University of North Carolina, Chapel Hill, USA
[2]Department of Chemistry, University of North Carolina, Chapel Hill, USA

The iridium pincer complex is the first efficient homogeneous catalyst that does not require photon or sacrificial hydrogen acceptors to drive the reaction. In this study, Three coordinated, T-shaped (PXP)Ir(I), (X=C or N), PCP = η^3-1,3-C_6H_3-$(CH_2PR_2)_2$, POCOP= = η^3-1,3-C_6H_3-$(OPR_2)_2$, PNP =2,6-C_5H_3N-$(CH_2CR_2)_2$, PONOP=2,6-C_5H_3N-$(OCR_2)_2$, as well as their reactivity for intermolecular C-H activation have been studied by DFT methods. We found that four pincer complexes are structurally and spectroscopically different from their iso-electronic structure compounds. A few quantitative linear relationships have been discovered between C-H bond activation energies, charge distributions, and DFT chemical reactive indices.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Quick, surfactant free synthesis of micron sized, porous CdO cubes and its photoelectrochemical properties

Dipak V. Shinde 한성환

한양대 화학과

Cadmium oxide (CdO) is one of the most promising wide band gap semiconductor due to its high electrical conductivity and visible light transparency. Porous CdO nanoarchitecture can be useful for the deposition of other functional materials utilizing its high conductivity and high surface area. In this study we report on the quick, surfactant free fabrication of porous cadmium oxide architectures. These architectures showed supercapacitor behavior. Controlled ion exchange of the cubes with selenium ions yielded porous CdO-CdSe architectures with tunable composition and with visible light photoactivity.

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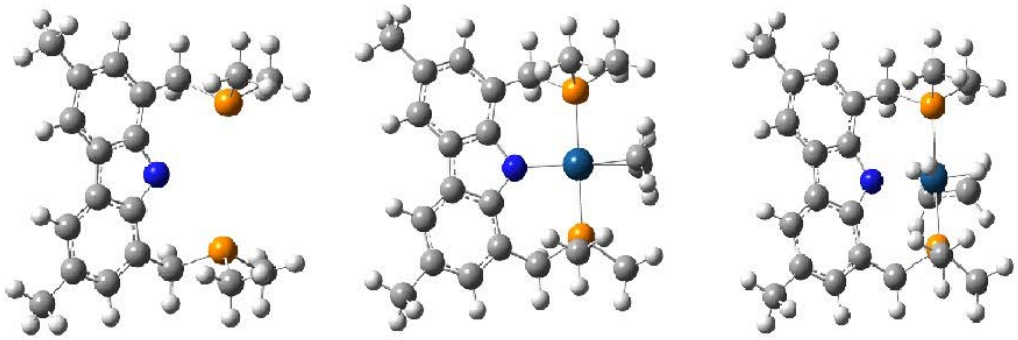
Synthesis and Characterization of new Carb-PNP pincer iridium complex: Mechanistic study of alkene hydrogenation by DFT calculations

김봉곤 Chen Cheng[1] Damien Gruironnet[1] Maurice Brookhart[1]

경상대 화학교육과 [1]Department of Chemistry, University of North Carolina, Chapel Hill

In an effort to rationally design better PXP-type iridium complexes for hydrogen transfer reactions, DFT calculations were used to evaluate the effect of X-atom on PXP-type iridium pincer complexes with regard to methane C-H activation. New carbazolide (1) pincer ligand and iridium complex 2 were synthesized, and individual steps of stochiometric hydrogenation reaction using 3 were investigated both by experiments and DFT calculation.



Car-PNP(L) [Ir(L)(CH2CH2)] [Ir(L)H2(CH2CH2)]

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강유전체 메모리 박막용 PZT 전구체의 제조 및 전환 특성 분석

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한양대 화학공학과 [1]한양대 수소연료전지공학과 [2]한양대 화학공학

1950 년대 후반에 발견된 Lead-zirconate-titanate (PZT) 화합물은 perovskite 형태의 구조를 갖는 piezoelectric 재료로 알려진 ceramic 물질로, 박막형태의 경우 high frequency piezoelectric transducers, surface acoustic wave device substrates 및 non-volatile random access memories 등에 사용되고 있다. 1986 년경까지 PZT film 은 주로 rf-sputtering 이나 ion beam deposition 등과 같은 물리적인 증착 방법이 주로 사용되어 왔으나, 최근에 와서 CVD, ALD 및 sol-gel process 와 같은 화학적 방법을 이용한 박막 제조가 점차 중요한 공정으로 대두되고 있다. 이러한 화학적 방법을 사용한 PZT film 제조의 경우 원하는 전기적 특성을 구현하기 위하여 추가적인 열처리를 통하여 ceramic 구조로의 전환 하는 공정을 필요로 하는 바 이 경우 낮은 소결 온도 및 고밀도 박막의 형성이 중요한 변수로 떠오르고 있다. 저온 소성이 가능한 양질의 PZT film 을 제조하는 데 있어서 전구체 물질의 특성과 더불어 증착 및 소성과정에서 일어나는 물리/화학적 변화에 대한 명확한 이해가 필수 불가결한 분야인데, 이를 위해서는 다양한 구조 및 화학적 조성을 갖는 전구체의 제조뿐만 아니라 제조된 전구체들의 명확한 물리적, 화학적 특성 분석이 요구되고 있다. 이 밖에도, PZT 와 같은 복합조성의 ceramic film 의 경우 전구체들간의 물리적 또는 화학적 상호 작용 또한 최종 박막의 특성에 중요한 영향을 주는 바 이들에 대한 조사 또한 각각의 전구체들의 합성과 더불어 고려하여할 중요 변수이다.본 연구에서는 다양한 구조 및 조성을 갖는 Pb, Ti 및 Zr 전구체들을 제조하여 이들에 대한 물리, 화학적 특성을 비교, 분석하였다. 이를 위하여 여러 형태의 β-ketonate 리간드 및 alkoxide 를 갖는 lead complex 전구체를 합성하였고 분광학적인 방법을 이용하여 이들의 구조 및 화학적 성질을 조사하였다. 또한 합성한 lead complex 전구체들을 기존의 Ti/Zr complex 들과의 화학적 또는 물리적인 상호작용 이용하여 복합전구체를 제조 한 후, 화학적 방법을 통하여 박막을 형성하고 소결을 통하여 ceramic

PZT film 을 제조 한 후, 이들 전구체들이 소결 반응 및 형성된 PZT 박막에 미치는 영향에 대하여 조사하였다.

대 한 화 학 회
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A New Hydrogen Uptake Mechanism in Nano-porous Materials Investigated by In-situ Neutron Scattering and Grand-Canonical Monte-Carlo Simulation

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현재, 저온(액체 질소온도(약 77K)) 수소 저장에 대해서 phsisorption 에 의한 나노 기공 물질내의 흡착자리에 의한 표면 흡착은 잘 알려져 있지만 그 이상 더 정확한 흡착 메커니즘은 알려져 있지않다. 본 연구에서는 50K 중수소 isotherm 에 대한 실상황(in-situ) 중성자 회절 실험을 통하여 Na-X/Y zeolite, MOF-5, MOF205 등과 같은 나노 기공 물질에서 표면 흡착이외에 액체와 비슷한 분자 상태로 저장되는 메커니즘을 발견하였고, 실제 액체 중수소 중성자 회절 실험으로써 이를 비교, 확인하였다. 이와같은 발견되지 않았던 새로운 저장 메커니즘은 나노 기공 물질내에 수소분자가 느슨하게 갇혀있어서, 이 수소 분자와 흡착된 수소분자사이의 interaction 이 액체 상태와 비슷한 회절 패턴으로 보이게 된다. 새로운 저장 메커니즘을 중성자 패턴으로 보인 나노 기공 물질에서는 수소의 kinetic energy(50 K)와 비슷한 얕은 potential 이 연속적으로 존재함을 Grand Canonical Monte-Carlo(GCMC)simulation 으로 계산하였다. 액체와 비슷한 상태으로 수소를 저장할 수 있는 나노 기공 물질들과 그 환경을 이 연구를 통하여 보이고자 한다.

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Heat Inducing Magnetic Nanoparticles in Biomedical Applications

정희영 유동원 천진우

연세대 화학과

Advances in nanoparticle technology have created new paradigms for biomedical applications such as magnetic resonance imaging (MRI), drug delivery, and cell actuation. Especially, magnetic nanoparticle mediated hyperthermia has brought tremendous attention in the context of heat-based treatment strategies owing to their ability to generate heat when subjected to an alternating magnetic field. Their non-invasive and localized, selective heat generating ability with minimal side effects makes them promising in modern cancer therapy. We have demonstrated that the high magnetism of metal ferrite nanoparticles (MNPs) can be modulated and achieved by Zn2+ dopant control to act as highly efficient hyperthermia agents compared to conventional MNP agents. By introducing these MNPs to smart drug container, we have successfully shown selective drug delivery system which could release anticancer drugs via heat generated by MNPs.

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Arsonic Acid as a Robust Anchor Group for the Surface Modification of Iron Oxide Nanoparticles(Fe_3O_4)

안지훈 문두식 이진규

서울대 화학부

Iron oxide (Fe_3O_4) nanoparticles are used in various fields including high density storage, bio-imaging, cell/catalyst separation, drug delivery, and hyperthermia treatment. For stable and effective use in these fields, the surface modification which gives colloidal stability and additional function to the nanoparticles is necessary. When one wants to modify the surface of iron oxide nanoparticles by functional molecules, the molecules should contain anchor group which have affinity to the surface. So far, carboxylic acid and catechol have been frequently used as anchor group for the surface modification of iron oxide nanoparticles. However, these conventional anchor groups show some problems such as low affinity, oxidative reaction with the surface. In this study, we investigated arsonic acid as a new anchor group. Although the high affinity of arsonic acid to the iron oxide is already known, there are few attempts to use arsonic acid for the surface modification. By using 4-azidophenylarsonic acid, it was possible to immobilize azide group on the surface of iron oxide nanoparticles by the arsonic acid. Then, desired functional molecules can be introduced to the surface by Copper Catalyzed Azide Alkyne Cycloaddition (Click reaction). By quantifying and comparing the amount of adsorbed anchor on the surface, it was found that arsonic acid shows better affinity than the conventional anchors. Also, we examined whether the anchors on the surface desorb in some conditions such as washing, various pH, and presence of displacing anchors. It was uncovered that arsonic acid maintains the stability in extensive conditions.

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Tandem Catalysis with Bifunctional Site-Isolated Lewis Acid-Brønsted Base Metal-Organic Framework, NH_2-MIL-101(Al)

홍순상 윤민영[1] Raghunandan Hota 김용휘 김기문

포항공과대 화학과 [1]University of California, Berkeley, Department of Chemistry

Metal-Organic Framework (MOF), NH_2-MIL-101(Al), without any post-synthetic modification, is demonstrated to function as a bifunctional site-isolated heterogeneous catalyst for tandem Meinwald rearrangement?Knoevenegal condensation reactions. The Lewis acidic Al(III) sites catalyze Meinwald rearrangement of epoxides with remarkable selectivity for substrates, which generate aldehydes via benzylic 3° carbocation, and the Brønsted basic amino groups in organic linkers catalyze Knoevenagel condensation of resulting aldehyde with malononitrile in tandem.

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발표분야: 무기화학

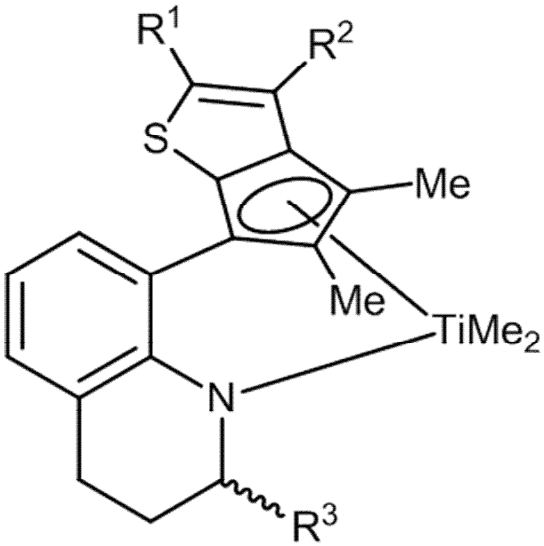
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of half-titanocenes of thiophene-fused cyclopentadienyl ligands for ethylene/a-olefin copolymerization

전성해 이분열

아주대 분자과학기술학과

During the course of development of the ortho-phenylene bridged complexes, tetrahydroquinoline-derived complex showed good catalytic performances. Directed ortho-lithiation of the lithium carbamates generated from tetrahydroquinoline or tetrahydroquinaldine enables one-step preparation of thiophene-fused and tetrahydroquinoline-linked cyclopentadienes[2-R^1-3-R^2-4,5,dimethyl-6-(2-R^3-2,3,4,5-tetrahydroqinolin-8-yl)-4H-cyclopenta[b]thiophene (R^1, R^2, R^3 = H or methyl)], from which titanium(IV) and zirconium(IV) complexes are prepared. The Me_2Ti-complexes, 14 and 15 (R^1 = R^3 = Me, R^2 = H) show excellent activities (62 and 54 × 10^6 g/molTi·h) in ethylene/1-octene copolymerization, even when activated with small amount of MAO (Al/Ti = 1000). Nonbridged half-titanocene complexes also have drawn much attention as a homogeneous Ziegler catalyst in olefin polymerization. Methylthiophene-fused or dimethylthiophene-fused trimethylcyclopentadienyltitanium trichloride compexes, (η^5-Me_4RC_7S)$TiCl_3$ (R = Me or H), are prepared, from which a chloride ligand is replaced with 2,6-diisopropylphenoxy, di(tert-butyl) ketimide, or tri(tert-butyl)phosphinimide ligand to yield (η^5-Me_4RC_7S)$TiXCl_2$. (11, R = Me, X = $iPr_2C_6H_3O$- ; 12, R = H, X = $iPr_2C_6H_3O$- ; 13, R = Me, X = tBu_2C = N- ; 14, R = H, X = tBu_2C = N- ; 15, R = Me, X = tBu_3P = N- ; 16, R = H, X = tBu_3P = N-).



	R^1	R^2	R^3
14	Me	Me	Me
15	Me	H	Me

Figure 1. Bridged half-metallocene complexes.

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Study on Graphene-Metal Composites

오영희 김경안 홍성국[1]

동의대 화학과 [1]동의대

Graphene/transition metal nanostructured composites have been prepared from the graphene, and metal salts in alcoholic solution. Morphology and the structures and properties of the composites have been examined.

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Synthesis, Characterization and Structural Correlation of Novel Li-Containing Polar Intermetallic Compound $La_{11}Li_{12}Ge_{16}$

정야호 유태수

충북대 화학과

A novel Li-containing polar intermetallic compound $La_{11}Li_{12}Ge_{16}$ has been synthesized using high-temperature reaction method and characterized by both single-crystal and powder X-ray diffractions. The compound crystallized in the orthorhombic crystal system (space group *Immm*, *Z* = 2, Pearson symbol *oI78*) with fifteen crystallographically unique atomic positions in the asymmetric unit, and the lattice parameters are refined as *a* = 4.5244(4) angstrom, *b* = 6.9932(6) angstrom, and *c* = 53.043(5) angstrom. The complex crystal structure of title compound can be described as the 2:1 intergrowth of two closely related compounds: $La_2Li_2Ge_3$ ($Ce_2Li_2Ge_3$-type) and $La_3Li_4Ge_4$ ($Zr_3Cu_4Si_4$-type) acting like "*building-blocks*" along the *c*-axis. Six La sites are categorized into three distinct types based on the local coordination environment showing the coordination numbers of 12-14. Three unique Li sites are placed in the centers of local tetrahedra formed by four Ge atoms which eventually construct Ge_2 dimers or 1-dimensional *cis-/trans*-Ge chains. Theoretical investigations using tight-binding linear muffin-tin orbital (LMTO) method provide rationales for an improved structural stability and for unique local coordination geometries established by anionic elements including [$LiGe_4$] tetrahedral, *cis-/trans*-Ge chain and Ge_2 dimers.

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Selective CO_2 adsorption in a metal?organic framework constructed from an organic ligand with flexible joints

홍대호 백명현

서울대 화학부

We have synthesized a porous metal-organic framework (SNU-110) by using an organic ligand containing flexible joints. Framework SNU-110 has a 3D pillared-layer structure generating 1D channels with window size of 4.4 × 3.7 $Å^2$. On activating SNU-110 with supercritical CO_2 fluid, desolvated solid $[Zn_2(mpm\text{-}PBODB)_2bpy]_n$ (SNU-110') results, which has the unit cell volume reduced by 8.8%. SNU-110' hardly adsorbs N_2 and H_2 gases at 77 K, indicating its smaller window size than the kinetic diameter (2.89 Å) of H_2. However, it uptakes 97 cm^3 g^{-1} of CO_2 at 195 K despite that CO_2 has much larger kinetic diameter than H_2, indicating that CO_2 can open up the gate of the flexible MOF due to its much higher polarizability and quadrupole moment than N_2 and H_2. SNU-110' shows a two-step CO_2 adsorption curve related with structural transformations on CO_2 adsorption, together with a big desorption-hysteresis. Expansion of the framework by CO_2 adsorption is evidenced by powder X-ray diffraction data measured under CO_2 stream at 248 K. The selectivities for CO_2 adsorption over N_2, H_2, and CH_4 at 195 K are 35:1, 61:1, and 15:1, respectively.

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Metal Complexes with a Pyridine Substituted N-Heterocyclic Carbene Ligand; Synthesis and Catalytic Application

배호연

전북대 화학과

Recently, N-heterocyclic carbenes(NHCs) have become a very important class of ligands in organometallic chemistry and catalysis. Furthermore, metal complexes of N-heterocyclic carbene(NHCs) have become extremely important in catalytic processes such as cross-coupling, metathesis, and C-H bond activation. Especially the readily available AgI-NHC complex is the most commonly used NHC transfer reagent. A great number of metal complexes have been obtained via transmetalation from AgI-NHCs. Here we have described a convenient method for the synthesis of metal-complexes using AgI-NHC complexes as the carbene sources. AgI-NHC complexes are very useful precursors for other metal-NHCs complexes. We are planning to synthesize a variety of transition metal and we are going to survey the potential applications of these new NHC complexes as materials or homogeneous catalysts.

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Property of Cu(II) Complex with N,N'-dimethyl-N,N'-bis(pyridin-2-yl)methanediamine (DPMA) and Anion Sensing

정현진 박경세[1] 이동헌

전북대 화학과 [1]군산대 화학과

Anions play an important role in various areas including nature, industry, and medicine. Especially, A colorimetric anion sensing utilizing coordination compounds continues to be major research efforts for the environmental and biomedical relevance. The design and synthesis for the molecular sensors that can detect the anions selectively are always of major interest. The interaction of N,N'-dimethyl-N,N'-bis(pyridin-2-yl)methanediamine (DMPA, 1) ligand with $Cu(ClO_4)_2$ salts yields compound of stoichiometry $[(DMPA)_2Cu](ClO_4)_2$, 2. Complex 2 was tested as potential anion sensors toward ions such as SCN^-, Cl^-, Br^- and I^- in organic solvents by utilizing a colorimetric method and was found to be feasible candidates for colorimetric detection of anions. Slow decomposition of 2 in methanol unexpectedly led to the formation of an alkoxo-bridged tetranuclear copper(II) cubane, 3. 3 is product of an oxidative N-dealkylation reaction, which took place on DMPA and methanol used as a solvent under the used conditions. The compound was characterized by a single crystal X-ray crystallography. Two copper ions of the tetranuclear copper(II) cluster each are five-coordinated in a square-planar geometry while the other two copper ions are six-coordinated in a octahedral geometry.

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Design, Synthesis and O_2 Reactivity Studies of Copper Complexes with an Aminoacid-Based Chelate.

이수연 정현진 이동헌

전북대 화학과

The involvement of a sulfur atom as a ligand in transition metal complexes is currently of considerable interest in bioinorganic chemistry. A sulfur atom as a ligand at the active sites of various metalloenzymes has been well documented. DβM (dopamine β-monooxygenase) and PHM (peptidyl glycine α-hydroxylating monooxygenase) each contain a methionine residue as one of the lignads at the catalytic site. The nonheme iron enzyme CDO(cysteine dioxygenase) catalyzes the oxygenation of cystein by O_2 to give cystein sulfinic acid. A cysteine-bound high spin FeII center occurs CDO as a reaction intermediate. We have synthesized a sulfur containing ligands derived from L-methionine ethyl ester (L = 2-Ethylthio-N,N-bis(pyridine-2-yl)methylethanamine) and it's copper(I) complex. The Cu(I) complex reacted with O_2 to produce sulfoxide derivative of thioether-amine ligand. We plan to study other new sulfur containing ligands derived from L-methionine and cysteine. And this research rendered service to an understanding of the discovery and influence of sulfur containing ligands with metal complexes reactivity.

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Simple Synthesis of Supramolecular Cages

이휘현 박가현 고민정 이준승

전남대 화학과

Supramolecular chemistry has provided a great contribution in the design and synthesis of various two-(2D) and three-(3D) dimensional architecture in nano scale. 2D molecules including triangle1, rectangle, pentagon and hexagon, and 3D complexes covering trignonal bipyramidal and admentanoid, cubooctahedron, and dodecahedron have been synthesized successfully by coordination driven self assembly. Particularly, 3D cage molecules including trigonal prism and tetrahedral have special interests because of their well-defined useful inner spaces. These cavities have been used in many research areas such as host-guest chemistry and catalysis.At this presentation, we present various 3D supramolecules having D3h or D4h Symmetry using simple tri- or tetra- pyridine donors. The compounds have been characterized by NMR spectroscopy and electrospray ionization mass spectrometry. Their structural properties and host-guest chemistry will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced isosteric heat, selectivity, and uptake capacity of CO_2 adsorption in a metal-organic framework by impregnated metal ions

박혜정 백명현

서울대 화학부

We demonstrate by experimental and theoretical studies that the impregnation of various metal ions in the pores of an anionic MOF, $[Zn_3(TCPT)_2(HCOO)][NH_2(CH_3)_2]$ (SNU-100') significantly enhances isosteric heat, selectivity, and uptake capacity of the CO_2 adsorption in the MOF without the heating process for reversible regeneration. Due to the electrostatic interactions between CO_2 and the extra-framework metal ions, the isosteric heats of CO_2 adsorption are increased to 60.4 - 40.8 kJ/mol and the adsorption selectivities of CO_2 over N_2 at room temperature are increased to 36.4 - 28.4, compared with 28.9 kJ/mol and 20.7 of the parent MOF (SNU-100') containing $[NH_2(CH_3)_2]^+$ cations.

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Well-dispersed MWCNTs / syndiotactic polystyrene composite using single site titanium catalyst anchored to MWCNTs

고민정 이휘현 박가현 이준승

전남대 화학과

A well-dispersed multiwall carbon nanotube (MWCNT)/syndiotactic polystyrene (sPS) composite was prepared by simple in-situ polymerization of styrene using pentamethylcyclopentadienyltitanium(IV) trimethoxide (Cp*Ti(OMe)3) attached to the shortened and functionalized MWCNT (f-MWCNT). The attachment of Cp*Ti(OMe)3 to the f-MWCNT was confirmed by thermogravimetric analysis, X-ray photoelectron spectroscopy, Fourier transformed infrared spectroscopy, and energy dispersive X-ray spectroscopy. Cp*Ti(OMe)3 attached to pristine MWCNT in the presence of methylaluminoxane (MAO) did not produce PS, whereas Cp*Ti(OMe)3 attached to f-MWCNT showed a high catalytic activity for the syndiospecific polymerization of styrene under the same polymerization conditions. Obtained sPS showed a narrow molecular weight distribution (PDI ?2), a high SI value (≥90%), and a high melting point (?272℃). Scanning electron microscopy and transmission electron microscopy images showed that MWCNT strands were well dispersed in the MWCNT/sPS composite. Such composites had greatly improved thermal stability compared to normal sPS polymers.

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Facile Preparation of Multifunctional Nanotube by Sequential Stacking of Nanoparticles

Fang Qiling WANGLULU[1] Linxiangde[1] 송기일[2]

경원대 화학공학과 [1]경원대 Bionano [2]경원대 바이오나노학과

Qiling Fang, Lulu Wang, Xiangde Lin, Gill Song, and Sang Jun Son*Multifunctionality is one of essential elements which enable nanomaterials to be employed in the field of nanobiomedical applications. Since simple integration of differently functioning NPs in a confined space could lead to malfunction or interference between the NPs, a method that can spatially isolate the NPs and can be applied to a wide range of NPs is highly required. In this work, we developed an efficient method that can be used to stack SNTs with various NPs for the prepation of multifunctional nanotube, which is involved with hydrophobic interaction between NPs and the inside walls of SNTs. In addition, we successfully demonstrated that barcode nanotube coded by different colored QDs and multifunctional SNTs with versatile magnetic, fluorescent, and SERS-active properties can be fabricated using the stacking method.

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Crystal Structure, Site-Preference and Structural Correlation of Intermetallic Compound $EuZn_{1.18\ (2)}In_{2.82}$

남근우 유태수[1]

충북대 화학부 화학과 [1]충북대 화학과

$EuZn_{1.18\ (2)}In_{2.82}$ has been synthesized using the In-flux method and characterized by both powder and single-crystal X-ray diffractions. The title compound crystallized in the tetragonal space group *I*4/*mmm* ($BaAl_4$-type structure, Pearson code *tI*10) with lattice parameters of *a* = 4.5463(3) Angstrom, *c* = 12.0279(18) Angstrom. The 18-vertex Fedorov polyhedron composed of Zn and In atoms is considered as a basic building unit for the crystal structure, where Eu atoms are embedded at the center of the polyhedron. Zn and In atoms show the specific site-preference between two available anionic sites on the Fedorov polyhedron, which is more substantially influenced by the size factor than the electronegativities, and only the apical-site displays the mixed-occupation of Zn and In. The crystal structure of $EuZn_{1.18\ (2)}In_{2.82}$ can be considered as a product of the structural transformation from the monoclinic $EuIn_4$-type structure to the tetragonal $BaAl_4$-type structure caused by In substitution with Zn, which can be understood based on the ionic size ratios between anionic elements. Theoretical investigations using tight-binding linear muffin-tin orbital (TB-LMTO) method provide understandings for the observed site-preference between anionic elements and suggest a possibly wide phase-width for the title compound.

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Effect of Li-Substitution on the Metal-Rich RE_5Tt_4 Family: Site-Preference and Crystal Structure of Er_4LiGe_4

남근우 전지은[1] 유태수[1]

충북대 화학부 화학과 [1]충북대 화학과

A new member of theRE_5Tt_4 family (*RE* = rare-earth metals, *Tt* = tetrels), Er_4LiGe_4 has been synthesized and characterized using powder and single crystal X-ray diffractions. The title compound crystallized in the orthorhombic space group *Pnma* (Pearson code *oP*36, *Z* = 4) and adopted the Gd_5Si_4-type structure, where all interlayer Ge-Ge distances fall within the range of the single-bonded dimer distance. The lattice parameters are observed as follows: *a* = 7.04(4) angstrom, *b* = 14.52(8) angstrom, and *c* = 7.62(5) angstrom. There exist six crystallographically unique asymmetric sites including two Er-sites, one Li-site and three Ge-sites. The overall crystal structure of Er_4LiGe_4 consists of two basic components: (1) the flat layered structure of the Er_2LiGe_2 slab adopting the Mo_2FeB_2-type structure and (2) Ge_2 dimers connecting two such layered structures. A Li atom on the Er_2LiGe_2 slab is primarily surrounded by eight Er atoms forming a distorted cubic coordination environment, and then it is further connected to six Ge atoms shaping a slightly distorted octahedral coordinates. The particular site-preference of Li atoms is also investigated using the coloring problem based on the theoretical approach by TB-LMTO method.

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The design and test of micrograting for an IR correlation spectroscopy

김태성 김성규

성균관대 화학과

A micrograting can be used in an IR correlation spectrometer in order to identify a target gas. The shape of micrograting can be designed by several methods such as the phase retrieval algorithm, the extended-phase retrieval algorithm, or the conjugated gradient method. These methods are compared for their effectiveness with the target gases such as ethylene, SO_2, ammonia, and SF_6. The micrograting for each gas spectrum is produced by MEMS and tested in a setup where a colliminated scannable monochromatic IR beam is incident onto the micrograting and the diffraction off it is collected at a fixed angle 15° before focused on a slit/MCT detector. The implication of this setup and its alignment is to be explained

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Preparation of Titanium Dioxide by Pulsed Laser Ablation in Liquid(PLAL) and Photocatalytic Applications

홍성민 최명룡

경상대 화학과

TiO_2 nanostructures were prepared by pulsed laser ablation (PLA) of a Ti metal plate in aqueous solution. In this case, the two-step experiments were conducted in a way and TiO_2 nanomaterials were formed to spherical, filamentous and cubic shapes, depending on the PLA experimental conditions. In this study, pure anatase, mixture of anatase/rutile and pure rutile of TiO_2 were fabricated by changing the nitric acid solution concentration. The structural and morphological characterization was conducted by X-ray diffraction (XRD) and field emission scanning electron microscope (FE-SEM), and UV-Vis spectroscopy. The photocatalytic activities of TiO_2 prepared in this study were investigated and discussed.

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Dynamic Heterogeneity of Solvation dynamics in coarse-grained model of room-temperature ionic liquids and all-atom model of acetonitrile : Red-edge effect

김대건 정연준 **Hyung J. Kim**[1]

서울대 화학부 [1]Department of Chemistry, Carnegie Mellon University

We study solvation dynamics of two systems which are a coarse-grained model of room temperature ionic liquids, 1-ethyl-3-methylimidazolium hexafluorophosphate (EMI^+PF6^-), and all-atom model of acetonitrile with a diatomic solute pair as a probe molecule by performing molecular dynamics simulations. For a diatomic solute pair, two different state of charge distribution are used, a neutral pair (NP) and a ionic pair (IP) with each atom have opposite charge 0.6364*e* and -0.6364*e*. We calculate the normalized time-dependent Stokes shift function in a non-equilibrium solvation dynamics simulation, using a concept of isoconfigurational ensemble to explore the effect of structure in solvation dynamics, after Frank-Condon transition from NP to IP and vice versa, especially in case of $\Delta E_{i\to f}$ equals to $<\Delta E_{i\to f}>$. $\Delta E_{i\to f}$ is defined by difference of total energy of RTIL-solute system, where *i* and *f* mean initial and final solute state. We also perform similar simulation in case of red edge condition and to find specific reasons of dynamic heterogeneity of solvation dynamics.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Density functional theory (DFT) study of the hydrated CO2 adsorption on barium oxide (BaO)

이왕로

전북대 기초교양교육원

CO2 adsorption on mineral adsorbents has been focused on the reduction of CO2 emission into the atmosphere. Flue gas steam in the fossil fuel power plants mainly contains CO2 and steam balanced with N2; thus. most adsorbents are sensitive to water due to its high affinity to adsorbents rather than CO2 which can be surrounded H2O in the system. This hydrated CO2 are important to understand the competitive CO2 and H2O adsorption on the adsorbent surface. This study applied a density functional theory (DFT) study of the hydrated CO2 adsorption on barium oxide (BaO) to investigate the role of H2O surrounded CO2 for adsorption on the (2x2; 11.05 ?x11.05 ?) BaO (100) surface because BaO adsorbs CO2 in a high reactivity. We investigated the adsorption properties (e.g., adsorption energies and geometries) of a single CO2 molecule surrounded a number of H2O molecule on the surface to achieve molecular structures and molecular reaction mechanisms.

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The O_2/CO_2 hybrid gas for Lithium-air battery system: mechanism and application

임형규 김형준[1] 임희대[2] William A. Goddard III[3]

KAIST(KAIST) EEWS [1]KAIST EEWS 대학원 [2]서울대 재료공학부 [3]California Institute of Technology, U.S.A

Considerable attentions have been emerged on Lithium-air battery with the thirst for a high energy density storage system. Conventional Lithium-air battery has been studied in a pure oxygen atmosphere excluding other contamination species such as H_2O and CO_2. However, considering that a genuine Lithium-air battery means the cell which is inevitably operated in ambient air,H_2O has to be eliminated thoroughly since it causes many side reactions. Although CO_2 concentration in ambient air is less than 400ppm, the solubility of CO_2 in organic electrolyte is 50~60 times larger than that of O_2. Therefore, it is essential to investigate the effect of CO_2 on Lithium-air cell system. Furthermore, recent research about Lithium-air battery using the mixed gas of O_2 and CO_2 reported that CO_2 has significant effect on the cell performance. However, fundamental understanding on the detail mechanism is still insufficient and rechargeability of the mixed gas system also remains unsolved. Therefore, fundamental understating of the effect of CO_2 on Lithium-air cell is necessary to make current system more practical. In this study, we proposed the reaction mechanism of $Li^+/O_2/CO_2$ fundamentally based on the DFT calculation, and proved it experimentally. Also opening of the new concept of 'Lithium-O_2/CO_2 battery' could be an important step forward in further designing of a practical Lithium-air battery.

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ZnO nanostructures grown on various Si and SiO_2 substrates

이승진 이상훈 이휘건

한양대 화학과

ZnO nanorods are grown on Si-based substrate by chemical bath deposition method in aqueous solution using zinc nitrate hexahydrate. Various substrates having different surface morphology are used to evaluate their effect on growing ZnO nanorods, such as flat Si(100) wafer, textured Si wafer, porous silicon, flat SiO_2 wafer, textured SiO_2 wafer. The length, diameter, geometry, and coverage density of ZnO nanorods are investigated by field-emission scanning electron microscopy. Grazing-angle X-ray diffraction and photoluminescence are also measured for each nanorod grown on various substrates.

		Zn/ f-Si	ZnO/ f-SiO_2	ZnO/ PS	ZnO/small texturized-Si	ZnO/small texturized-SiO_2	ZnO/large texturized-Si	ZnO/large texturized-SiO_2
Big	Length(μm)	1.19	3.16	2.97	2.14	3.50	2.45	3.65
	Diameter(μm)	0.16	0.37	0.69	0.30	0.35	0.11	0.34
	Coverage density(%)	20	20	40	5	5	5	5
Small	Length(μm)	none	0.59	none	0.90	0.62	0.75	0.55
	Diameter(μm)	none	0.09	none	0.12	0.08	0.12	0.06
	Coverage density(%)	none	75	none	> 95	> 95	> 95	> 95

Table 1.
Length, Diameter and Coverage density of Big and Small ZnO on various substrates

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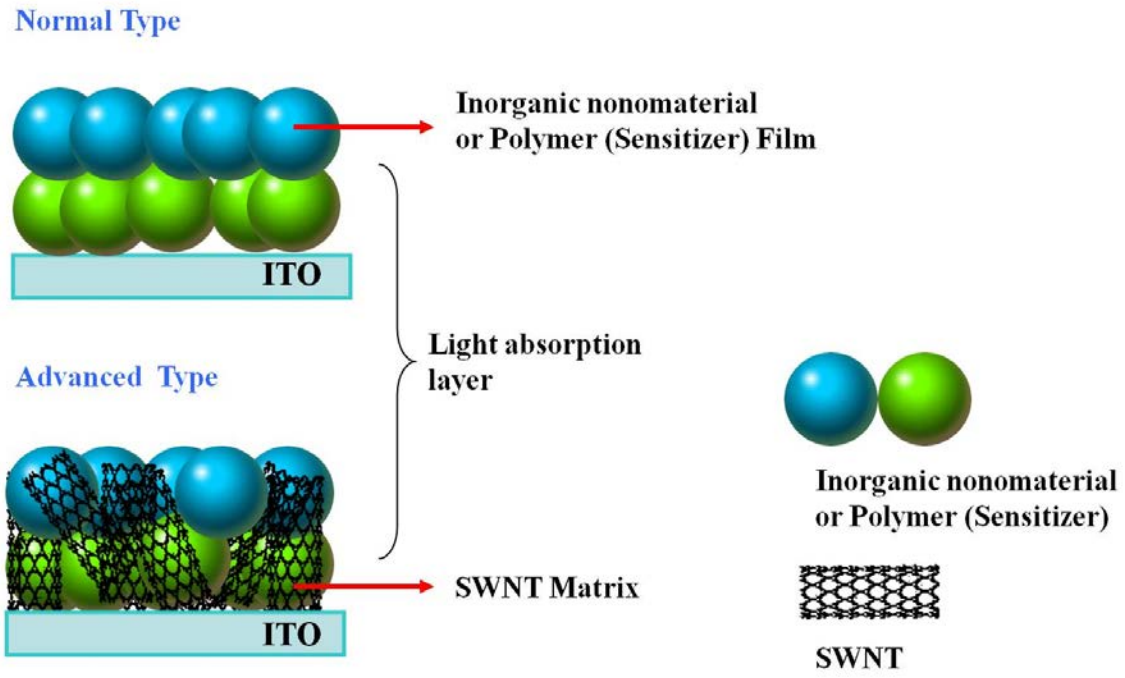
Study of conversion efficiency In_2O_3/In_2S_3 Photochemical cell using on Single wall carbon nanotube.

김희수 박현준 이휘건

한양대 화학과

Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure. The chemical bonding of nanotubes is composed entirely of sp2 bonds. In particular, owing to their extraordinary thermal conductivity and mechanical and electrical properties, carbon nanotubes find applications as additives to various structural materials. So we used In_2O_3 which has wide bandgap energy used for semiconductor for many application. and In_2S_3has less toxic and more environmentall than CdS,CdSe. and also it have narrow bandgap energy 2.0eV. Therefore we use SWNT for Photochemical cell and study how to increase efficiency.



대한화학회
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Fabrication of Infrared sensor using 3-dimensional single-walled carbon nanotube networks suspended on ZnO Nanorods

이종택 박태희 이휘건

한양대 화학과

Optoelectronic materials that are responsive at the wavelengths in the near-infrared (NIR) region (800~2000nm) are highly desirable for various demanding applications such as telecommunication, thermal imaging, remote sensing, thermal photovoltaics, and solar cells. Single-walled carbon nanotubes (SWNTs) have strong absorptions in the NIR region owing to the second optical transition (S22) of semiconducting nanotubes, which offer the possibility of an infrared (IR) sensor and are considered as material for IR photo response. We synthesize single-walled carbon nanotubes (SWNTs) suspended on zinc oxide (ZnO) nanorods on textured Si substrate using thermal chemical vapor deposition (CVD). SWNTs suspended on ZnO nanorods, are treated as 3-dimensional network structure. The IR sensitivity of the sample above are investigated by measuring ON/OFF ratio on IR illumination and compared with SWNTs synthesized on ZnO film on textured Si substrate using CVD. The IR sensitivity from 3-D SWNTs is more enhanced than that from SWNTs of film type by reducing intertube junctions as forming network structure. From this result, we conclude that SWNTs suspended on ZnO nanorods are individually separated and have more efficient structure for IR photo response.

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Photophysical behavior of cyclometalated Ir (III) complexes with (ppz)2acac ligand series.

김연희 윤승수 안태규[1] 김성규

성균관대 화학과 [1]성균관대 에너지과학과

We have investigated the photophysical behavior of phosphorescent cyclometalated Ir(III) complexes with diphenylpyrazolacetylacetonate (ppz)2acac ligand series in solution. A steady-state luminescence spectrometry and a time-correlated single photon counting (TCSPC) have been the main experimental tools. The quantum yields were measured very low and the lifetimes were in general shorter than 1 μs even after samples were degassed. To explain such observations, we performed density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations to characterize the excited singlet state and the triplet state. We believe that a non-radiative decay channel from the emitting triplet state, in which Ir-N bond is elongated and a twisting of pyrazol ring is open, is responsible for the shortening the lifetime and the extinguishing the phosphorescence. The calculation also shows that the degree of the coupling between the excited singlet state and the triplet state with the metal 5d character maybe partially responsible for the variations of the phosphorescent intensities throughout the complex series.

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Vibrational Spectroscopic Determination of Solvation Structure and Dynamics of 2,3,4-Cyanophenol

이주용 조민행

고려대 화학과

2,3,4-Cyanophenol (2CP, 3CP, 4CP) solutes form two-types of hydrogen bond in aprotic polar solvent. The complexes simultaneously in that 2CP hydroxyl has intra-molecular hydrogen bond and unusual forms are inter-molecular hydrogen bond with neighboring 2CP molecule when they are dissolved in dichloromethane and chloroform. This can be viewed as a simple prototype model system for a Watson-Crick base pair formation. Thus, studying such a cyclic dimer formation process in the condensed phase will provide us with information on the time scale and mechanism of the hydrogen-bonding dynamics. So we are trying to carry out 2D-IR chemical exchange experiments to study possible dimer formation-dissociation dynamics of certain 2CPs in a polar aprotic solvent. Also, the vibrational anharmonic frequency shifts, intrinsic lifetimes, and bandwidths of the nitrile stretch mode and the combination mode in these molecular systems are fully characterized, and their relationships with resonance structures are discussed.

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Following single-molecule reaction kinetics in individual gap-junctions

최한규 김지환

고려대 화학과

We studied the photochemical reduction kinetics of 4-nitrobenzenethiol (NBT) into 4,4'-dimercaptoazobenzene (DMAB) using the gap-plasmons formed at Ag nanoparticle and a Au thin-film junction. The photochemical reaction is initiated by irradiating light at λ= 633 nm and the subsequent evolution of DMAB product molecules are monitored by the surface-enhanced Raman scattering (SERS). While the ν_s(NO) peak shows continuous pseudo 1st-order decay kinetics of many (~200) molecules, the bands (9b, 3, and 19b) of the product show discrete steps of intensities. We also observed a spectral signature of long-lived nitrobenzene anion radials ($R\text{-}NO_2^-$) intermediates. In addition, the dynamics of the product steps are strongly correlated to the decay of the ν_s(NO) peak. Furthermore, the sizes of the steps show remarkable consistency among different hot-spots. These, together with the statistical analysis of the trajectory confirm that the "quantized" steps of the products indeed represent the buildup of individual DMAB products. Also, we could identify isomer (*o*-NBT, *m*-NBT) dependent reaction kinetics. The result constitutes the first observation of photochemical reaction of unlabeled individual molecules.

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Synthesis of GeSxSe1-x Nanocrystals and their Photo-Induced Cation Exchange Reaction

명윤 박정희 임형순[1] 김창현 정찬수 조용재 장동명 김한성 백승혁 임영록

고려대 소재화학과 [1]고려대 미세소자공학협동/마이크로소자공학

GeSxSe1-x (0≤x≤1) nanocrystals (NC) were synthesized using a novel gas-phase photolysis method. The composition of NC was simply controlled by the gas-phase composition of TMG, H2S, and DMS. Remarkably, the amorphous ligand-free GeSxSe1-x NC efficiently transformed into a series of corresponding crystalline Cd, Zn, Pb, and Ag chalcogenide NC via the photo-induced cation exchange reaction in aqueous solution. The S/Se composition of NC coincides with that of GeSxSe1-x NC. The present cation exchange reaction is governed by the thermodynamic driving force based on solubility, in which product with a lower solubility drives the exchange of cations. This effective synthesis strategy promises the development of cost-effective excellent optoelectronic devices.

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Dynamics of Molten Globule State of Apomyoglobin Binding to Nile Red Investigated by Fluorescence Correlation Spectroscopy

박성철 임만호

부산대 화학과

The dynamics of the binding reaction of nile red (NR) to molten globule state of apomyoglobin has been investigated by fluorescence correlation spectroscopy (FCS). When a ligand is small enough that the diffusion of the macromolecule is unaffected by the ligand binding and if we assume pseudo-first-order conditions with an abundance of ligand, the on-off rate coefficients for binding of the ligand to the protein can be determined directly.[1] To take pseudo-first-order conditions, it is necessary to separate the autocorrelation function (ACF) of individual components of bound and free ligand. NR strongly fluoresces when it is within the hydrophobic heme pocket of the protein but is weakly fluorescent in solution. Even the weak fluorescence from the free NR was significant and was removed. The fluorescence lifetime correlation spectroscopy method, a fusion of time correlated single photon counting and FCS, makes possible to separate bound and free NR and we can extract the on and off rate constants from the fit of the ACF.[2] Apomyoglobin is stable in its native state at pH 7 and the conformation changes from native state to molten globule state, the partly folded intermediate, at pH 4. This molten globular state was investigated by FCS of NR that binds heme pocket of the apomyoglobin.

References

[1]Don C. Lam *Biophysical Journal* 2000, 79, 1129-1138.
[2]Peter Kapusta *J.Fluoresc.* 2007, 17, 43-48.

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고상반응법을 이용한 $SrTiO_3:Sm^{3+}$의 합성과 광특성 연구

홍경수 정의덕[1]

한국기초과학지원연구원 하이테크부품소재연구지원센터 [1]한국기초과학지원연구원 부산센터

Strontium titanate ($SrTiO_3$) is of great interest to many kinds of integrated devices. Since it has several characteristics such as fast dielectric response, low leakage/low loss, and longer life time, $SrTiO_3$ has been applied to the integrated capacitors, strong capacitors in long-scale integrated dynamic random access memories, monolithic microwave integrated circuits, and pyroelectric IR sensors and piezoelectric microactuators. In this presentation, we synthesized Sm^{3+}-doped $SrTiO_3$ by using the solid state reaction method. In order to obtain the best crystallinity, we have optimized the synthesis conditions by measuring the physical properties of the synthesized powder with XRD and SEM. Also we have studied luminescent properties by taking absorption, excitation, and emission spectra. A red-orange luminescence corresponding to $^4G_{5/2} \rightarrow {}^6H_{7/2}$ transition of Sm^{3+} for near ultra-violet excitation is observed.

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Dynamics of Geminate Rebinding of NO with Cytochrome c in D_2O Solution

김주영 박재홍 이태곤 임만호

부산대 화학과

We investigated the rebinding dynamics of NO to cytochrome c (Cytc) and a model heme, microperoxidase-8 (Mp), after photodeligation of CytcNO in D_2O solution and MpNO in an 81% glycerol/water (v/v) mixture at room temperature using femtosecond vibrational spectroscopy. The stretching mode of the NO band in CytcNO revealed an asymmetric structured band that peaked at 1619 cm^{-1} with an FWHM of ca. 27 cm^{-1}. The structured NO band in CytcNO, well described by the sum of three Gaussians, did not evolve with time and its amplitude decayed exponentially with a time constant of 7 ± 1 ps. Rebinding of NO to Cytc was much faster than the rebinding of NO to myoglobin (Mb). When the deligated NO was constrained near the Fe atom either by a viscous solvent or by the protein matrix, it rebound to heme Fe much faster than CO, suggesting that NO has a higher propensity for binding to heme Fe and the high reactivity governed the rebinding kinetics. Moreover, the faster ligand rebinding in Cytc than in Mb suggests that Cytc does not have a primary docking site-like structure found in Mb that suppresses rebinding by restraining ligand motion.

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Near-field Study on a Multiferroic Bismuth Ferrite Film

김진욱 김덕수[1] 김지환 조문호[2]

고려대 화학과 [1]고려대 기초과학연구소 [2]연세대 신소재 공학부

We demonstrate a near-field imaging of a multiferroic BiFeO3 (BFO) film with scattering-type apertureless near-field scanning optical microscopy (ANSOM). BFO film contains various concentration of oxygen vacancy ($BiFeO_{3-\delta}$) and shows switchable photocurrent behavior with reorientation of local ferroelectric domain by exposing different directions of the electrical bias. Near-field approach on BFO film may be helpful to understand multiferroic behaviors and the connection between the oxygen vacancy and local ferroelectric domains.

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High yield Expression, Purification, and Structural Characterization of human transmembrane Proteins.

박유근 김용애

한국외국어대 화학과

Human transmembrane proteins(hTMP) are known to play an essential role in a variety of biological function. These proteins constitute about 30% of all proteins in eukaryotic cell and are involved in major disease processes in the body. 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 tried to produce large amounts of several Human transmembrane proteins(hTMP) like amyloid-?(hAb? protein that is related to the dementia and melanocrotin-4 receptor protein that is related to the obesity. The human amyloid protein(hAb? transmembrane is membrane-bound oligomeric state, and the Ca2+-permeable ion channel formation of non-fibrillar in the cell membrane. To determine the three dimensional structures of the intact hAb-TM, the isotopically labeled protein must be produced and purified in sufficient quantity. We succeed to produce large amounts of the hAb-TM. Structural characterizations of the hAb -TM in the membrane-like environments were obtained by solution and solid-state NMR spectroscopy.Human melanocortin-4 receptor (hMC4R) has a critical role in part of energy homeostasis. Heterozygous mutations in second transmembrane domain of hMC4R relate in genetic cause of severe human obesity. We succeed to produce the second trans-membrane domain from the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). But, the purified protein contains decent amounts of KSI fragment somehow. Therefore, we spend a lot of time to optimize the purification schemes. Circular Dichroism and MALDI-TOF MS spectroscopy were used to identify the initial secondary structures and purity. We obtained high resolution solution NMR spectra of hMC4R TM2.

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Efficient expression, purification, and NMR Structural Studies of Syndecan4-TM

송주영 최성섭 김용애

한국외국어대 화학과

Syndecan-4 plays important roles that may affect tissue development and repair as well as the pathogenesis of numerous diseases. It is composed of four transmembrane heparan sulfate proteoglycans found in most cell types and includes an extracellular domain, a transmembrane domain and a cytoplasmic domain. Today, plentiful studies regarding the structural information and biological functions for cytoplasmic and extracellular domain of syndecan-4 have been reported but, prior efforts to elucidate the structure and function of its transmembrane domain (Syd4-TM) have been relatively hindered by deficient yields and low solubility. Here, we report an efficient method for the recombinant expression and purification of Syd4-TM. Peptide was isolated from the KSI-fused protein and then purified by semi-preparative reversed-phase HPLC. Finally, over 5mg of Syd4-TM was obtained from 1L of M9 minimal media under optimized conditions with high purity. Previously, three- dimensional structural determination, biophysical properties were studied by circular dichroism (CD), mass spectrometry and nuclear magnetic resonance (NMR) spectroscopy. The CD spectra show that Syd4-TM adopts a stable α-helical structure in micelle environments. And solution NMR studies display Syd4-TM forms an asymmetric dimer in micelles. For further studies, we research not only mutant syndecan-4 which has a partially modified sequence of Syd4-TM, doesn't present dimerization but is comprised of monomer, but also Syd4-eTC which has extracellular, transmembrane and cytoplasmic domain of syndecan-4. We also report an optimized method for the recombinant expression and purification of mutant Syd4-TM and Syd4-eTC peptide. Consequently, we verified that mutant Syd4-TM forms a monomer and Syd4-eTC does a dimer.

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The First Result of Time-of-Flight Neutron Spectrometer DC-TOF in HANARO.

소지용 김은혜[1]

한국원자력연구소 중성자과학부 [1]한국원자력연구소 중성자과학연구부

The Disk Chopper Time-of-Flight Spectrometer (DC-TOF) is the first cold neutron Time-of-Flight spectrometer in Korea at the research reactor HANARO. Time-of-Flight spectrometer can measure wide range of dynamic range : from 20 ueV to 50 meV in energy, from 0.0 to 6.0 A^{-1} in momentum.In addition, one can choose the dynamic rangeSimilar kinds of instruments have been intensively used for the wide range of research field : magnetism, superconductivity, molecular dynamics of macromolecule and hydrogen storage meterials. In this presentation, we wil report the result of first experiments including standard vanadium, hydrogen storage material and simple molecules.

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Solvation energy and solvation shell of the metal complexes in mixed solvent

김형준 이윤섭

KAIST 화학과

The metal complexes are widely used as redox flow battery (RFB) active materials. These take advantage of high open circuit voltage (OCV), high efficiency and less pollution. These are dissolved in aqueous or organic solvents. High solubility and OCV can be expected when dissolved in water solvent but the RFB working voltage range is overlapped with water dissociation. Organic solvent such as acetonitrile (ACN) , gamma-butylolactone (GBL) and propylene carbonate (PC) are reasonable substitutes for water due to their stability under the charging process. Mixed solvent of ACN, PC and GBL are simulated using GROMACS package. The molecular force field parameters for PC and GBL are from OPLS/AA and the one for ACN is developed by Nikitin and Lyubartsev.(1) We refined the parameters to reproduce the experimental density and heat of vaporization by scaling partial charge. Assuming that parameter for pure solvent will work in the case of mixed solvent, the various mixing ratio for all the possible combination are tested. The dielectric constant property which is important in predicting solvation energy is thoroughly examined. The 1st and 2nd solvation structure, solvation energy of transition metal complexes (TMCs) are examined. The solvent molecules behavior is analyzed in terms of radial distribution function and their angle distribution. The candidates for TMCs are [Fe(bpy)3]2+ and [Fe(phen)3] 2+ and [Fe(terpy)3] 2+. (bpy=2,2’-bipyridine, phen=1,10-phenanthroline, terpy=2,2’;6’,2’’-terpyridine) The force field for metal complexes is selected from the ruthenium poly pyridinyl analogous.(2)References[1] A. M. Nikitin, A. P. Lyubartsev, J. Comput. Chem., 2007, 28, 2020[2] P. Brandt, T. Norrby, B. Akermark, Inorg. Chem., 1998, 37, 4120

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-370**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Luminescence Properties of Silica Nanospheres Incorporated with[Eu(dbm)4]- and [Eu(dbm)3?phen]

정용광 강준길

충남대 화학과

Eu(III) complexes with dbm (dibenzoylmethanido) and phen (1,10-phenanthroline) were synthesized, and their crystal structure and luminescence properties were characterized. Furthermore the complexes were incorporated to SiO2 nanospheres (NSs) as outer-shell and core-shell. The morphology of Eu(III) complex-incorporated SiO2 NSs were confirmed by FE-SEM and TEM. Luminescence properties of the SiO2 NSs were investigated as a function of temperature. The Eu(III) complexes excited at UV and emitted sensitized luminescence via the energy transfer from dbm to Eu(III). The efficiency of the sensitized luminescence was markedly enhanced by incorporating as outer-shell. The luminescence enhancement could be associated with the surface extension of the complex, resulting in the reduction of nonradiative transitions.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Nano-patterning of PEDOT:PSS layer and its effect on the absorption of subsequently deposited ZnPc thin films

한지영 임상규 이진호 최수나

국민대 생명나노화학과

Zinc phthalocyanine(ZnPc) is one of the most widely used electron donor materials in small-molecule organic photovoltaic(OPV) devices. The thickness of the ZnPc thin films in the device is, however, quite limited due to the significantly short exition diffusion length of the material. In this context, efficient absorption of incident light is of great importance to enhance the generation of photocurrent and power conversion efficiency(PCE) of the device.In this work, we fabricated 2-dimensionally (2D) nano-patterned surface of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOST:PSS) films using capillary method and nanoimprinting technology at the scale of several hundred nanometers.While the surface nanopatterning of low-conductive-grade PEDOT:PSS layer was successfully carried out by both methods, only the capillary method was effective for high-conductive-grade PEDOT:PSS layer.It is expected that the photonic crystal effect of this nano-patterned PEDOT:PSS layer alternates the direction and increases the path length of the incident light and consequently enhance the absorption of subsequently deposited ZnPc thin films. Acknowledge: This work was supported by the korea foundation for the Advancement of Science & Creativity(KOFAC) grant funded by the Korean Government(MEST).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon Capacitor: Effect of Pore Size in CNT-Sucrose Systems

김용빈 장락우

광운대 화학과

Supercapacitors are emerging as an ideal solution to electrical energy storage applications that require high power density and extraordinary recyclability. However, the key factor limiting the widespread deployment of supercapacitors in everyday technology is their moderate energy density. Carbon supercapacitors, which are energy storage devices that use ion adsorption on the surface of highly porous materials to store charge, have numerous advantages over other power-source technologies, but could realize further gains if their electrodes were properly optimized. In this study, we performed molecular dynamics simulations to investigate the effect of pore size on capacitance in the carbon nanotube (CNT) and sucrose system.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Dynamics Simulation Studies of CEA-Binding ssDNA Aptamers

이준성 장락우

광운대 화학과

Carcinoembryonic antigen (CEA) is expressed in many types of cancer cell. For example, its overexpression promotes hepatic metastasis of colon cancer cells. DNA aptamer candidates capable of binding to CEA were identified by using an optimized Systematic Evolution of Ligands by Exponential Enrichment (SELEX) procedure for diagnostic and therapeutical applications. In this study we performed all-atom molecular dynamics simulations of these ssDNA aptamer candidates to investigate their stable conformations at ambient temperature and provide some insights into their binding behavior.

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

QM/MM Studies of CALB-Catalyzed Dimerization of Methyl Lactates

김성훈 장락우

광운대 화학과

Candida Antarctica lipase B (CALB) has enantio-selectivity in the dimerization reaction of methyl lactates in organic solvents: CALB only catalyzes the dimerization of D-lactate. However, its mechanism is not still well understood. In this study, we performed quantum mechanics/molecular mechanics (QM/MM) simulations of atomistic models of enzyme-substrate complexes including several tetrahedral intermediate forms to understand the catalytic mechanism of CALB. The QM part consists of Ser-105 and His-224 along with the substrate and the MM part comprises the rest of the system. Transition states and free energy profiles along the reaction coordinate were calculated for both enantiomers, which would provide significant insights into the enantio-selectivity of the enzyme.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

DFT Study of Dye Regeneration Mechanism in Dye- Sensitized Solar Cells

전지원 김형준[1] 박영춘[2] 이윤섭[2]

KAIST EEWS [1]KAIST EEWS 대학원 [2]KAIST 화학과

Since Dye-Sensitized Solar Cell (DSSC) using iodide/triiodide (I-/I3-) couple as redox mediator produces high power conversion efficiency which is ~11%, I-/I3- couple is so far the most popular redox mediator. Interaction of this redox couple with dye (D) is important as this is involved in the dye regeneration process. As a matter of fact, although I-/I3- couple has significant effect on the performance of the DSSC, the interaction mechanism between redox couple and dye has not fully been understood due to its complexity to investigate via calculation and experiment. Before starting to study the interaction, a systematic study on I, I-, I2, I2-, I3, and I3- is carried out using different density functional methods (hybrid, GGA, and LC) and basis sets (aug-cc-pVDZ-pp, aug-cc-pVTZ-pp, and aug-cc-pVQZ-pp). Furthermore, we discuss the spin-orbit contribution for the open shell structures.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The effect of an external electric field on diffusion-influenced irreversible geminate ion recombination

김재훈 이상엽

서울대 화학부

The geminate recombination of the electron and the radical cation is one of the most important phenomena in the primary process of radiation chemistry. This subject has been investigated intensively in an effort to make more efficient solar cells. In this work, we employ the recently proposed solution method for Fredholm integral equations of the second to treat the diffusion-influenced irreversible geminate ion recombination under the external electric field. The merit of our theory is the simplicity of the solution. In previous theories, the geminate recombination probability was expressed as an infinite series of two complicated functions, each of which was also expressed as an infinite series. The formula also involved coupling constants which must be determined by solving a set of complicated linear equations. Our expression for the geminate recombination probability requires a single numerical quadrature.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Cu Oxide Nanofiber

박주연 빈준형[1] 강용철

부경대 화학과 [1]일진베어링 R&D센터 Polymer material팀

The Cu oxide/PVA nanofibers were synthesized by sol-gel and electrospinning technique. The obtained Cu oxide/PVA nanofibers were calcinated to remove the PVA compound at 673 and 873K. The ultrafine Cu oxide nanofibers were analyzed by 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 method and the diameters of Cu oxide nanofibers were 100-450 nm at room temperature. XRD results indicated that the crystal structure was changed from amorphous to monoclinic CuO through cubic Cu2O. TEM images also verified the crystal phase of Cu oxide nanofibers. XP spectra and X-ray induced Auger electron spectra were taken to assign the oxidation state of Cu in the Cu oxide nanofibers.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of highly stable superhydrophobic TiO2 surfaces with completely suppressed photocatalytic activity

김영독 서현욱 심종기 정명근 김대한 박은지

성균관대 화학과

TiO2 nanoparticles with a mean size of 20-30 nm were covered by ultrathin polydimethylsiloxane (PDMS) film, which shows hydrophobic properties. Surfaces consisting of the PDMS-coated TiO2 particles showed water contact angles close to 170o. In contrast to the hydrophobic films consisting of organic molecules, which can be photocatalytically decomposed on TiO2 in the presence of UV light, PDMS-coating on TiO2 was highly stable. These samples were shown to be resistant towards acidc and basic conditions. The PDMS-coating completely suppressed the photocatalytic activity of TiO2. The unique properties of PDMS-coating can be exploited for UV protection layer and self-cleaning surfaces.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

새로운 냉중성자 산란장치 : 디스크쵸퍼 비행시간 분광장치 (Disk Chopper Time-of-Flight, DC-TOF)

김은혜 소지용[1]

한국원자력연구소 중성자과학연구부 [1]한국원자력연구소 중성자과학부

디스크쵸퍼 비행시간 분광장치(DC-TOF)는 한국원자력 연구소의 연구용 원자로인 하나로에 설치된 국내 최초의 중성자 비행시간 분광장치이다. 2003 년에 개발이 시작되었으며 2012 년에 첫번째 중성자 빔 입사실험에 성공하였다. 원자로 내에 설치된 냉중성자원에서 발생한 중성자는 총 6 기의 디스크 쵸퍼를 거쳐 특정 파장을 갖는 중성자 펄스가 되어 시료에 산란되며, 산란된 중성자를 넓은 면적에 걸쳐 분포된 위치민감형 검출기를 이용하여 검출한다. 비행시간 분광법을 이용하여 중성자의 에너지 및 운동량 변화를 측정함으로서 물질의 동역학을 측정 할 수 있다. 본 장비는 냉중성자를 이용하여 20 μeV ~50 meV 의 에너지 영역과 0 ~ 6 Å-1 의 운동량 영역을 측정 할 수 있어서 자성체, 초전도체, 나노물질, 생체물질, 고분자물질, 수소 저장물질등 다양한 물질의 동역학을 측정 할 수 있다. 본 발표에서는 디스크쵸퍼 비행시간 분광장치의 장치 특성, 개발 현황 및 향후 계획에 대해 논의할 것이다.

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Theoretical Investigation of Para-substitution Effect on the Electronic Transition, A 2B2 ← X 2B1 of Thiophenoxyl Radical

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KAIST 화학 [1]KAIST 화학과

High level ab initio level calculation is performed to estimate the para-substitution effect on the electronic transition, A 2B2 ← X 2B1 of thiophenoxyl radical. Electron donating group, -F or -CH3 in the para position of thiophenoxyl radical increases the X -A energy gap by significantly stabilizing the X state energy. Electronic conjugation between the unpaired electron of S atom and ring π system plays a great role in characterizing the electronic structure of thiophenoxyl radical. Due to different orbital alignment of both studied electronic states, the degree of manipulating the electronic structure by para-substitution is quite different.

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Electrochemical Synthesis and characterization of Anodized TiO2 nanotubes Arrays/ZnFe2O4 Electrode

Haider Zeeshan 강영수

서강대 화학과

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. Although self assembled titania nanotubes arrays carry many advantages as compared to conventional TiO2 nano particle film such as better electron transportation, less wall thickness, tunable pore diameter and length as well as high aspect ratio, However in spite of several significant structural features there are also several short comings such as uv-absorption characteristics as well as recombination of charge carrier which causes hindrance to achieve highly efficient photovolitc device. In addition to other strategies, hetero structuring of titania with secondary materials having suitable position of band edges and having visible light absorption properties can significantly boost the photoelectrohcmial characteristic of titania nanotubes. In this study we have focused on the facile synthesis of coupling TNTA with p-type Zinc Ferrite by electrochemical method, which enabled to decorate TNTA with Zinc Ferrites particles without pore clogging of the nano channels. Reference:[1]. Hou, Y.;, Li, X.Y.; Zhao, Q-D.; Quan, X.; Chen, G-H, Adv. Funct. Mater.2010, 20,13, 2165.

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Further Kinetic Studies of Solvolytic Reactions of Isobutyl chloroformate in solvents of high Ionizing Power under Conductmetric conditions

류준하 김문무

동의대 화학과

AbstractSolvolyses of isobutyl chloroformate (4) in 43 binary solvent mixtures including highly aqueous media, water, D2O, CH3OD, 2,2,2-trifluoethanol (TFE) as well as aqueous 1,1,1,3,3,3-hexafluoro-isopropanol (HFIP) solvents were performed at 45oC, in order to further investigate the recent results of D`Souza, M,J1.et. al. (2011. Beilstein J. Org. Chem.); solvolyses of 4 are found to be consistent with the proposed mechanism (AdE). The variety of solvent systems was extended to comprise highly ionizing power solvent media (YCl > 2.7 excepted for aqueous fluorinated solvents and pure TFE solvent) to investigate whether a mechanistic change occurs as solvent compositions are varied. However, in case of 18-solvent ranges having aqueous fluorinated solvent systems (TFE-H2O and HFIP-H2O) excepted as well as YCl > 2.7 solvent systems, the solvent effect on reactivity for those of 4 are evaluated by the multiple regression analysis as competition with SN2 - type mechanism. And in pure TFE and 97 w/w % HFIP solvents with high YCl and weak NT, these solvolyses are understood as reactions which proceed through an ionization (SN1) pathway.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Live-cell imaging with novel, biocompatible fluorescent photoproducts of resveratrol and its derivative

이종우 양일승[1] 황선진[1] 이정은[1] 이준[2] 황도익 임은학[1] 금영삼[3] 김성근[1]

서울대 생물물리 및 화학생물학과 [1]서울대 화학부 [2]동국대 화학과 [3]동국대 약학대학 약학과

Resveratrol and resveratrol glucoside often found in grapes, berries, and nuts are well known to be antioxidant, anti-inflammatory, and anti-carcinogenic. We found that both of these nonfluorescent compounds can be easily converted to highly fluorescent forms by a photochemical reaction induced by simple UV irradiation. The photoproducts are deemed very desirable in fluorescence imaging due to their large Stokes' shifts, high fluorescence quantum yields, and large two-photon absorption cross sections. Furthermore, we found that these photoproducts have no cytotoxicity, while, in particular, the glucoside form boasting hydrophilicity. With these characteristics playing advantageous roles, both photoproducts are expected to be ideal bio-compatible fluorophores for live-cell imaging. Using these compounds, we demonstrate live fluorescence imaging of E. coli, S. cerevisiae, a mammalian cell, and a zebrafish embryo.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Controlled Morphosynthesis of Hematite for Photoelectrochemical Water Splitting

van thanh khue 강영수

서강대 화학과

The capping agent plays a critical function for the anisotropic crystal growth to induce polyhedral morphology of a nanocrystal. Uniform and single-crystalline α-Fe2O3 polyhedral nanoparticles in the hexagonal single crystal system named truncated hexagonal bipyramid for the first time was successful synthesized by a facile one step hydrothermal method with the aid of carboxymethyl cellulose and hydrazine molecules. The appearance and crystal structure of these iron oxide nanoparticles were characterized in detail by physicochemical methods. The results show that the as-synthesized α-Fe2O3 particles are bound by twelve same side-crystalline facets {101} and two other same facets {001} at tops. These obtained iron oxide particles belong to a pure hematite phase and the particle size is around 400 nm. The optical property of the as-synthesized product was analyzed and a determined indirect bandgap value Eg is 2.08 eV. The magnetic property studies of truncated hexagonal bipyramid hematite particles have shown that this kind of α-Fe2O3 possess a weak ferromagnetism under the TM and the saturation points do not reach up to the maximum applied magnetic field. Role of the reactants was discussed and investigated systematically in the work. Furthermore, a schematic illustration for the probable formation of this α-Fe2O3 morphology in whole of the synthetic process was also proposed.References [1] Thanh-Khue, V.; Cha, H. G..; Cuong, K. N.; Kim, S. W.; Jeong, M.H..; Kang, Y.S.. Cryst. Growth Des. 2012, 12, 862 ? 868.

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single molecule fluorescence study on kink and fork : increasing tension in the short dsDNA

김철희 김재열 이남기[1]

포항공과대 물리학과 [1]포항공과대 시스템생명공학부/물리학

Understanding to DNA property is important for biological process. Short dsDNA bending, among the many characteristic, is significant step of DNA packing on nucleosome, transcription control step and viral genome packing in the cell. Nevertheless, how strong tension applied to short dsDNA spontaneous sharply bent is well unknown. We prepared D-geometry samples that decreased the cyclization of ssDNA(60bp~34bp) and partial dsDNA region is fixed at 30bp. Then, cyclization of ssDNA part shorter, dsDNA part take to tension is increased. We have tested using single molecule ALEX(Alternating laser excitation)-FRET technique and computer simulation. Measured by single molecule ALEX FRET, we were able to make accurate calculation of FRET value, it was analyzed. Here, we found the bifurcation point fork state and bend state. In order to confirm these state, we use magnesium ion gradient and augment number of mismatch in the center of dsDNA part. And we get tension to bifurcation point and dsDNA going from bend state to kink state by theoretical calculation for equilibrium to between bending energy and stretching energy.

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A novel, fatigue-resistant photochromic fluorophore with fluorescence excitation decoupled from switching

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서울대 생물물리 및 화학생물학과 [1]서울대 화학부

The diarylethene family and their fluorescent derivatives are some of the most interesting photochromic molecules due to their excellent fatigue-resistance and thermal stability. However, nearly all diarylethene-based fluorophores have significant coupling between fluorescence excitation and switching wavelengths, and thus cannot act as a non-destructive optical memory. In this experiment, we combine fluorophore derived from well-known natural compound (‘resveratrol’) with diarylethene by simple UV irradiation. Because this fluorophore have strong absorption in the wavelength region where photochromic reaction of diarylethene does not occur, these new compounds exhibit nearly complete decoupling between fluorescence excitation and switching, which makes them an ideal candidate for fluorescence switching in nondestructive, fatigue-resistant optical memory. We demonstrate this possibility with optical writing and reading on photochromic compound-doped PDMA-based optical on/off system.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Raman Spectroscopy Study of Diffusion of Water through Graphene/SiO_2 Interface

이대웅 류순민

경희대 응용화학과

친수성 기판과 소수성 그래핀(graphene) 계면에서의 물의 확산 현상은 호기심을 자극할 뿐만 아니라 그래핀 소자의 특성을 좌우하는 전하도핑(charge doping) 현상을 이해하는데 중요한 모델이 된다. 본 연구에서는 라만 분광법을 이용하여 그래핀/SiO_2 계면에서의 물의 확산 현상과 그에 따른 정공 밀도 변화를 탐구하였다. 열처리된 그래핀은 기판과의 상호작용에 의해 높은 밀도의 정공(electron hole)으로 도핑되어 있기 때문에, 물이 계면을 통해 확산하게 되면 정공의 밀도를 감소시킬 수 있게 된다. 본 실험에서는 이차원 라만 분광법을 통해 물 속에 담겨진 그래핀의 정공 밀도의 공간적인 분포를 확산 시간에 따라 조사하였다. 물의 확산은 시료에 따라 수 시간에서 수 일의 시간대에 걸쳐 그래핀 가장자리에서 중앙으로 이루어진다는 사실을 확인하였다. 또한 물의 계면 확산으로 인해서 전하 밀도가 감소한다는 사실은 열처리된 그래핀의 정공 도핑을 유발하는 산소가 그래핀/SiO_2 계면에 존재한다는 것을 증명한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Contribution of RNAP polymerase to gene expression noise in E.coli

양소라 이남기[1]

포항공과대 물리학과 [1]포항공과대 시스템생명공학부/물리학

A population of cells has different level of proteins even if their genomes are identical. This causes a phenomenon called “gene expression noise” or cell-to-cell variation. According to the origins, “noise” can be classified into two factors of intrinsic and extrinsic noises. Intrinsic noise occurs due to the stochastic nature of chemical reactions, while extrinsic noise by various cell-to-cell variations, such as protein numbers and glowing conditions. Among the possible sources of extrinsic noise, the number variation of RNA polymerase (RNAP) has been considered as one of the major noise sources. In this work, we studied the effect of RNAP concentration on the downstream protein noise in E. coli cells. We found that RNAP concentration indeed has a major effect only on the extrinsic noise, not on the intrinsic noise. At high expression levels, the protein noise is dominated by the extrinsic noise originated from fluctuations in RNAP concentration. Our result clearly demonstrates that RNAP at transcription plays a significant role on determining the cell-to-cell variations at protein level.

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Structures and Properties of Polythiophene Derivatives : Theoretical Approaches

이수빈 구인선 박종근

경상대 화학교육과

Cyclic n-thiophene derivatives (n=4～26) and their complexes (n=6～18) with the carbon dioxide were optimized at the HF/3-21G and B3LYP/6-31G* levels. Geometric structures, bond lengths, atomic charges, and HOMO-LUMO gaps of the neutral and the cationic derivatives were investigated. There are two types of the cyclic thiophenes : one is in-type, while the other is out-type. In the neutral thiophene derivatives, the structures of in-type (n=4～12) are planar. But, with increasing n (n>14), the structures vary to the curved geometry. In the cationic thiophene derivatives (n=14～26), the structures are similar to the neutral thiophene derivatives. With increasing the cationic number (+1, +2), the structures are circularly planar. The polythiophene derivatives substituted with carboxyl group are more planar than the corresponding polythiophene derivatives. These structures interact with the carbon dioxide through hydrogen bond. The binding energy of 12-thiophene derivative bonded with two carbon dioxides is about 0.097 eV.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Tetragonal LaVO4 and Its Application to Downconversion Phosphor of Dye-Sensitized Solar Cell

김두경 강영수

서강대 화학과

Lanthanide orthovanadate crystals have two types of morphology that is tetragonal phase with zircon structure and monoclinic phase with monazite structure. Generally tetragonal LaVO4 is a better host for rare-earth activators. The charactericstic of downconversion phosphor enables to convert UV into Visible light. This phenomenon is expected to enhance the efficiency of DSSC (dye-sensitized solar cell) and stability of dye which is easily photooxitized. LaVO4 was prepared using La(NO3)3?6H2O, Dy(NO3)3?6H2O, NH4VO3, oleic acid and ethanol by hydrothermal method.[1] The adsorption of oleic acid on certain surfaces make nanoparticle as a plate shape which is 40*40*10 nm. Using oleic acid as a surfactant makes nanoparticles well disperse into the organic solvents. This property makes allows LaVO4 nanoparticles to be applied to dye-sensitized solar cell through coating method such as a spin coating or a doctor blading. Properties of nanoparticles have been checked by XRD, TEM and photoluminescence (PL). References: [1]Junfeng Liu,' Yadong Li. Advanced Materials. 2007, 19, 1118-1122

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Fast dynamics of single-biomolecule with sub-millisecond resolution with tens of millisecond observation time

김재열 김철희 이남기[1]

포항공과대 물리학과 [1]포항공과대 시스템생명공학부/물리학

Fluorescence detection has been widely used for biochemical studies, such as enzymatic reaction, folding, protein-protein interaction, and so on. Advance in fluorescence techniques allowed even detecting fluorescence from a single-molecule. Single-molecule fluorescence resonance energy transfer (smFRET) is one of most useful techniques to measure the dynamics of biomolecules. However, smFRET has limited time resolution (~10 ms) for immobilized TIR measurement. Diffusion-based smFRET can achieve millisecond time resolution but it suffers from short observation time (~1ms). Here, we applied a new strategy on diffusion-based smFRET (ALEX-FRET) to overcome the resolution and observation time limits by using liposome. By tethering molecules on liposome, we increased diffusion time from ~1 ms to ~20 ms. As a result, we observed fast dynamics of DNA Holliday junction with sub-milisecond time resolution.

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Kinetics and Mechanism of the Pyridinolysis of Dimethyl Isothiocyanophosphate in Acetonitrile

Adhikary Keshab Kumar Hasi Rani[1] 김찬경 이해황

인하대 화학과 [1]인하대 물리화학과

The kinetics and mechanism of the pyridinolysis (XC_5H_4N) of dimethyl isothiocyanophosphate are investigated in acetonitrile at 55.0°C. The Hammett and Bronsted plots for substituent X variations in the nucleophiles exhibit two discrete slopes with a break region between X = 3-Ac and 4-Ac. These are interpreted to indicate a mechanistic change at the break region from a concerted to a stepwise mechanism with a rate limiting expulsion of the isothiocyanate leaving group from the intermediate. The relatively large β_X values imply much greater fraction of frontside nucleophilic attack TSf than that of backside attack TSb. The steric effects of the two ligands play an important role to determine the pyridinolysis rates of isothiocyanophosphates.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Native strain-dependent photoluminescence in single-layer MoS_2

고택영 박광희 류순민

경희대 응용화학과

When MoS_2 is thinned to single layer (1L), photoluminescence (PL) quantum yield drastically increases due to emergence of direct band gap. A recent theory predicts that the electronic structure of 1L MoS_2 is very sensitive to its lattice constants. We investigated the effects of native strain on PL of 1L MoS_2 supported on SiO_2 substrates using spatially resolved PL and Raman spectroscopy. Changes in the lattice constants were monitored by the Raman frequency of the in-plane (E_{2g}) mode. Systematic correlations between PL and Raman spectral features, revealed in the preliminary results, will be further tested with samples on other substrates and against thermal stress. The results will be also discussed in regard to the theoretical predictions.

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Photodetector based reduced graphene oxide film for visible and intrared

최종완 형은수 윤수진 문인규[1] 김낙중

한양대 화학과 [1]서강대 인공광합성 연구센터/나노물질연구소

Reduced graphene-oxide (rGO) is considered to be a promising material for optoelectronic devices due to exceptional electrical and photonic properties; 2-D spread structure andmechanical flexibility. More interestingly, rGO also has the ability to absorb photons over a wide spectrum from visible to near infrared, which is significant for making optoelectronicdevices. Here in this work, we prepared a rGO paper through vapor-phase reduction for graphene with HI/acetic acid. We also fabricated a photodetector using the gold (Au) electrodeswhich were attached to both sides of rGO sheet. The photocurrents were measured with a laser (632.8 nm or 1550 nm) depend on the position of the laser spot. The final results clearlyshow that macro-scale thick films of rGO can serve as a position photosensing at the. range of visible through rear infrared.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Kinetics and mechanism of the anilinolysis of aryl ethyl isothiocyanophosphate in acetonitrile

Hasi Rani Adhikary Keshab Kumar[1] 김찬경[1] 이해황[1]

인하대 물리화학과 [1]인하대 화학과

Abstract: The nucleophilic substitution reactions of Y-aryl ethyl isothiocyanophosphates with substituted X-anilines and deuterated X-anilines are investigated kinetically in acetonitrile at 75.0 oC. The free energy relationships with X in the nucleophiles exhibit biphasic concave downwards with a break point at X = H. A stepwise mechanism with a rate-limiting bond formation for more basic anilines and with a rate-limiting bond breaking for less basic anilines is proposed based on the negative and positive ρXY values, respectively. The deuterium kinetic isotope effects (DKIEs; kH/kD) are gradually changed from primary normal with more basic anilines, via primary normal and secondary inverse with aniline, to secondary inverse with less basic anilines. Primary normal and secondary inverse DKIEs are rationalized by a frontside attack involving hydrogen bonded four-center-type TSf and backside attack involving in-line-type TSb, respectively.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Different Morphologies of Upconverting β-NaYF4 Prepared by a Facile Hydrothermal Method and Their Application into Dye-Sensitized Solar Cells

이재호 강영수

서강대 화학과

Upconversion is a process where low-energy photon is converted into a high-energy photon[1]. By using upconverting nanoparticles, infrared light can be converted into visible light. Therefore these materials can be a possible candidate to overcome the spectral mismatch of dye-sensitized solar cells (DSSC)[2]. Upconverting nanoparticles such as β-NaYF4 doped with Yb, Er, Ho are the possible candidates for application since they have excellent upconverting efficiencies along with emissions around ~550 nm, which can be efficiently absorbed by the N-719 dye. By making different morphologies of β-NaYF4(Yb,Er,Ho) by a simple hydrothermal method, we can apply it to different parts of the DSSC and enhance its efficiency by using not only visible light, but also infrared light. Different morphologies of β-NaYF4 doped with ytterbium and erbium was synthesized by a facile hydrothermal method using rare-earth nitrate precursors. Further investigation of their optical properties have to be clarified, along with new ideas for their application into DSSC.References[1]Haase, M.; Schafer, H. Angew. Chem. Int. Ed. 2011, 50, 5805-5829.[2]van der Ende, B. M.; Aartsa, L.; Meijerink A. Phys. Chem. Chem. Phys. 2009, 11, 11081-11095.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] Synthesis process of BiOBrxCl1-x that and active features as photocatalytic

나율이 손영구

영남대 화학과

발 표 취 소
본 논문은 발표취소된 논문입니다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Observation of Vibronic Emission Spectrum of Jet-Cooled 2-Chloro-m-Xylyl Radical Generated during Corona Discharge

윤영욱 이상국

부산대 화학과

The jet-cooled 2-chloro-m-xylyl radical was generated and vibronically excited in a corona excited supersonic expansion from precursor 2-chloro-m-xylene seeded in a large amount of inert carrier gas helium for the first time. The well-resolved vibronic emission spectrum of the jet-cooled 2-chloro-m-xylyl radical was recored using a long path monochromator in the visible region. The spectrum was analyzed to obtain an accurate measurement of the energy of the D1→D0 electronic transition and the frequencies of vibrational modes in the ground electronic state by comparison with those of ab initio calculations and known spectroscopic data of 2-chloro-m-xylene.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Substituent effects on the electronic structures and pKa of Substituted tert-Butylbenzene: A Theoretical Study

한인숙 김창곤 김찬경 이해황 손창국[1] 유유희[2]

인하대 화학과 [1]전남대 화학교육과 [2]전남대 과학교육학과

To investigate the origin of substituent effects on the acidity and physical properties of substituted tert-butylbenzene, a series of substituted species have been examined theoretically at various levels of theory. A more satisfactory agreement with the experimental values was obtained at the G3(+)MP2 level on the MP2/6-31+G* geometries. To make accurate predictions of pKa values in aqueous solution, the structures and the Gibbs free energies of solvation were examined by use of the conductor-like polarizable continuum model (CPCM) with various cavity models: UA0, UAHF, UAKS, UFF, BONDI and PAULING, and by use of a discrete/continuum solvation model at the MP2/6-31+G* levels. Geometries of the stationary point species in aqueous solution and in the gas-phase have been fully optimized and characterized by frequency calculations. All the calculations were performed with the Gaussian-03 program.

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Fabrication of CoSe nanowires using Au catalysts by an atmospheric pressure chemical vapor deposition (APCVD)

김진일 방수경 김태규

부산대 화학과

Cobalt selenide (CoSe) nanowires were grown on Si(100) substrate coated with Au catalyst by using an atmospheric pressure chemical vapor deposition (APCVD) method. Au thin film induces an Au-catalyzed vapor-liquid-solid (VLS) growth of CoSe nanowires. We used cobalt chloride (CoCl2) beads and selenium (Se)-graphite mixture as precursors. Graphite powder was used to vaporize two precursors simultaneously. The synthesized nanowires were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive x-ray spectroscopy (EDS) and x-ray diffraction (XRD) analysis. Electron microscopic results show the typical diameter and length of single CoSe nanowires is 60-100 nm and 10-20 μm, respectively. Energy dispersive x-ray spectroscopy (EDS) data suggest the homogeneous character of CoSe nanowires. In addition, x-ray diffraction (XRD) pattern indicates that the obtained CoSe nanowires are in the hexagonal phase.

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Fabrication of Three-dimensional Network of Carbonnanotubes coated with Polydiacetylene for HCl Gas Seonsor

안도연 서정은 조석진 조용덕[1] 김종만[2] 이해원

한양대 화학과 [1]한양대 나노융합과학과 [2]한양대 응용화공생명공학부

Carbonnanotube has been applied to a lot of applications because of its unique structural, mechanical, electrical properties. And Fabrication of three-dimensional network of carbonnanotubes was achieved by growing carbonnanotubes between Silicon Pillars. This unique structure shows highly dense and uniform structure which has a strikingly large surface area. On the other hand, Pi-conjugated polymer presents unique color change and fluorescence when exposed to some external impetus. Due to this characteristic, this polymer has been widely applied to sensors and detecting devices. In this study, three-dimensional network of carbonnanotubes was coated with pi-conjugated polymer. By doing so, we was able to observe an increase of fluorescent intensity relative to the previous instance.

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Preparation and Characterizations of Photofunctional Metal Alloy for Bio-applications

왕강균 김봉진 정지혜 권재덕 김용록

연세대 화학과

Metal alloys have widely been used for the biomedical applications in cardiology, orthopedics, and dentistry due to its good wear resistance and pitting resistance to human body. However, the metal alloys may induce the occurrence of neointimal hyperplasia and unnecessary cell proliferation by immune system. In recent years, It has been reported that reactive oxygen species (ROS) can be used for suppression of neointimal hyperplasia and cell proliferation. The use of ROS in photodynamic inactivation (PDI) is particularly attractive due to its high efficiency for deactivation of target organism and less side effect. In this work, we report the fabrication of photofunctional metal alloy plate that is prepared by a simple modification process. Microstructure and elemental composition of the metal alloy plate were checked with scanning electron microscopy (SEM) and energy dispersive X-ray spectrometer (EDS). Properties of the photofunctional metal alloy were confirmed with various spectroscopy method. Also, reactive oxygen generation from the photofunctional metal alloy plate was confirmed by using the chemical decomposition reaction. To demonstrate its application as a photodynamic material for biological systems, the fabricated photofunctional metal alloy is applied to the decomposition of cells.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Single-Crystalline Monoclinic BiVO4 by the Seed Layer Assisted Growth on FTO Glass

손영석 김창우 강영수

서강대 화학과

Presently, 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 superior charge transport properties. 1-D semiconductor nano-architectures have been synthesized by a number of chemical and physical techniques, including vapor-liquid-solid, dielectrophoresis, Langmuir-Blodgett, anodized aluminum oxide template, hydrothermal, lithographically patterned nanowire electrodeposition, molecular beam epitaxy etc. Among various semiconductors, BiVO4 is a promising material to achieve efficient water photoelectrolysis with visible light illumination. BiVO4 has been widely reported with controlled morphology from spherical particle to pyramidal shape. However few researches have been reported about single crystalline BiVO4. Moreover it is very few to report BiVO4 films as photoanode. In this study, we report BiVO4 nanoparticle film on the FTO by hydrothermal method. Using seed layer by spin-coating, BiVO4 nanoparticle film with various morphologies was grown on the seed layer. We demonstrated 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 regionKeywords: BiVO4, Photoanode, Photocatalyst.

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A new sub-diffraction-limit optical nanoscopy technique: Dual-point illumination AND-gate microscopy on nanodiamonds (DIAMOND)

권지웅 임영빈[1] 정지원[2] 김성근[2]

서울대 생물물리 및 화학생물학과 [1]서울대 생물물리 및 화학생물 [2]서울대 화학부

We introduce a new, easily implementable sub-diffraction-limit microscopy technique utilizing the optical AND-gate property of fluorescent nanodiamond (FND). We demonstrate that when FND is illuminated by two spatially-offset lights of different wavelengths, fluorescence emission comes only from the region of their overlap, which is used to reduce the effective point spread function from ~300 nm to ~ 130 nm in lateral plane, well below the diffraction limit.

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Near-field Optical Microscopy of quantum dots with an Up-Conversion Nanoparticle attached tip as a Point Light Source

김주영 김지환

고려대 화학과

We demonstrate the use of up-conversion nanoparticles (UCNPs) as local point light source for optical imaging of quantum dots via FRET (Fluorescence resonance energy transfer) between UCNPs and Qdots (Quantum dots) as donors and acceptors, respectively. The UCNPs have core@shell Yb3+/Er3+@NaYF4 structure and produce strong dual fluorescence at 540 nm and 660 nm with cw-excitation at 980 nm. Because they do not have significant photo-bleaching or blinking, they are best suited as a point light source for near-field optical imaging. The UCNP-tip is made by chemically linking the UCNPs at the apex of the Si-tip using APTMS (Aminopropyltrimethoxysilane) linkers, and the emission at λmax = 540 nm is non-radiatively transferred to Qdots via the FRET process. We observe that the FRET images show features that are smaller than the optical diffraction limit of the excitation (980 nm) or emission wavelengths (540 and 660 nm), which demonstrate that the UCNP-tip indeed serve as a near-field (incoherent) point light source and an effective donor as well. Based on such UCNP-FRET microscopy technique, possibility for the nanometric imaging of individual molecules is also explored.

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Synthesis of Dendritic Fe, Co and Ni Alloy for O2 Evolution and Methanol Oxidation

Zheng jin you 강영수

서강대 화학과

The vertical dendritic FeCo, FeNi, CoNi and FeCoNi alloy array films were prepared on Ni foil substrates by electrochemical deposition. The morphologies of as-obtained alloy films were characterized by scanning electron microscopy, which shows that the dendrites with micro size are uniform. In addition, the ratio of metal elements was analyzed by energy-dispersive spectroscopy; it indicates that the amount of elements in metal alloys is equal (ca. 1:1 or 1:1:1). The dendritic metal alloy films can be transformed into metal oxide films without destroying the dendritic structure and morphology by thermal oxidation. The electrodes were used for O2 evolution and methanol oxidation, which were carried out by the cyclic voltammetric (CV) technique in NaOH solution or NaOH with methanol solution.Keywords: metal alloy, O2 evolution, methanol oxidation, dendrite, electrodeposition

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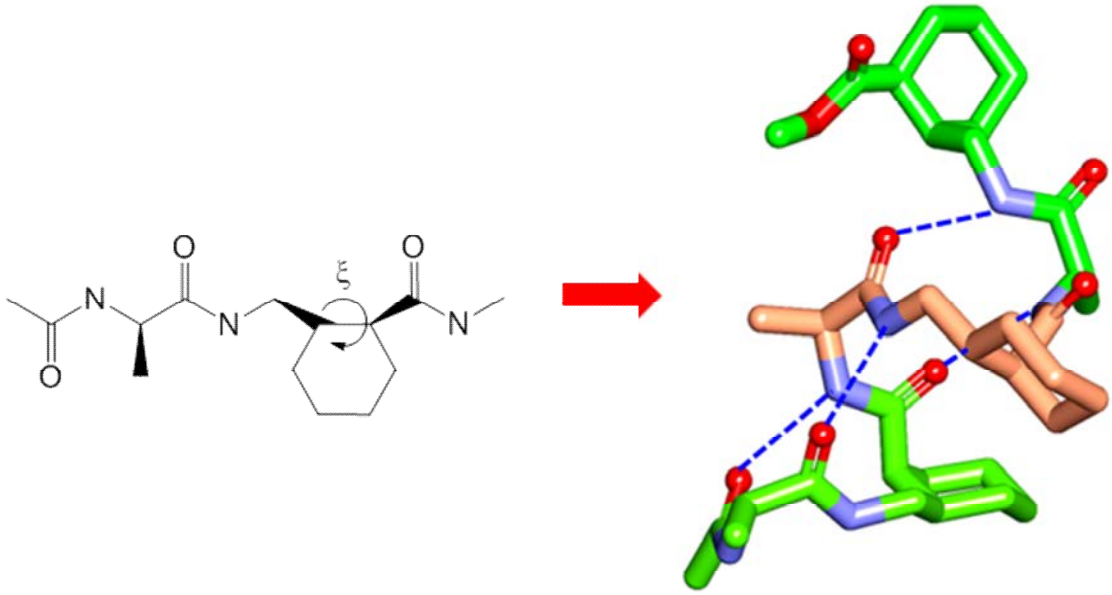
Theoretical Insights into Helix Formation in α/γ-Hybrid Peptides

이주연 채종학[1] 강영기

충북대 화학과 [1]한국화학연구원 신물질연구본부/신약플랫폼기술팀

γ-amino acid building blocks a ring containing at least one backbone bond are of particular interest because cyclic constraints were documented to be useful in stabilizing specific secondary structures among foldamers. Gellman et al. reported that asymmetric synthetic routes to γ-amino acids with a cyclohexyl constraint at the Cα-Cβ bond (ξ torsion angle), which provide derivatives of the *cis* and *trans* γ-amino acid diastereomers, each in highly enantioeriched form. And they have recently provided crystallographic evidence for the 12-helix in α/γ-hybrid peptides that contain γ-residues with a *cis* cyclohexyl constraint on the Cα-Cβ bond. Crystal structures revealed a strong helix-forming propensity for the *cis* γ-residue. The present study was conducted to calculate for conformational preferences of Ac-(Ala-γAmc_6)n-XMe, α/γ-hybrid dipeptides (n=1, X=NH), tetrapeptides (n=2, X=O), and hexapeptides (n=3, X=O), respectively, in order to analysis available conformations and then propose new types through an insight into helix formation in α/γ-hybrid peptides.[Figure] Structure of α/γ-hybrid dipeptide and hexapeptide optimized at the M06-2X/6-31G* in the gas phase



대 한 화 학 회
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Structural and Electronic Characteristics Induced by Carbonization Control of Mesoporous Carbon Nanofibers

임지은 **LIJING** 노중석 김용록

연세대 화학과

Porous carbons have become one of the important materials that are actively investigated. Especially, mesoporous carbon materials with a high surface area and ordered mesostructure have quickly attracted wide attentions due to their potential applications of gas sensor, natural gas storage, fuel cells, and electrodes in electrochemical devices. In this study, we report a successful strategy to provide the precise control and enhance electrochemical characteristics of mesoporous carbon nanofibers (MCNFs) for the gas sensing properties. The carbonization temperature is a key factor to control the structural characteristics and the electronic properties of MCNFs. The band gap energies of MCNFs are estimated to be 0.040, 0.018, and 0.0072 eV at the carbonization temperatures of 600, 900, and 1200 °C, respectively. In addition, as the carbonization temperature increases, the conductivity of MCNF increases due to the enhanced values of L_c, L_a, and L_c/d.

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The Photodissociation of 2-bromopropene near 234 nm : Ion-Imaging Studies

김현국 **Paul Dababrata** 김태규

부산대 화학과

The photodissociation dynamics of 2-bromopropene have been investigated near 234 nm using a velocity map ion imaging technique coupled with a state selective [2+1] resonance-enhanced multiphoton ionization [REMPI] scheme. The nascent Br atoms stem from the primary C-Br bond dissociation leading to the formation of C_3H_5 and Br($^2P_{3/2}$) and Br*($^2P_{1/2}$).Total translational energy distributions have been well fitted by a single Boltzmann and two Gaussian functions for both Brand Br* formation channels. Based on the recoil anisotropy and distribution width of each component, trimodal translational distributions of Br and Br* channels have been assigned to the direct and indirect dissociation mechanisms originating from the initially excited (π,π^*) and (n,σ^*) states.

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DFT studies of [16]annulene configurational isomers for their interconversion mechanisms and binding properties to various neutral and cationic nickels

장효원

순천대 화학과

We identified two separate reaction paths each connecting the most stable pseudo-planar [16]annulene conformer and a higher-energy pseudo-capsule-shape conformer, respectively. One path involves two elementary steps associated with Moebius aromatic transition states where the single and double bond-shift occurs. It is interesting to note that nickel cation and dimeric nickel cation stabilize the higher energy pseudo-capsule-shape conformer to a greater extent than it does to the most stable pseudo-planar conformer while neutral and dicationic nickel does not. We try to find the possible explanations behind these observations where appropriate.

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Photodegradation of methyl orange catalysed by phosphomolybdic acid encapsulated Zeolite Y in presence of Ag^+-N-TiO_2 nanochains under visible light irradiation

박기성 **Radhakrishnan Sivakumar**[1]

충남대 화학과 [1]Department of chemistry, National Institute of Technology, Tiruchirappalli, India

Phosphomolybdic acid ($H_3PMo_{12}O_{40}$; PMo12) encapsulated zeolite Y with surface adsorbed Ag^+-N-TiO_2 nanochains were successfully designed to locate photocatalytically active sites in zeolite for enhanced photodegradation of organic dyes. Diffuse reflectance spectroscopy, Inductively coupled plasma atomic emission spectroscopy, X-ray photoelectron spectroscopy techniques were used to confirm the encapsulation of PMo12 in the cavities of zeolite. X-ray diffraction analysis reveals the retention of the crystallinity of zeolite Y upon encapsulation of PMo12. A uniform distribution of directly synthesized PMo12 within zeolite Y pore channel was also confirmed by SEM and TEM images. These photocatalysts were investigated for the photodegradation of methyl orange and found that higher Ag^+-N-TiO_2/PMo12Y shows higher photodegradation rate when compared to Ag^+-N-TiO_2-PMo12, suggesting the crucial role of zeolite in enhancing the charge carrier separation.

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Individual chlorophyll characteristic in Photosystem II core complex

이은 안태규[1]

성균관대 에너지과학 [1]성균관대 에너지과학과

Part of the functionality of the photosystem II comes from the transfer of energy between chlorophylls. These are connected in to a complex network where the coupling strength is related to both the geometry of the chlorophyll and their spatial orientation. We investigate how much of the photosystem II in Thermosynechococcus vulcanus that can be explained by the network topology of this network. We calculate the excitation-energy coupling strength by using F?rster energy transfer theory. We use the calculated excitation-energy coupling strength as the basis for constructing a network of possible excitation transfer pathways. We find that network centrality measures can characterize the role of individual chlorophylls in the excitation-energy transfer network. By using the network-structural measures betweenness centrality, closeness centrality and clustering coefficient, we can predict the different functionality of individual chlorophylls. Among other things, we can infer that the chlorophyllcomplex CP47 has the role of a bridge in excitation energy transfer . We can infer that most of chlorophylls in pigment-protein complex CP47 have heightened probability to absorb the energy compared with other chlorophylls. The so-called A-branch special pair in the reaction center is characterized by a high closeness centrality, a high betweenness centrality and a low clustering coefficient. This implies that this component is able to get more energy than other component of special pair.

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Violation of Stokes-Einstein Relation and Component Decoupling of Multicomponent Metallic Glasses

김정민 성봉준

서강대 화학과

The breakdown of Stokes-Einstein relation (SER), $D \sim \tau_\alpha^{-1}$, near glass transition has been an issue of significance in colloid dynamics and materials science, where D is a diffusion coefficient and τ_α is a translational relaxation time. Fractional Stokes-Einstein relation, $D \sim \tau_\alpha^{-\xi}$ with $\xi_{43}Cu_{27}Ni_{10}P_{20}$ alloy [1] reported a strong component decoupling of diffusion coefficients upon super-cooling between the largest component Pd and others. To elucidate the connection between the breakdown of SER and the component decoupling, we perform molecular dynamics simulations for hard sphere mixtures modeled after $Pd_{43}Cu_{27}Ni_{10}P_{20}$ melts. We find that the volume fraction ($?_{SE}$) is 0.59 when SER starts to fail. Fractional SER is well fitted with ξ=0.84±0.03. As the volume fraction approaches $?_{SE}$, the diffusion coefficient of P becomes about 20 times larger than that of Pd. And, a particle displacement distribution shows clear component decoupling between a slow component of Pd and a mobile component of P. Reference[1] A. Bartsch, Phys. Rev. Lett. 104, 195901 (2010)

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Impedometric Estrogen Biosensor based on Estrogen Receptor Alpha-immobilized Gold Electrode

LIJING 임지은 김병건 이원용 김용록

연세대 화학과

A label-free impedometric biosensor has been developed for the detection of estrogen hormone 17b-estradiol. The electrochemical biosensor has been fabricated by immobilizing both estrogen receptor-a and bovine serum albumin on gold electrode surfaces. The binding of 17b-estradiol to the estrogen receptors on the fabricated biosensor has increased the electron-transfer resistance which has been directly monitored by electrochemical impedance spectroscopy in the presence of 5.0 mM $K_3Fe(CN)_6/K_4Fe(CN)_6$ (1:1, v/v) redox couple. The association constant between the 17b-estradiol and the estrogen receptors has been found to be ca. $1.8\times10^{11}M^{-1}$, which indicates that the estrogen receptors are well formed on gold electrode surfaces not only with high density but also with good specificity to its corresponding 17b-estradiol. The present biosensor gives a linear response (r^2 = 0.992) for 17b-estradiol concentration from 1.0×10^{-13} to 1.0×10^{-9} M with a detection limit of 1.0×10^{-13}M (S/N = 3), which is much lower compared to those obtained with other detection methods. The present biosensor exhibits good stability, in which the biosensor has retained 88 % of its initial activity after 3 weeks of storage in 50 mM phosphate buffer at pH 7.0.

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Synthesis of Cu2O/SiO2 Core-shell using the sol-gel process

경동현 윤혜수 김종규

단국대 화학과

Core-shell particles of Cu2O/SiO2 were synthesised via two-step process. First, particles of Cu2O were synthesised via sol-gel process. The Cu2O precursor was prepared with Copper acetate monohydrate, oleic acid and D-(+)-glucose. Secondly, uniformly shelled Cu2O with SiO2 synthesized with tetraethyl orthosilicate(TEOS). So, a very thin SiO2 condensed on the Cu2O. By repeating this process, particle size and morphological changes were examined by increasing the thickness of the SiO2. Observed changes in the surface of the product were characterized by using scanning electron microscopy (SEM). The crystallization mechanism and the chemical composition were investigated with X-ray diffraction (XRD).

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Studies of Reaction Mechanism on the Solvolyses of Allyl Chloroformate

고한중

전주교육대 과학교육과

The solvolysis rate constants of allyl chloroformate in 30 different solvents are well correlated with the extended Grunwald-Winstein equation, using the N solvent nucleophilicity scale and Y solvent ionizing scale, with the sensitivity values of 0.93±0.05 and 0.41±0.02 for l and m, respectively. These l and m values can be considered to support a SN2 reaction pathway. The activation enthalpies and the activation entropies which is also consistent with the proposed bimolecular reaction mechanism. The solvent kinetic isotope effect of 2.16 was also in accord with the SN2 mechanism. The values of product selectivity (S) for the solvolyses of allyl chloroformate in alcohol/water mixtures was 1.3 to 3.9, which is also consistent with the proposed bimolecular reaction mechanism.

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Label-Free Molecular Histology by Coherent Raman Microscopy

임상현 김형훈[1] 김선만[2]

광주과학기술원 환경공학부 [1]광주과학기술원 화학소재전공 [2]광주과학기술원(GIST) 화학소재전공

Coherent Raman Microscopy (CRM) can map out distributions of multiple chemical species via intrinsic vibrational responses of sample molecules, thus allowing label-free observation of the chemical distributions in cells and tissues. We have developed a novel CRM method that can rapidly obtain distributions of lipids (fat cell or sebaceous gland) and proteins (Collagen or Keratin) through their characteristic vibrational spectra. Our CRM method allows us to observe cells or tissues without any staining nor sample preparation. Technical details and preliminary histology data will be presented.

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Crystal growth of Zinc Oxide coating ITO glass as using spin coater

박병천 진훈열 김종규

단국대 화학과

Zinc Oxide(ZnO) thin film has the way of applications such as dye sensitized solar cell, photo diode device, gas sensor and piezoelectrode etc. Method of basic pre-treatment is of coating on substrate before devices are made. To study basic theory of coating technology, spin coater was used which relatively has a lower operating cost than existing coating equipment compared to thermal decomposition, beam sputtering. The ZnO was synthesized on Indium Tin Oxide(ITO) glass at different rpm times using spin coating. ZnO sol was dropped on ITO glass by using Micropipette. Crystalline structure and components of ZnO on ITO glass was identified through X-ray diffraction(XRD). Tendency of layer growth was found as applying debye-scherrer equation. Surface morphology and cross section of selected area were obtained by operating field emission scanning electron microscopy (FE-SEM).

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Thermogravimetric investigation of volatility of dioctyl phthalate on plasticized PSSA ionomers.

고광환 박혜련[1] 김준섭[2]

조선대 첨단부품소재공학과 [1]조선대 화학과 [2]조선대 응용화학소재공학과

Ionomers are polymeric materials containing small amounts of ionic groups em bedded with relatively less or non-polar polymer matrix. The process of volatilization of dioctyl phthalate (DOP) plasticized poly(styrene-co-styrenesulfonate) ionomers was studied by the method of isothermal thermogravimetry in the temperature range of 80-150 ℃. Addtion level of DOP to ionomers are 0, 5, 10, 20, 30 wt%. The rate constant of the process can be regarded as the characteristic of the physical process of DOP volatilization on plasticized PSSA.

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Preparation and Characterization of Photofunctional Film for the Bio-applications

김봉진 왕강균 손현아 김용록

연세대 화학과

Reactive oxygen species (ROS) are utilized in various fields due to their high activity and good selectivity. ROS can be generated by hydrogen peroxide or Fenton reactions, and also photo-physical reactions. The advantage of photo-induced ROS generated from energy transfer and/or charge transfer processes of photo-exited photosensitizer (PS) is the control factor of ROS generation which depends on photon power and irradiation time. In order to have such control factor in precise way, all other subsidiary factors are removed by isolating the PS in the inert environment of polymer, resulting the photofunctional film. The photo-physical properties of the fabricated photofunctional films were investigated by various time and steady state spectroscopies. The films were applied to the inactivation study of cells, which is affected only by the induced ROS, excluding the cell uptake factor, etc. The purpose of the study is to demonstrate that such photofunctional film can be utilized for medical applications.

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Photodissociation dynamics of oxalyl bromide at 234 and 265 nm

Paul Dababrata 김현국 이경석[1] 김태규

부산대 화학과 [1]한국표준과학연구원 분석화학표준센터

The photodissociation dynamics of oxalyl bromide at 234 and 265 nm have been investigated using a velocity mapping technique coupled with a state-selective [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme. To obtain the detail dynamics, the translational energy distribution and recoil anisotropy of Br(^2P_J , J = 3/2, 1/2) atom formation process are extracted from the acquired two dimensional ion images. The nascent Br($^2P_{3/2}$) atoms stem from the primary C?Br bond fission as well as secondary dissociation of their corresponding C_2O_2Br radicals which are energized from the ultrafast primary photodissociation steps at both excitation wavelengths. On the basis of the proposed mechanism in the formation of each component, the ultrafast primary one of the C?Br bond dissociation of $C_2O_2Br_2$ leads to the high velocity component and other translation distributions are originated from the subsequent secondary dissociation of C_2O_2Br radicals (from primary Br and Br^* pathways).

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Investigation of ciliary substructure using STED nanoscopy

김남두 김형준 김성근[1]

서울대 화학부 [1]서울대 화학부, 서울대 생물물리 및 화학생물학과

Primary cilium is a microtubule-based subcellular organelle which is critical to cellular signaling processes. Abnormality of proteins in cilia leads to many human diseases including retinal degeneration, cystic kidney disease, skeletal defects, and obesity. There are nine microtubule dimers that make up the core structure, which has been elucidated by electron microscopy and fluorescence microscopy. However, ciliary substructure remains unclear to date due to its small size (< 100 nm). Here, we investigated the ciliary substructure with STED nanoscopy to understand the origin of selective transport between cytosol and primary cilium.

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

Designing the size of nanorings by peptide self-assembly

박성병 신석민

서울대 화학부

Interests in artificial bio-nanostructures, including peptide-based nanostructures, have been very intense. Controlling the sizes of bio-nanostructures is very important for various applications. Recently, nanorings with highly uniform diameters were synthesized from self-assembling β-sheet-forming peptides (WKWEWYWKWEW) with the hydrophilic oligoether dendron. We have performed MD simulations, using all-atom AMBER force field 96 under the implicit solvation condition, on the various β-barrel like peptides with the selective W to F mutations. It was found that nanorings with different sizes can be obtained by introducing such mutations. Smaller nanorings with the inner-pore diameters of ca. 2-4 nm were obtained after all or half of TRPs were replaced by PHEs. Analyses for the simulation results suggest that important factors determining the β-barrel like structures include H-bonding between backbones of monomers, the electrostatic interactions between Lys and Glu residues, and the alignments of aromatic rings in TRPs or PHEs. Understanding the basic driving force for peptide self-assembly is expected to be useful in designing new functional bio-nanostructures.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Supercapacitors based on reduced graphene oxide electrodes in organic electrolyte: A computer simulation study

박상원 정연준 Hyung J. Kim[1]

서울대 화학부 [1]Department of Chemistry, Carnegie Mellon University, USA

Supercapacitors with two reduced graphene oxide (RGO) electrodes in the parallel plate geometry are studied via molecular dynamics (MD) computer simulations varying coverage of hydroxyl groups attached on graphene sheets . A 1.1 M solution of 1-ethyl-3-methylimidazolium tetrafluoroborate ($EMI^+BF_4^-$) in acetonitrile are considered as prototypes of organic electrolytes. Electrolyte structure, the number of hydrogen bonds, charge density, and associated electric potential are investigated by varying the charges of the two electrodes. Multiple charge layers formed in the electrolytes in the vicinity of the electrodes are found to screen the electrode surface charge almost completely. As a result, the supercapacitors show nearly an ideal electric double layer behavior, i.e., the electric potential exhibits essentially a plateau behavior in the entire electrolyte region except for sharp changes in screening zones very close to the electrodes. Due to its small size and large charge separation, BF_4 is considerably more efficient in shielding electrode charges than EMI^+. Acetonitrile also plays an important role by aligning its dipoles near the electrodes; however, the overall screening mainly arises from ions. The protruding structure of hydroxyl groups in graphene sheets hinder the opposite ions from layering near the electrodes, which makes capacitance lower as the coverage of hydroxyl groups increases. At lower OH coverage anions screen more effectively than cations due to its small size and hydrogen bonding, but at higher OH coverage hydrogen bonding does not affect the capacitance. Ion conductivity obtained via the Green-Kubo (GK) method is found to be largely independent of the electrode surface charge and OH coverage.

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발표코드: **PHYS.P-425**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction of Polyethylene glycol (PEG) with Water Solvents and its Osmotic Behavior

신혜영 김형준 William A. Goddard[1]

KAIST EEWS 대학원 [1]California Institute of Technology

Understanding of polymer-water interaction has its own importance for various applications in pharmaceutical excipients, water-soluble packaging, polymer based forward osmosis technique, and etc. However, detailed investigation of the structure of the water soluble polymer and its interaction with water solvent molecules from the atomistic level has been limited from experimental techniques (e.g. SLS or SANS), when the polymer density is above the dilute regime, and also limited from theoretical calculations for the large size of polymers (due to the computational cost). Here, we develop a new computational protocol to sample polymer configurations having a wide range of sizes in solution phase by introducing a concept to scale the non-bond interactions between atoms, named as a scaled non-bond cohesive energy density (SNB-CED) method. By using this method combining with first-principle based force fields, we extensively study the structural dynamics of PEG-20kDa in aqueous solution, its interaction with water, and thermodynamic changes using two-phase thermodynamic (2PT) method. We find that the strong solvation interaction is developed by forming a shell structure covering the polymer backbone surface. This enables the substantial fluctuation of PEG configurational dynamics, but simultaneously immobilizes the water molecules reducing the entropy of the system. Without considering this entropic cost term, we find that the conventional Flory-Huggins (FH) theory cannot explain the experimental osmotic behavior of PEG, hence, we suggest a modified FH model to include the entropic cost term that is quantized by using 2PT analyses.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical Properties and Photodynamic Activity of Pheophorbide-a Derivatives

황정욱 왕강균 정승진 송형완 이창희[1] 김용록

연세대 화학과 [1]강원대 화학과

Photodynamic therapy (PDT) is a recently developed method for an alternative clinical cancer treatment. It has been focused to the selection of effective and selective photosensitizers. One of the most desirable properties is the long-wavelength absorption of photosensitizers since light penetrates the tissue more deeply with minimal light loss to biological cells in long wavelength region. The high singlet oxygen quantum yield of photosensitizer is also desirable due to its high tumor killing efficiency. This study provides the discussion on the photophysics of the pheophorbide-a derivatives (PaDs) which are excited by red light and relates the properties to their photodynamic biological activity *in vitro*. The steady-state and time-resolved spectroscopies resulted the lifetimes and quantum yields of the fluorescences, and the quantum yields of the triplet states and the singlet oxygen. In addition, the killing efficiency of tumor cell was also investigated with respect to the singlet oxygen quantum yields of PaDs. Understandings of the photodynamic factors are one of the important factors for the development of the photosensitizer that is effective for a specific application of PDT.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-resolution fluorescence microscopy for morphological image processing of amyloid fibrils

허현 이진우[1] 홍성철[1] 김성근[2]

서울대 화학부 [1]서울대 물리학부 [2]서울대 화학부, 서울대 생물물리 및 화학생물학과

Fluorescent microscopy has two distinctive advantages, non-destructivity and high detection efficiency, which enable visualization of living cells and their structures. Sub-diffraction-limit optical nanoscopy further enhances the above merits of fluorescence microscopy. In order to address the pathological effects of molecular aggregates, in particular amyloid fibrils and oligomers, we introduce a high-resolution optical nanoscopic technique called binding assistant localization microscopy (BALM) using fibril specific binding dyes.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

KPACK: Relativistic Two-component *Ab Initio* Electronic Structure Program

김인구 이윤섭

KAIST 화학과

We report a newly developed relativistic electronic structure program package: KPACK, designed for the two-component *ab initio* calculations in either Kramers restricted or unrestricted formalism in the framework of relativistic effective core potentials, and intended for the molecular calculations containing heavy atoms, for which the effect of spin-orbit coupling is significant. The spin-orbit coupling is entered into calculation at the HF stage and therefore, treated in a variational manner. The two-component molecular spinors are generated as the one-electron eigenfunctions, which are then utilized for the correlated calculations. As correlated methods, KPACK provides the two-component MP2, CI and CASSCF methods.

K Relativistic
Two-component
Ab initio
PACK Electronic structure program

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장소: 부산BEXCO
발표코드: **PHYS.P-429**
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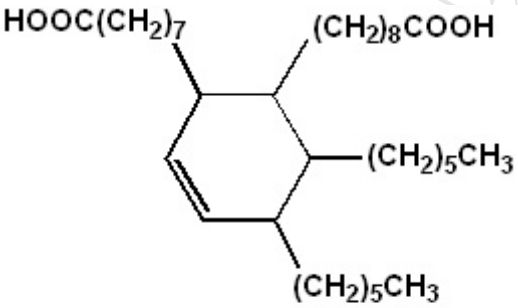
발표종류: 포스터, 발표일시: 수 16:00~19:00

A study of thermogracimetic of volatility on the vegratable-oil based Na-neutralized aromatic dicarboxylate of styrene ionomer.

고광환 박혜련[1] 김준섭[2]

조선대 첨단부품소재공학과 [1]조선대 화학과 [2]조선대 응용화학소재공학과

Since recently environmental regulations on industrial consumption have been tightened up, our research team have been working on the developement of vegetable oil-based environmental-friendly products. In the present work, we investigated the process of loss of plasticizer from PSSA ionomers using method of isothermal thermogravimetry in the temperature range 80-150 ℃. The samples contained ca, 0-40 wt% dimer acid. The rate constants of the process of loss of plasticizer were calculated and the dependence of the rate constant on temperature. On the initial concentration plasticizer in plasticized PSSNa ionomer were mathematically defined.



monocyclic

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-430**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Manganese Doping on the Hematite Single Crystal: Band Gap Energy and Size

노현석 차현길 강영수

서강대 화학과

We have developed a hydrothermal process to synthesize crystalline manganese doped Fe2O3 crystals and control their morphology. Manganese doped hematite crystals were prepared in an aqueous solution containing iron chloride and sodium hydroxide at 150 ?C for 4 h with additional transition metal solution. Mn:Fe2O3 crystals having cubic shapes were homogeneously nucleated and precipitated in solution. Crystal growth and preferential growth facets were controlled by the concentration of adding metal solutions. Morphological control in this system will contribute to the development of solution chemistry for inorganic materials and future metal oxide devices. Morphology and crystal structure of the obtained product was comparatively with XRD, TEM, SEM, and XPS.

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발표코드: **PHYS.P-431**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

염기성을 갖는 MOFs의 합성, 안정성 및 특성 연구

전재우 정성화

경북대 화학과

Zirconium 과 1,4-benzendicarboxylate (BDC) 이 반응하여 만들어지는 다공성을 가진 구조체인 UiO-66 에 amino group 의 contents 를 달리하는 UiO-66s (UiO-66, UiO-66-NH2)를 합성하여, amino group 의 contents 에 따른 합성 속도의 차이를 조사하였다. 합성 된 UiO-66 와 UiO-66-NH2 의 amino group 의 contents 에 따른 특성과, 산성 및 염기성 조건 그리고 열에서의 안정성 차이를 분석하였고 흡착 및 반응에 미치는 염기성 작용기의 효과를 연구하였다.

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발표코드: **PHYS.P-432**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Photofunctional Nanocomposites and Their Bio-application of Anti-microbial Effects

신언필 왕강균 진형빈 김용록

연세대 화학과

The continuous spread of microbial pathogens with antibiotic-resistance has led to a growing interest in the design and development of new materials that are effective in elimination of harmful organisms. Photodynamic Inactivation (PDI) is a promising approach for elimination of antibiotic-resistant harmful organisms. Targeting of therapeutic agent to the harmful organisms is required to improve efficiency and avoid possible damage of normal organisms. In this study, we synthesized the nanocomposites (Fe_3O_4@PS/RP) conjugated with photosensitizers (PS) and receptor proteins (RP) and characterized to check the application possibility as a new and effective antimicrobial therapeutic agent. The nanocomposites are capable of selective elimination of harmful organisms from aqueous solution. As the specific harmful organisms are exposed to the appropriate wavelength, the nanocomposites localized to the harmful organism surface effectively eliminate them at a low power density light. Such novel nanocomposites can be applied in various medical applications, such as in magnetic resonance imaging (MRI) diagnosis, bio-separation, target delivery, and PDI.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Kinetic Studies of Type II Restriction Enzyme on Methylation Modified Recognition Site Using Total Internal Reflection Fluorescence

박소영 김성근[1]

서울대 화학부 [1]서울대 화학부, 서울대 생물물리 및 화학생물학과

TIRF (Total Internal Reflection Fluorescence) is a useful tool to verify the dynamics of a hundreds of nanometer proteins at a single molecule level. In this experiment, we try to discriminate multiple steps of restriction enzyme on a methylated recognition site. Type II Restriction enzyme cleaves the specific site after recognizing short sequences. First, fluorescent dye labeled DNA was immobilized on the quartz. When the restriction enzyme binds to the specific site on DNA, the fluorescence signal increases and it decreases as it cleaves and dissociates the DNA. As a result, the binding and cleavaging rate can be calculated and the methylation effect on kinetics of restriction enzyme can be more accurately understood.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Laser-Induced Breakdown Detection of Capillary Electrophoresis for Nanoparticle Analysis

이자연 최중길

연세대 화학과

The Laser-induced Breakdown Detection (LIBD) technique has been known to possess a remarkably low detection limit of several nanometer size and ppt concentration range for the nanoparticles. From previous study in our laboratory, it has proved that the LIBD system can distinguish the size difference of 14 nm for the aqueous polystyrene particles. In this report, we introduce the capillary electrophoresis (CE) to the LIBD method to detect the size-mixture of nanoparticles more effectively. Firstly, the mixture of polystyrene nanoparticles in different sizes is separated in time by the CE. The single sized sample separated is then detected at the end of the capillary by the LIBD, using specially designed the waste reservoir of CE as a detection cell. This study sequentially demonstrates the use of a CE-LIBD complex system to detect nanoparticle mixture according to the sizes of samples as well as to the nature of materials with high efficiency and selectivity.

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발표코드: **PHYS.P-435**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Removal of benzothiophene from fossil fuel by liquid phase adsorption over copper-benzenetricarboxylate loaded by phosphotungstic acid

imteaz ahmed Nazmul Abedin Khan 정성화

경북대 화학과

Sulfur compounds affect drastically to the environment and currently the removal of these compounds from fossil fuel is a great concern [1]. To understand the effect of adsorption of basic contaminants over phosphotungstic acid (PWA), liquid phase adsorption of benzothiophene (BT) was carried out over PWA loaded copper-bezenetricarboxylate (Cu-BTC, a porous metal-organic framework) [2]. The maximum adsorption capacity (Qo) increases upto 26% with increasing PWA loading up to a W/Cu (wt./wt.) ratio of 0.22 in PWA/Cu-BTCs compared with virgin Cu-BTC. The surface area and pore volume of virgin and PWA loaded Cu-BTC was nearly same. So, there is some effect of PWA over the increase of the adsorption and this can be explained by acid-base interaction between acidic PWA and basic BT [3]. Based on this result, it can be suggested that MOF (metal-organic framework)-type materials, modified suitably, can be used in the adsorptive desulfurization of fuels.AcknowledgementThis 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 (grant number 2012004528). References[1] V.C. Srivastava, RSC. Adv. 2 (2012) 759. [2] N.A. Khan, S.H. Jhung, Fuel Process. Technol. 100 (2012) 49?54.[3] Y. Yang, H. Lu, P. Ying, Z. Jiang, C. Li, Carbon 45 (2007) 3042?3044.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Implications of the Dye-Iodine Interactions on Open-Circuit Voltage in Dye-Sensitized Solar Cells

김동희 Mannix Balanay Enopia Camille Marie 이상희

군산대 화학과

We presented a computational investigation based on density functional theory to model the dye-iodine interactions in organic dye-sensitized solar cells. We evaluated the binding of I2 to the various electron-donating sites in organic sensitizers, such as in thiophene, furan, or cyano moieties. We consider the extent of I2 binding between the furan- and thiophene-containing dyes in order to explain the decrease of the open-circuit voltage observed in thiophene-containing dyes. Our results indicated that the thiophene-containing dye has a greater tendency to form charge-transfer complexes with I2 species in the electrolyte rationalizing the increase in charge-recombination.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

다공성 Cr-benezenedicarboxylate를 이용한 bisphenol-A 흡착 제거

박은영 정성화

경북대 화학과

Chromium 과 benezenedicarboxylate (BDC) 이 반응하여 만들어지는 다공성을 가진 구조체인 MIL-53(Cr)을 합성하여 이를 bisphenol-A 의 흡착실험에 적용하였다. Bisphenol-A 의 농도변화와 흡착 시간을 변화시켜 MIL-53(Cr)를 이용한 bisphenol-A 의 흡착량을 조사하였다. Bisphenol-A 의 농도가 증가할수록, 흡착 시간이 길수록 MIL-53(Cr)에서의 bisphenol-A 의 흡착량이 증가되는 경향을 보였다.MIL-53(Cr)은 다른 구조체인 MIL-100s, MIL-101(Cr) 들에 비해 bisphenol-A 의 높은 흡착량을 보였다. 또한 MIL-53(Cr)은 전형적인 흡착제인 활성탄에 비해서도 우수한 흡착 결과를 보였다. MIL-53(Cr)를 이용한 bispheol-A 의 흡착실험을 다양한 온도에서 수행하여 흡착의 열역학적 인자도 연구하였다.

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발표코드: **PHYS.P-438**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Photosensitized TiO_2-based Multicomposite Photocatalysts

김혜리 임지은 **LIJING** 김용록

연세대 화학과

Titanium dioxide (TiO_2) has widely used in photocatalysis because of its high photocatalytic activity and durability. Many researches have been performed to enhance photocatalytic efficiency of TiO_2. In this study, we synthesized porous TiO_2-based multicomposite photocatalysts. The morphology was characterized by SEM, TEM, XRD and BET. The photophysical properties of the TiO_2-based photocatalysts were characterized by UV?Vis spectrophotometer and spectrofluorometer. The fabricated muticomposite photocatalysts are expected to improve visible-light photocatalytic activity due to their large surface area and wide range of absorption spectra.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermodynamic stability of gas hydrates for CO_2 exchange: Molecular dynamics study

엄태대형 김형준 William A. Goddard[1]

KAIST EEWS대학원 [1]California Institute of Technology

To improve the sustainability of human beings, capturing and storing technology of carbon dioxide have been great importance. One interesting and promising idea here is to replace the methane hydrate in the deep ocean to carbon dioxide in order to (1) store the CO_2 while making (2) CH_4 to be available. To investigate this swapping mechanism from the atomistic level, it is important to understand how the carbon dioxide hydrate can be more stabilized over the methane hydrate in terms of free energy quantities. Here, we carried out molecular dynamics (MD) simulations to study the effect of guest molecules in the thermodynamic of gas hydrate systems. We used two-phase thermodynamics theory for fast and accurate evaluations of free energy values. From the atomistic MD simulations, we figured out the different entropy of the guest molecules leads the relative stability among the gas-hydrate systems, leading the swapping from methane to CO_2 to be possible.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

질량분석실험을 통한 amyloid fibril structure을 형성하는 활성 peptide oligomer인 VEALYL와 NFGAIL의 초기 stacking structure pattern 연구.

김수아 이은숙 강예송 김호태

금오공과대 응용화학과

당뇨병, 알츠하이머병들의 공통점은 활성 peptide oligomer 들이 amyloid fibril structure 을 형성한다는 것이다. 본 연구는 amyloid fibril 을 형성하는 것으로 알려진 peptide oligomer VEALYL 과 NFGAIL 의 질량분석기 실험을 통하여 VEALYL 와 NFGAIL 의 초기 stacking structure 을 알아보려는 시도를 하였다. ESI Mass Spectrometer 을 이용하여 VEALYL 와 NFGAIL 의 MS 실험과 MS/MS 실험을 진행하였다. Gaussian program 을 이용하여 각 oligomer structure 의 안정화 energy 를 구하고, 실험결과의 설명에 적합한 구조를 찾는 시도를 하였다.

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장소: 부산BEXCO

발표코드: **PHYS.P-441**

발표분야: 물리화학

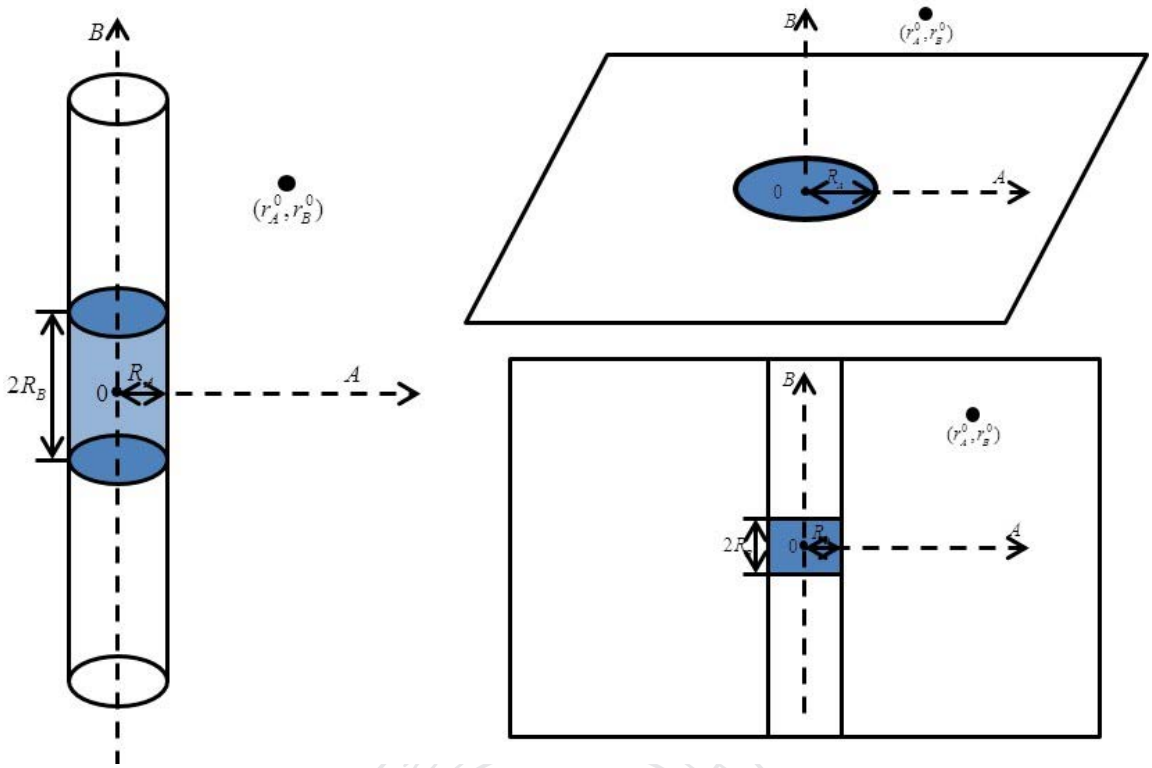
발표종류: 포스터, 발표일시: 수 16:00~19:00

Generalized theoretical and computational approaches for dimension reduction problems in biological reactions

김태준 김효준

동아대 화학과

The generalized theoretical and computational approaches are presented to study facilitated diffusion effects on ubiquitous dimension-reduction problems, which include the protein-DNA binding, the plane-meditated diffusion, and line-meditated surface diffusion models. This rigorous theoretical approach can deal with the coupling between diffusive motions of two subsystems. For a simplified model, we show that the approach predicts numerically exact results by comparing with results of the lattice-based Monte Carlo simulations.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure and electronic properties of endohedral C20 and C20H20 complexes and its ions with H2, H3, HF, and N2

전성기 조인수[1] 이설 이기학[1]

원광대 생명나노화학부 [1]원광대 화학과

Structures of endohedral doped C20 and C20H20 fullerenes and its ions with H2, H3, HF, and N2 were optimized with the B3LYP hybrid density functional method and the 6-31G(d,p) basis set. We have also investigated electronic properties. For endohedral complexes, charge transfer is from H3 to cage, but it is reversed in the other doped molecules. We discussed the change of bond lengths of encapsulated molecules in cages.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

How can we relate the experimental reaction rate to the reaction probability in Monte Carlo computer simulations?

안서연 김효준

동아대 화학과

Even though the imperfect trap problems have a large variety of applications in physics, chemistry, and biology, it is not easy to relate the experimental reaction rate to the reaction probability in computer simulations since the relationship between the two is ambiguous yet. By comparing theoretical and simulation results, we try to establish the simple relationship between two parameters in one, two, and three regular dimensions. This can increase greatly the versatility of the lattice-based Monte Carlo simulation methods to be straightforwardly applied to more realistic diffusion-reaction systems.

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발표코드: **PHYS.P-444**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparative Kinetic Studies of Photo-induced Reactive Oxygen Species in Solution

정지혜 왕강균 김봉진 김용록

연세대 화학과

Reactive oxygen species (ROS) have been widely studied for the applications of photodynamic therapy, wastewater purification, stereospecific synthesis of organic compounds. The photo-induced ROS are initially 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. The quantitative and qualitative analyses for the effects of the two components are not yet investigated in details. In this study, we carried out chemical kinetic analyses with photolysis experiments by using different types of ROS generating photosensitizers and a ROS indicator in solution. The photochemical kinetic analyses were also investigated with time resolved near IR spectroscopy. From the results, we could determine the quantitative decomposition mechanisms of singlet oxygen and super oxide radical molecules in solution phase. We believe that this study provides the valuable fundamental information on the many application researches based on photo-induced ROS generation.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

H2O@C24 와 CH3@C24에 대한 원자구조와 안정도

전성기 이설 황용규[1] 이기학[2]

원광대 생명나노화학부 [1]원광대 반도체.디스플레이학부 [2]원광대 화학과

혼성 범 밀도 함수법(B3LYP/6-31G(d,p))을 사용하여 H2O@C24 와 CH3@C24 의 원자 구조와 안정도를 Gaussian 03 프로그램을 이용하여 수행하였다.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An Efficient Synthesis and electronic properties analysis of ZnP-Tri-SWNT via Click Chemistry

WENPING YIN YanCui 신희원[1] 양정운 안태규

성균관대 에너지과학과 [1]성균관대 신개념융복합에너지과학연구소

The most ambitious target of artificial photosynthetic mimics is to get the greatest extent of charge separated (CS) net rates. In this work, we have synthesized a triazole-based electron donor-acceptor conjugate, which connected zinc(II) porphyrin (ZnP) and single wall carbon naotube (SWNT) through a central triazole moiety (Tri) using click chemistry method. According to XPS, FTIR, Photoluminescence and TCSPC and transient absorption analysis, there is a rapid excited-state deactivation of ZnP via through-band photoinduced charge transfer to SWNT, which in return, indicates the electronic properties of the ZnP-Tri-SWNT conjugate.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Field Effects in one-dimensional Monte Carlo Simulations

허윤석 김효준

동아대 화학과

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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발표종류: 포스터, 발표일시: 수 16:00~19:00

Guest Changes Host : Gas Adsorption in Metal Organic Frameworks Shrinks Their Volume

주재용 한상수[1] 김형준[2]

한국표준과학연구원(KRISS) 나노소재평가센터 [1]한국표준과학연구원 나노소재측정센터
[2]KAIST EEWS대학원

Recently, metal-organic frameworks (MOFs) are receiving many attentions for hydrogen storage due to their remarkable porosity (*e.g.*, high surface area of ~10,000 m^2/g). Here, their crystalline structures are formed by using organic linkers and metal atoms or cluster. Until now, many researchers have tried to clarify the nature of the MOF-H_2 interaction by density functional theory (DFT) calculations. However, it is well-known that the DFT generally fails to describe accurately systems where the van der Waals (vdW) interactions are dominant. Here we show that DFT-ulg method in which corrections of the vdW interactions are added leads to accurate description of the hydrogen adsorption sites and binding energies in MOFs. According to our PBE-ulg calculations on MOF-5, H_2 adsorption energies are 5.5 kJ/mol for the Cup site, 5.4 kJ/mol for the ZnO_3, 4.8 kJ/mol for the ZnO_2, and 3.7 kJ/mol for the Hex, which is very close to the reported experimental value (4.7-5.2 kJ/mol). On the other hand, the LDA calculation tends to seriously overestimate H_2 binding (15.4 kJ/mol for the Cup site) and the PBE calculation underestimates H_2 binding (2.1 kJ/mol for the Cup site). These results indicate that DFT-ulg method is indeed very powerful to predict H_2 binding in MOF systems. Furthermore, we have found an interesting structural property of the MOF-5. Contrary to our intuition, the lattice parameter of MOF-5 is contracted upon H_2 uptake, where more H_2 loading leads to larger shrinkage.

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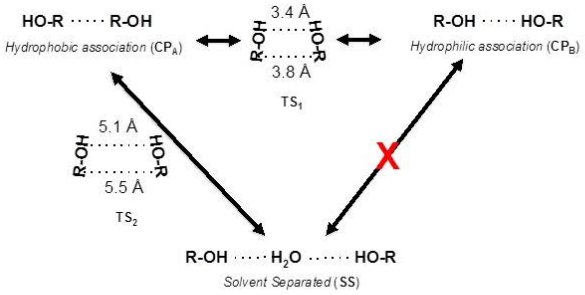
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrophobic and Hydrophilic Associations of Methanol Pair in Aqueous Solution

Manik Kumer Ghosh 최철호

경북대 화학과

The association dynamics of methanol pair in aqueous solution were theoretically studied with QM/EFP-MD and quantum mechanical methods. Stable contact pairs and solvent separated configurations (SS) were found from simulations with the free energy barrier of 2 kcal/mol, revealing the strong tendency of association. The stable contact pairs were further identified as the hydrophobic (CPA) and hydrophilic (CPB) species, with the CPA having a larger population. Although the free energy difference between the CPA and CPB is negligible with virtually no associated free energy barrier, the slow isomerization dynamics of intermolecular rotations ensures their individual identity. Preferred intermolecular torsional angle (C-O"?" O-C) of -60° ~ 60° in the contact pairs illustrates their restricted conformations due to the solvent. Further mechanistic analysis revealed that only the CPA has a direct path to the SS, showing that hydrophobic attraction initiates the association process. A subsequent intermolecular hydrophilic attraction isomerizes CPA and CPB. Therefore, our results show that both of the hydrophobic and hydrophilic attractions between methanol molecules play important roles in the association dynamics. The former operates on the longer intermolecular distance, while the latter is effective in contact pairs.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-450**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Kinetics and Mechanism of Reaction of 2-Adamantyl Chlorothioformate under Solvolytic Conditions and a comparison with 2-Adamantyl Chloroformate Solvolysis

양기훈 성미혜 박경호 경진범

한양대 응용화학과

The specific rates of solvolysis of 2-adamantyl chlorothioformate (2-AdSCOCl, 1) have been measured at 25.0^{o}C in hydroxylic solvents. These gave the satisfactory correlation over the full range of solvents when the exteded Grunwald-Winstein equation [log (k/k_o) = $lN_T + mY_{Cl} + c$], with incorporation of the solvent nucleophilicity and the solvent ionizing power, is applied. The selectivity values for reactions of 1 under solvolytic conditions in ethanol, TFE and ethanol-TFE mixtures and in a range of composition for binary aqueous mixtures with ethanol and TFE are calculated. The kinetic solvent isotope effect of 1 are similar to those previously observed for 1-adamantyl chlorothioformate solvolysis. The small negative values for the entropies of activation are consistent with the ionization nature of the proposed rate-determining step. These observations are compared with those reported earlier for 1-adamantyl and 2-adamantyl chloroformates.

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장소: 부산BEXCO

발표코드: **PHYS.P-451**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of 2-methylpyrazine

강도원 이지혜 홍용준[1] 황현석 김홍래 권찬호

강원대 화학과 [1]국방과학연구소 국방신기술센터/융복합기술부

One-photon mass-analyzed threshold ionization (MATI) spectrum of 2-methylpyrazine was obtained by using vacuum ultraviolet (VUV) radiation. The VUV radiation was generated by four-wave difference mixing in Kr. The adiabatic ionization energy of 2-methylpyrazine has been determined to be 9.0406 eV by field free approximation of the 0-0 band in the MATI spectrum. To analyze this spectrum, the quantum chemical calculation of vibrational frequencies and Franck-Condon factors was done at the B3LYP/cc-pVTZ levels. Several vibrational modes of 2-methylpyrazine in ionic ground state were assigned with the aid of the performed calculation. In particular, the prominent peaks in the spectrum were proved to the progression of the 6a mode.

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장소: 부산BEXCO

발표코드: **PHYS.P-452**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrical properties of honeycomb-patterned poly(ε-caprolactone)-reduced graphene oxide composite film

PHUNG XUAN THINH

인제대 화학과

In this study, a novel biocompatible composite of poly(ε-caprolactone) (PCL) was synthesized via in situ ring-opening polymerization method of ε-caprolactone monomer in the presence of reduced graphene oxide (RGO). Fourier transform infrared, and X-ray photoelectron spectroscopy (XPS) studies support a strong interaction between PCL and RGO. The crystallization behavior and thermal stability of these composites were studied using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), respectively. Honeycomb-patterned thin films were fabricated by casting the composite solutions under humid conditions. The scanning electron microscopy (SEM) images of the resulting honeycomb patterned films on the composites show a regular structure. The temperature-dependent DC conductivity of the honeycomb-patterned composite films was studied in the range of 290-330 K. DC conductivity of the patterned films was increased by increasing the concentration of RGO in the composites and in the increased temperature, which revealed a semiconducting behavior in the transport properties of the composite films. The prepared honeycomb-patterned composite films have many potential applications in biological, engineering, and medicinal fields.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Adsorption Reaction Mechanism of SO2 on Ice Surface: A Theoretical Study

Shoaib Mahbubul alam 최철호[1]

경북대 일반대학원 화학과 [1]경북대 화학과

Except in conditions of very low relative humidity, the atmospheric oxidation of SO2 to sulfuric acid is thought to occur predominantly within cloud droplets. The first step in this process is the entry of SO2 into the drop and its solvation and hydrolysis. At the molecular level the mechanism of SO2 hydrolysis is still unclear. Interestingly, recent studies suggest that an “SO2 surface complex” forms as a precursor to SO2 hydrolysis during the interaction of SO2 with water surfaces. We have carried out theoretical calculation of adsorption and reaction mechanism of SO2 on ice surface with the help of DFT/6-311++G(d,p) basis set. At first SO2 physically adsorbed on ice surface and then H2SO3 formed by chemical adsorption. Reaction barrier depends on surface heterogeneity as well as ice surface model and the net barrier of H2SO3 can be as low as 0.2 Kcal/mol. When another SO2 was added on preadsorbed H2SO3 afterwards, electron was passed and proton transfer occurred from H2SO3 to SO2 in the system and finally HOSO- and HSO3- can be found on the neutral surface. This reaction can be called Hydrogen Coupled Electron transfer (HCET) which can be important in the hydrolysis reaction. Furthermore, we have performed calculation of reaction mechanism of SO2 on Protonated ice surface.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Characteristics of biphenyl-2,2'-dicarboxylic acid adsorbed on silver surfaces: Comparing with the quantum chemical calculations

엄소영 김홍래 권찬호

강원대 화학과

Surface-enhanced Raman spectra of biphenyl-2,2'-dicarboxylic acid have been acquired by utilizing the colloidal Ag substrate nanostructured with the hot spot. The intuitively spectral feature revealed to the adsorption via the carboxyl group(s) tilt on silver surfaces from the appearances of the C-H stretching at 3054 cm^{-1} and the banding of the COO^- at 850 cm^{-1} in the SERS spectrum. However, the detailed vibrational assignments in the SERS spectrum of the large adsorbate such as the biphenyl derivative may be suffered in an effort to refer only the vibrational frequencies of the others. Thus, we demonstrate that the vibrational analyses in the SERS spectrum have been straightforwardly accomplished with the aid of the quantum chemical calculations of the Raman simulations related to the dihedral angles between two phenyl rings with each carboxylate form on Ag adatoms.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Estimating pka Values for acetic acid using ab initio Molecular Dynamics Simulations

Nizam Uddin 최철호[1]

경북대 일반대학원 화학과 [1]경북대 화학과

Accurate Prediction of the acidity dissociation constant (ka) is an important issue for the theory of proton transfer reactions, making first principle prediction of pka comparison with experimental values a benchmark of broad interest. The pka values are estimated by using QM/EFP Molecular Dynamics Simulation for the dissociation of acetic acid. The free energy profile for acid ionization and the corresponding pka values are calculated by QM/EFP molecular dynamics simulations utilizing the umbrella sampling technique by means of coordination constrained. The solvation state energy is determined for each component of the acid dissociation reaction.CH3COOH + H2O ? CH3COO- + H3O+The solution pka of acetic acid formed during the hydrolysis of acetic acid is estimated as pka=4.753

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Nanoparticle shape on the Plasmon-Enhanced Fluorescence

이은별 김지환[1]

고려대 [1]고려대 화학과

We investigated how the shape of the metallic nanoparticle influences the enhanced fluorescence of nearby molecules. For this end, nanoparticle@fluorophore core-shell structures are prepared. All of the nanostructures have similar diameters and similar dipolar resonances near the wavelength of 480 nm. The enhanced emission of individual structures are examined with correlated confocal / atomic force microscopy. We find that the nanoparticles with sharp edges show significantly brighter emission than in the case of smooth ones. The observed shape-dependent enhancement is likely to arise from the electromagnetic lightning-rod effect that occurs at the vertexes of the nanoparticles. Such enhancement in emission is compared with the numerical electromagnetic simulations.

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발표코드: **PHYS.P-457**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface-enhanced Raman scattering of 4-amino-4'-nitrobiphenyl on silver surfaces

류세림 이진철 김홍래 권찬호

강원대 화학과

We have measured the surface-enhanced Raman spectra of 4-amino-4'-nitrobiphenyl (ANBP) adsorbed on silver surfaces under the various pH conditions. The obtained SERS spectra have been analyzed with the aid of the Raman simulations and the normal modes obtained from the density functional theory (DFT) calculations for the molecules adsorbed on Ag adatoms. From the spectral analyses, the adsorption behavior of the ANBP on silver surface has been characterized to the changes of the orientation of the biphenyl ring against the silver surfaces according to the pH conditions. In addition, absence or presence of the C-H stretching bands in the SERS spectra was conclusively about the orientations of the ANBP adsorbed on silver surfaces.

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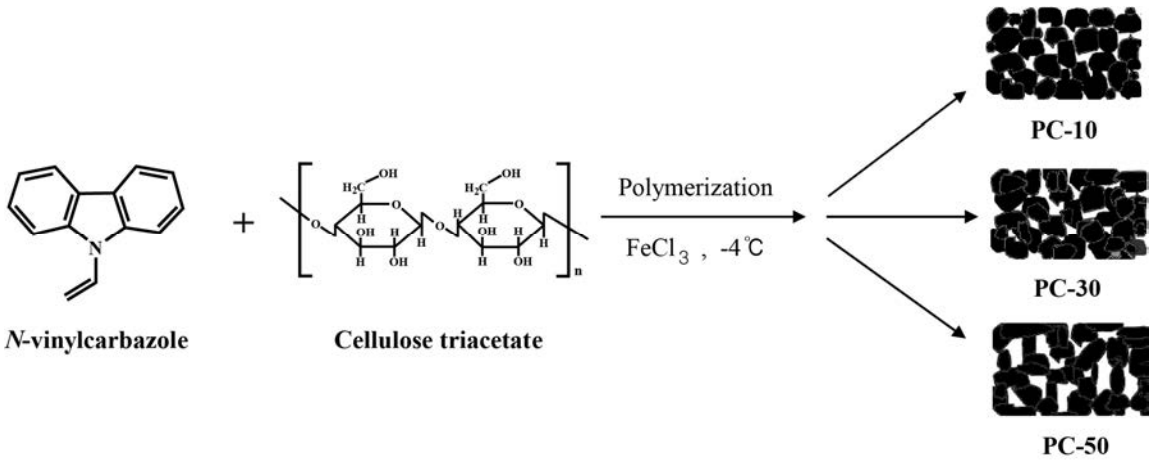
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of photo-controlled reduction of silver nitrate on honeycomb-patterned poly(N-vinylcarbazole)-cellulose triacetate composite thin films

김광일 노국태

인제대 화학과

Photo-controlled reduction of silver nitrate to silver nano-particles on the honeycomb-patterned poly(N-vinylcarbazole) (PVK)-cellulose triacetate (CTA) composite thin films was studies. The composites were prepared via the oxidative polymerization of N-vinylcarbazole with ferric chloride using different concentrations of CTA. Honeycomb-patterned film was fabricated by casting the composite solution under humid condition. The result showed that the homogeneously well distributed Ag particles were obtained by the composite film with a moderate concentration of CTA, however, aggregated Ag particles was observed in the film using so low concentration of CTA and under long time illumination.



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발표코드: **PHYS.P-459**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Excited-state Dynamics of Rhodamine 6G and DCM near plasmonic metal nanoparticles

이재범 이인구 이세복 박태리 방윤수

광주과학기술원 광공학응용물리학과

Metal-enhanced fluorescence (MEF) arising from the amplification of local electric field due to metal nanoparticles and plasmonic energy transfer from metal nanoparticles to chromophores can be useful especially for fluophores with low quantum efficiency. In order to find optimal nanoparticles/nanosurfaces for MEF of various chromophores, we synthesize various silver nanoparticles and nanosurfaces by reducing silver ions. Colloidal silver nanoparticles in a wide range of diameter (5-100 nm) have shown their absorption bands centered in the range of 380-460 nm. Very thin silver island films of absorbance maximum of 0.1-0.3 have shown the absorption band in 380-550 nm. We have observed enhancements in fluorescence and absorbance of various chromophores including rhodamine 6G, rhodamine B, and 4-dicyanomethylene-2-methyl-6-p-dimethylaminostyryl-4H-pyran (DCM) in the existence of colloidal silver nanoparticles and silver island films. Especially, silver island films are found to be most effective substrates for MEF of these chromophores. Transient absorptions and induced emissions from the excited states of chromophores near plasmonic metal nanoparticles have been measured to investigate ultrafast energy transfers between chromophores and silver nanoparticles and excited state dynamics of chromophores near metal particles.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-460**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photodissociation dynamics of H atom production from hydrogen peroxide at 205nm

박성만 강충만 권찬호 김홍래

강원대 화학과

Photodissociation dynamics of gaseous H_2O_2 at 205 nm has been investigated by measuring angular and energy distribution of H atom products. The spectrum of H was measured by laser-induced fluorescence from the 3s, 3d to the 2p state (Balmer-alpha line) induced by two photon absorption from the 1s state. Doppler profile analyses of the spectrum suggest that 1) the electronic transition of H_2O_2 at 205 nm should take place to mostly the A state where the transition dipole moment lies perpendicular to the O-O bond axis, 2) the dissociation should be fast along the repulsive potential energy surface, and 3) most of the available energy should be transformed into product translation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Early Detection and Small Molecular Inhibition Assay for Primary Aβ Aggregation Using Pyrene Fluorescence Analysis

이혜민 이민영[1]

이화여대 화학나노학과 [1]이화여대 화학나노과학과

This work focuses on the detection for the early stage of beta-amyloid (Aβ) aggregation and screening of its small molecular inhibitors through pyrene fluorescence analysis. Pyrene-labeled Aβ(11-25) (Py-Aβ) can be utilized to quantify the monomer-dimer equilibrium depending on the environments owing to the unique spectral features of pyrene. We developed the steady-state fluorescence assay system that is able to simultaneously monitor the time-dependent intensity of both monomer peak and excimer bands. We measured the aggregation inhibition efficiency of the drug candidates according to the excimer/monomer ratio, calculated by comparing the emission intensity of monomer peak with respect to the excimer band. Our assay explored a set of objectively chosen candidates that exhibit the high degree of anti-aggregation, which requires a molecular level understanding of small molcule-amyloid interactions.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

UV photolysis of ortho-halogenated thiophenol: Hydrogen bonding effect on photodissociation dynamics

유현식 임진선 김상규

KAIST 화학과

The experimental techniques of velocity-map ion imaging and resonance-enhanced multiphoton ionization spectroscopy have been used to investigate the dynamics of D atom loss processes from gas phase ortho-halogenated thiophenol-(d1), following photolysis at many wavelengths within the range of vibronic bands of S1 electronic state and further higher excited state. In case of 2-fluorothiophenol-(d1), a dependence of the relative yields of two reaction channels (ground and the first excited state of 2-FC6H4S? radical) is observed within S1 (ππ*) region. We've expected that molecular planarity by intramolecular hydrogen bonding of H???F affects bifurcation dynamics of the second CI, considering previous finding. And relative contribution of S1 (ππ*) & S2 (nσ*) electronic states is investigated along energetics. To shed light on this behavior, potential energy surface (PES) along related reaction coordinates (SD elongation & CSD bending angle & CCSD torsion angle), vertical excitation energy, Frank-Condon simulation and radical energetics are performed using CASPT2, SA-CASSCF, TD-DFT levels. According to chemical intuition, we are doing experiment on effects strength of hydrogen bond upon fragmentation mechanism using 2-chlorothiophenol-(d1). Comparison electronic spectrum of S1 (ππ*) state and branching ratio with the results of 2-fluorothiophenol-(d1) will serve to highlight intramolecular hydrogen bonding effect on photodissociation dynamics.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of pyrimidine

김재한 이지혜 홍용준[1] 황현석 김홍래 권찬호

강원대 화학과 [1]국방과학연구소 국방신기술센터/융복합기술부

Vibrational spectrum of the pyrimidine cation in the ground electronic state has been acquired by using a vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectrometry. From the observed MATI spectrum, the precise ionization energy of pyrimidine to the ionic ground state has been determined to be 9.3308 eV. In addition, the vibrationally resolved spectrum has been analyzed with the Franck-Condon analysis performed at the B3LYP/cc-pVTZ levels. Hence, the overall spectral feature in the 0～4000 cm^{-1} vibrational energy region was confirmed to the progression of the 6a mode caused by the structure deformation upon ionization.

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발표분야: 물리화학

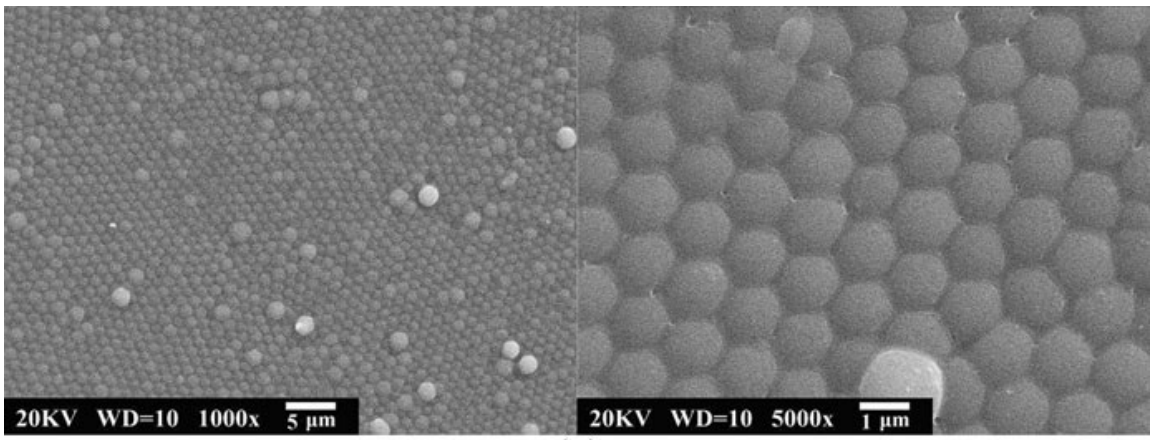
발표종류: 포스터, 발표일시: 수 16:00~19:00

characterization of smart hydrogel nanocomposites sensitive to oxidation-reduction

김진경

인제대 화학과

Honeycomb-patterned hydrogel films sensitive to environmental oxidation-reduction supporting nanoparticle by adsorption were fabricated through the photopolymerization of ruthenium(4-vinyl-40-methyl-2,20-bipyridine)bis(2,20-bipyridine)bis(hexaflurophosphate) and N-isopropylacrylamide. Nanoparticle adsorption by the hydrogel film was controlled by the dynamic changes in the surface morphology of the film in relation to environmental oxidation?reduction, which induces change ofthe oxidized and reduced states of ruthenium ion included in the hydrogel. For the adsorption of nanoparticles in the patterned hydrogel film, silver nanoparticles were immobilized in the hydrogel surface. Adsorptivity was obtained through measuring the released concentration of the silver nanoparticles using UV?vis spectroscopy in an aqueous solution. Desorption ofAg nanoparticles from the hydrogel surface was foundto be larger in the oxidizing solution than in the reducing solution.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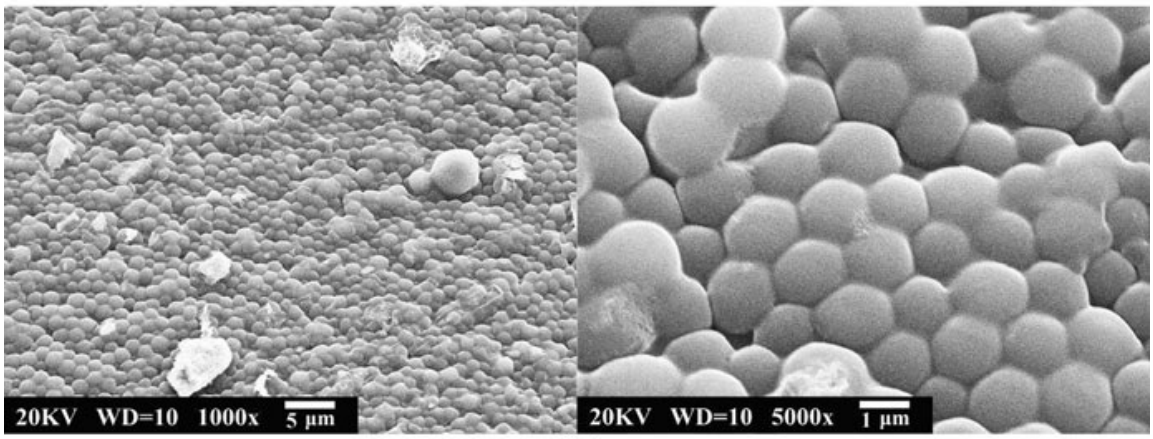
20KV WD=10 5000x 1 μm

(a)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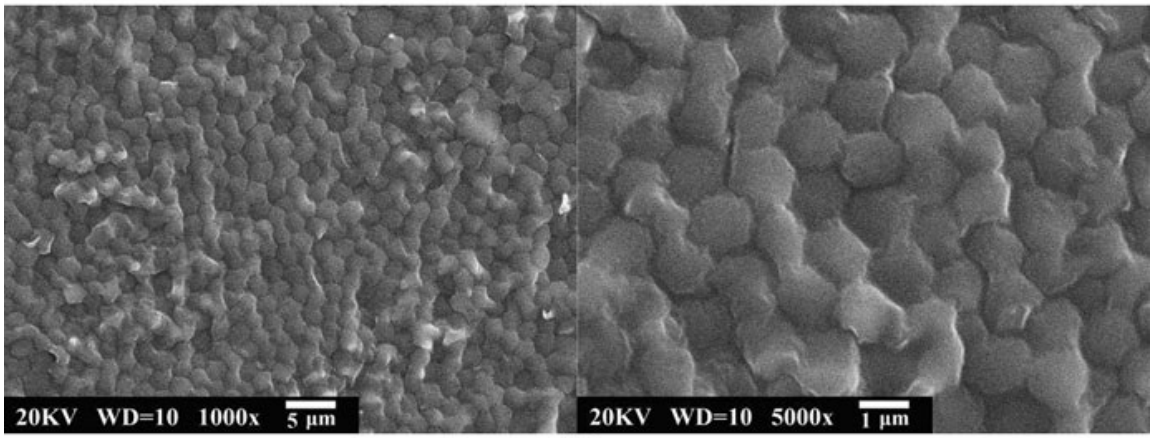
20KV WD=10 1000x 5 μm
20KV WD=10 5000x 1 μm

(c)

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Excited-state dynamics of Thioflavin T embedded in polymer nanowires

이유민 김유림[1] 김명화[2] 이민영

이화여대 화학나노과학과 [1]이화여대 자연과학대학 화학나노과학과 [2]이화여대 화학 나노과학과

Thioflavin T (ThT) is a fluorescence dye that has been used to probe formation of amyloid fibrils. The underlying mechanism is that the rigidness of amyloid aggregates blocks the internal twisting of the dye in the excited state. The increase of the fluorescence quantum yield or lifetime manifests the increase of the rigidity of the medium. This work first utilizes the photodynamics of ThT to investigate the mechanical properties of polymer. The poly(ethylene oxide) (PEO) and poly(acrylic acid) (PAA) fibers that contain ThT were prepared by electrospinning and the morphology of the sample was characterized by scanning electron microscopy. Subsequently, the excited-state dynamics of ThT in PEO and PAA fibers were elucidated by fluorescence lifetime imaging microscopy (FLIM). We have observed that ThT is an excellent dye to investigate the elastic modulus mapping of polymer fibers through FLIM.

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발표코드: **PHYS.P-466**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure and Dynamics of Nitroxyl(HNO) bound to Myoglobin

이태곤 임만호

부산대 화학과

Nitrosyl hydride (HNO) has been postulated to participate as an important intermediate in the heme-based catalysis involved in the global nitrogen cycle. Its interaction with heme or heme proteins was found to be fruitful in understanding biological nitrogen chemistry and identifying the elusive intermediate. HNO bound ferrous myoglobin (HNO-MbII) has been prepared by either reduction of NO bound ferric Mb with $NaBH_4$ or the trapping of HNO by deoxyMb. HNO-MbII was structurally characterized by ^{1}H NMR, resonance Raman, and X-ray absorption spectroscopy. Here, we prepared HNO-MbII and H^{15}NO-MbII and characterized the conformation of the protein by assigning the stretching mode of NO in HNO-MbII, which is located near 1350 cm^{-1}. Femtosecond time-resolved vibrational spectroscopy of NO mode after photoexcitation of HNO-MbII in D_2O with a 570 nm pulse showed instantaneous bleach in the NO fundamental mode that recovers on the picosecond time scale. More than 10% of the bleach does not recover in 1 ns, suggesting that some portion of HNO is photolyzed and does not rebind up to 1 ns. Full analysis of the time-resolved spectra and their implication will be presented.

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발표분야: 물리화학

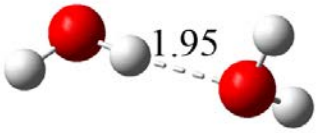
발표종류: 포스터, 발표일시: 수 16:00~19:00

Thoretical approach for the strucures, energetics and spectroscopic properties of $(H_2O_4)_n$ (n=1-3) clusters.

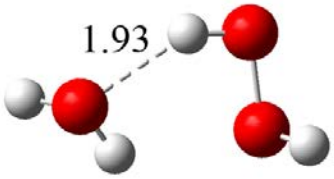
송희성 김승준

한남대 화학과

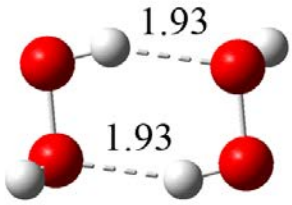
본 연구는 $(H_2O_4)_n$, (n=1-3)에 대해서 다양한 기저집합과 밀도 범함수이론(DFT)을 사용하여 최적화된 구조와 결합에너지, 조화진동수를 계산하였다. H_2O_3 와 H_2O_4 의 경우 trans 구조가 열역학적으로 가장 안정한 global minimum 으로 확인되었다. H_2O_4 의 여러 가능한 분자 구조를 최적화하고, 그 가운데 가장 열역학적으로 안정된 분자구조를 예측하였다. 이 때 이전의 DFT 방법에 대한 약점인 약한 결합을 갖는 클러스터들의 분자 구조를 정확히 예측하기 위하여 Gaussian 09 버전에서 long range interaction 을 보완하여 새로 제안된 DFT 방법 가운데 wB97X-D 및 MP2 방법 등을 사용하여 보다 정확한 구조적 특성과 결합에너지를 확인하였다. 나아가 H_2O_4-H_2O 의 결합에너지를 H_2O_3-H_2O 와 H_2O_2-H_2O 의 결합에너지 등과 비교 분석하여 용매 물속에서의 상대적인 열역학적 안정성 등을 연구하였다. 또한 H_2O_4-H_2O_n (n=1-4) 중합체의 결합에너지를 조사하여 수소결합의 세기와 열역학적 안정성을 예측하였다.



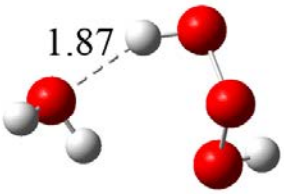
H_2O-H_2O



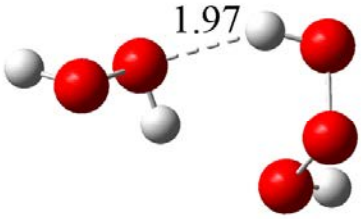
H_2O-H_2O_2



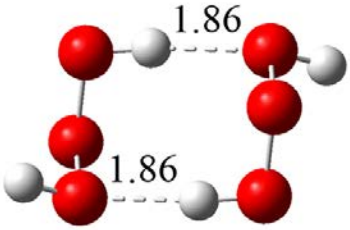
H_2O_2-H_2O_2



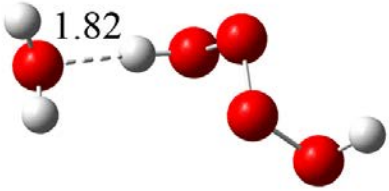
H_2O-H_2O_3



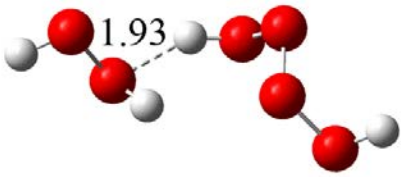
H_2O_2-H_2O_3



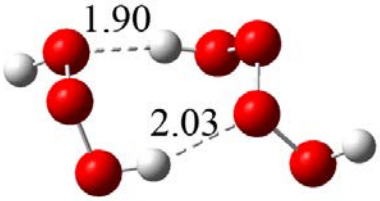
H_2O_3-H_2O_3



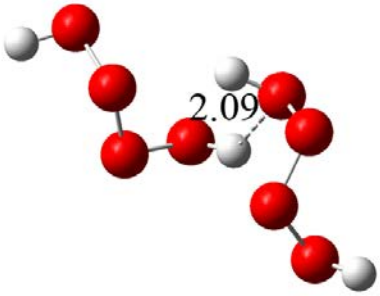
H_2O-H_2O_4



H_2O_2-H_2O_4



H_2O_3-H_2O_4



H_2O_4-H_2O_4

일시: 2012년 10월 17~19일(수~금) 3일간

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

General, quantitative description of the cell-to-cell variation of mRNA levels in E. Coli

박성준 임유림 성재영

중앙대 화학과

We present a new theoretical model for description of the cell-to-cell variation of mRNA level among isogenic cells. While most previous models in this field assume that the transcription dynamics for an activated gene is a simple Poisson process with a constant rate coefficient, the present theoretical model takes into account the dynamic fluctuation in the transcriptional rate coefficient of the activated gene, whose stochastic properties could be different from one system to another. We present exact analytic expressions for the mean and the variance of the cell-to-cell fluctuation in mRNA levels for the proposed model, and the prediction of our results is in an excellent agreement with the previously reported experimental data for m-RNA statistics for multiple promoters in E. Coli. We find that the fano-factor, or the standardized variance, of the m-RNA levels in the high expression limit increases with the fluctuation in the transcriptional rate coefficient of the activated gene, but decreases with the relaxation time scale of the transcriptional rate coefficient fluctuations and the lifetime of mRNA. Our analysis shows that fluctuations in the transcriptional rate coefficients of the activated genes are so significant that the experimental data could not be explained with the previously suggested model, in which the fluctuation in the transcriptional rate coefficient of the activated genes is neglected.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of mesoporous silica by controlled concentration of silica and surfactant

구병진 권재민 배재영

계명대 화학과

Mesoporous silica was prepared by sol-gel method. This method is using tri-block copolymer surfactant and CTACl. Preparation of mesoporous silica was the ratio of the concentration of silica and surfactant. Surfactant was removed by calcination. Brunauer-Emmett-Teller (BET) method, transmission electron microscopy (TEM) were used to characterize the mesoporous silica.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **PHYS.P-470**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Termini Substitution in the CID of Protonated Penta- and Octa-glycine

이수복 송기형[1]

한국교원대 화학교육과 [1]한국교원대 화학과

A QM+MM direct dynamics chemical simulation were used to study gas phase collision-induced dissociation (CID) of protonated pentaglycine and protonated amino-octaglycine with argon. The semiempirical models were used for intramolecular potential of peptides and analytic functions were used for intermolecular potential between argon and peptides. More than 20,000 trajectories were run for each reaction by VENUS coupled with MOPAC. Simulations were performed with collisional energy of 350 kcal/mol for both peptides. Trajectories were terminated after 40 ps. The result was compared with previous study that terminus of poly-glycine was substituted. Reaction ratio was 2.56% at C-terminus, 4.51% at N-terminus for protonated pentaglycine and 0.39% at C-terminus, 1.39% at N-terminus for protonated octaglycine. Correlation between final rotational and vibrational energies shows that trajectories with high vibrational energies were reactive regardless of termini effect. Many dissociative channels were observed including NH2CH2+ + rest of peptide channel.

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장소: 부산BEXCO

발표코드: **PHYS.P-471**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical approach for the structures, energetics and spectroscopic properties of $(H_2O_3)_n$ (n = 1-5) clusters

서현일 김승준

한남대 화학과

The geometrical parameters, vibrational frequencies, and binding energies for $(H_2O_3)_n$ (n = 1-5) have been investigated using various quantum mechanical techniques. The possible structures of the clusters (n=2-5) are fully optimized and the binding energies are predicted using energy differences at each optimized geometry. The harmonic vibrational frequencies are also determined and zero-point vibrational energies (ZPVEs) are considered for the better prediction of the binding energy. For n=2 and 3, linear structures with all trans forms of the HOOOH monomers are predicted to be the lowest conformations in energy, while the cyclic structures with all cis-HOOOH monomers are preferable structures for n=4 and 5.

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장소: 부산BEXCO

발표코드: **PHYS.P-472**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Cationic Polystyrene Particles with Controllable Size for Hollow Silica Spheres Application

권재민 구병진 배재영

계명대 화학과

Hollow silica spheres were prepared by non calcined process. This method is just based on a emulsion polymerization and subsequent sol-gel process. Synthesis of cationic polystyrene particles under the stabilizer-free condition and the use of AIBA. Hollow silica spheres were sol-gel coating process on the polystyrene, subsequently dissolved polystyrene using NH_2OH. The morphologies of the obtained products were characterized by transmission electron microscopy (TEM).

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장소: 부산BEXCO

발표코드: **PHYS.P-473**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Investigation on Asymmetric Diels?Alder Reactions of 2,4-Dienones Catalyzed by Trienamine Catalyst

su zhishan 이해황[1] 김찬경[1]

인하대 물리화학 [1]인하대 화학과

The mechanism and the origin of selectivity of asymmetric Diels-Alder reactions of 2,4-dienones have been investigated by B3LYP method with 6-31G* level. Calculations indicate that 9-amino-9-deoxyepiquinine reacts with dienone to form a key trienamine catalytic species, which could act as a diene in the DA reaction with an electron-deficient dienophile. The acidic additive (salicylic acid or trifluoroacetic acid) plays a key role to produce preferred conformation of trienamine by H atom transfer from δ-substituted methyl group to quinuclidine moiety in quinine. The protonated tertiary N atom of quinine activates dienophile substrate by hydrogen bonding. The transition state with the lowest energy barrier corresponds to the product with endo selectivity, which is in good agreement with experimental observations.

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장소: 부산BEXCO

발표코드: **PHYS.P-474**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ni and Ni/Pd bimetallic nanoparticles for dechlorination of m-Dichlorobenzene

이슬기 최명룡

경상대 화학과

We have synthesed of inorganic nickel nanoparticles by pulsed laser ablation in methanol. The prepared nanoparticles have fcc nanostructures which are known to have catalytic properties. Metal nanoparticles have a large surface area than micro-sized particles, thus have high catalitic activities on surface. Pure Ni and Ni/Pd bimetallic nanoparticles were synthesized for the dechlorination of m-dichlorobenzene(m-DCB). The structural and morphological properties of the Ni and Ni/Pd nanoparticles were characterized by x-ray diffraction (XRD), field-emission scanning electron microscope (FE-SEM), transmission electron microscope (TEM) and dechlorination reactions were analyzed by gas chromatography(GC).

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발표코드: **PHYS.P-475**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-Efficiency Dye-Sensitized Solar Cells Based on double layer Nanoporous Electrodes

박수경 배재영

계명대 화학과

Since Gr?tzel and co-workers developed a new type of solar cells based on the nanocrystalline TiO2 electrode, dye-sensitized solar cells (DSSCs) have been attracting much attention because of their high energy conversion efficiency and as a low-cost alternative to commercial Si-solar cells. It is necessary to further improve the energy conversion efficiency in order to commercialize DSSCs successfully.In this study, highly efficient DSSCs were fabricated using nitrogen-doped TiO2 (n-TiO2) nanoparticles and MgO as a bottom and a top layer, respectively. The properties of the n-TiO2 powder, MgO/n-TiO2 film, and solar cell were investigated.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표코드: **PHYS.P-476**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Visible Light Response of Silver 4-Aminobenzenethiolate and Silver 4-Dimethylaminobenzenethiolate Probed by Raman Scattering Spectroscopy

이승훈 김관[1] 신권수[2]

서울대 화학과 [1]서울대 화학부 [2]숭실대 화학과

Silver thiolate is a layered compound with a Raman spectrum that is known to change with time, becoming the same as the surface-enhanced Raman scattering (SERS) spectrum of the parent thiol molecule adsorbed on Ag nanoparticles. On this basis, the Raman scattering characteristics of silver 4-aminobenzenethiolate (Ag-4ABT) compounds were investigated to determine whether certain peaks that are identifiable in the SERS spectrum of 4-aminobenzenethiol (4-ABT) but absent in its normal Raman spectrum were also apparent in the Ag salt spectrum. For comparative purposes, the Raman scattering characteristics of silver 4-dimethylaminobenzenethiolate (Ag-4MABT) were also examined. Raman spectra acquired while spinning the sample were typified by only a1-type vibrational bands of Ag-4ABT and Ag-4MABT, whereas in the static condition, several non-a1-type bands were identified. The spectral patterns acquired in the static condition were similar to the intrinsic SERS spectra of 4-ABT or 4-dimethylaminobenzenethiol (4-MABT) adsorbed on pure Ag nanoparticles. Notably, the CH3 group vibrational bands were observable for Ag-4MABT irrespective of the sample rotation. In addition, no decrease in intensity during irradiation with a visible laser was observed for any of the bands, suggesting that no chemical conversion actually took place in either 4-ABT or 4-MABT.

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장소: 부산BEXCO

발표코드: **PHYS.P-477**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical study on reaction mechanism of desymmetrization of meso anhydrides catalyzed by bifunctional Bronsted Acid/Base organocatalyst

Li Jun 이해황 김찬경

인하대 화학과

The reaction between anhydride and methanol catalyzed by bifunctional Bronsted acid/base organocatalyst was investigated theoretically by B3LYP method with 6-31++G* basis set. Calculations indicate that the energy barrier is quite high without catalyst, i.e. 30.8 kcal/mol. In the presence of catalyst, the reaction proceeds through a concerted mechanism with the energy barrier of 14.1 kcal/mol. The pyridine moiety works as a Bronsted base to activate methanol substrate, and the N atom attached to P atom works as a Bronsted acid to activate anhydride by hydrogen bonding.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-478**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Excited-State Dynamics of Carotenoids Studied by Femtosecond Stimulated Raman Spectroscopy

이인구 이세복 이재범 박태리 방윤수

광주과학기술원 광공학응용물리학과

Femtosecond Stimulated Raman Spectroscopy (FSRS) is a useful spectroscopic technique for investigating time resolved vibrational dynamics of molecules in ultrafast time scale often observed in many photophysical and photochemical processes. We are trying to expand our understanding in excited state dynamics including electronic transitions and vibrational relaxations by developing a FSRS technique.FSRS requires two femtosecond pulses (actinic pump, Raman probe) and one picosecond pulse (Raman pump), all generated from a Ti:sapphire amplifier laser (1 kHz, 50 fs, 800 nm). Actinic pump pulses which create excited states of chromophores are generated from a non-collinear optically parametric amplifier (NOPA) at the wavelengths of 450-600 nm. Narrowband Raman pump pulses which specify the spectral resolution of stimulated Raman, are produced by a grating filter and broadband Raman probe pulses which specify the temporal resolution of the stimulated Raman process, by white light super-continuum generation in a sapphire window. This broadband probe can also provide a wide spectral window (1000~2000 cm-1) of molecular vibrational spectra. In this presentation, steady state stimulated Raman spectra of simple organic solvents (benzene and toluene) will first be provided, and excited state stimulate Raman results of photosynthetic pigments such as carotenoids and chlorophylls will be investigated in a near future.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **PHYS.P-479**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical study of hydrogen transfer process for some amino acids

박병호 김창곤 이해황 김찬경

인하대 화학과

Our previous research showed that the PAULING cavity model is the best choice in dealing with the glycine chemistry in aqueous solution. Although the activation energy barrier for intra-molecular hydrogen transfer process was more or less comparable to experimental value, the side chain in amino acids would affect the activation barrier. In this work, we investigated the effect of side chains on the hydrogen transfer process for some amino acids. In aqueous solution, the two NE conformers and ZW conformer were fully optimized at the CPCM-B3LYP/6-311+G(d,p) level adopting PAULING cavity model. All calculations were performed by using the Gaussian 03 program. The NE and ZW structures were verified as minima with no imaginary frequency and as a transition state with only one imaginary frequency, respectively.

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장소: 부산BEXCO

발표코드: **PHYS.P-480**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Extracting Frequency-frequency correlation function from Two-dimensional Infrared Spectroscopy

곽경원 여학민

중앙대 화학과

Two-dimensional infrared (2D-IR) spectroscopy can probe the fast structural evolution of molecules under thermal equilibrium. Vibrational frequency fluctuation caused by structural evolution produced the time-dependent line shape change in 2D-IR spectrum. A variety of methods has been used to connect the evolution of 2D-IR spectrum with Frequency-Frequency Correlation Function (FFCF), which connects the experimental observables to a molecular level description. Here, a new method to extract FFCF from 2D-IR spectra is described. The experimental observable is the time-dependent frequency shift of maximum peak position in the slice spectrum of 2D-IR, which is taken along the excitation frequency axis. The direct relation between the 2D-IR peak shift and FFCF is proved analytically. Observing the 2D-IR peak shift does not need the full 2D-IR spectrum which covers 0-1 and 1-2 bands. Thus data collection time to determine FFCF can be reduced significantly, which helps the detection of transient species.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-481**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic-Inorganic Hybrid Thin Film Fabrication as Encapsulation using TMA, Adipoyl Chloride and 1,4-Butanediamine at low temperature

김세준

한양대 화학과

We fabricate organic thin film for the purpose of encapsulation by molecular layer deposition(MLD) using Adipoyl Chloride(AC) and 1,4-Butanediamine. Ellipsometry was employed to verify self-limiting reaction of MLD. Linear relationship between number of cycle and thickness was obtained. We found that desirable organic thin film fabrication is possible by MLD surface reaction in monolayer scale. Purging was carried out after dosing of each precursor to form monolayer in each sequence. We also confirmed roughness of the organic thin film by atomic force microscopy. We deposit AC and 1,4-Butanediamine at 70 °C and investigated surface roughness with increasing thickness of organic thin film. We confirmed precursor's functional group by IR spectrum. We calculated WVTR of organic-inorganic hybrid super-lattice epitaxial layer using Ca test. WVTR indicates superlattice film can be possibly use as encapsulation in flexible devices.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-482**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Boron-11 solid-state NMR study of some boronic acids and their catechol cyclic esters

오세웅 David L. Bryce[1]

목포대 화학과 [1]University of Ottawa, Canada

Some arylboronic acids and their catechol cyclic esters are investigated using ^{11}B solid-state NMR spectroscopy at the three different magnetic field strengths (9.4, 11.7 and 21.1 T). Through the analysis of spectra of static and magic angle spinning samples, the ^{11}B electric field gradient and chemical shift tensors are determined. The effects of relaxation anisotropy and nutation field strength on the ^{11}B NMR line shapes are investigated. New X-ray crystallographic structures of some aryboronic acids are reported. Calculations of the ^{11}B NMR parameters are performed using cluster model and periodic gauge-including projectors augmented wave (GIPAW) DFT approaches and the results are compared with the experimental values.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-483**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical study on the effect of carbon dioxide solubility by substituted anilines

매방 이해황[1] 김찬경[1]

인하대 물리화학부/화학과 [1]인하대 화학과

Abstract: Aniline was selected as a substrate to study the effect of various functional groups on carbon dioxide adsorption. Physisorption is considered using the MP2/6-311++g(d,p)// HF/6-311++g(d,p) and BSSE is considered with "counterpoise" method. Effect of chain length, electron-withdrawing, and -donating groups on benzene ring were studied. Electron-donating group is favorable to carbon dioxide adsorption: the more this group, the higher binding energy. Electron-withdrawing group is bad for carbon dioxide adsorption, reducing binding energy. Details of calculation, functional groups, binding energy will be presented.

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장소: 부산BEXCO

발표코드: **PHYS.P-484**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

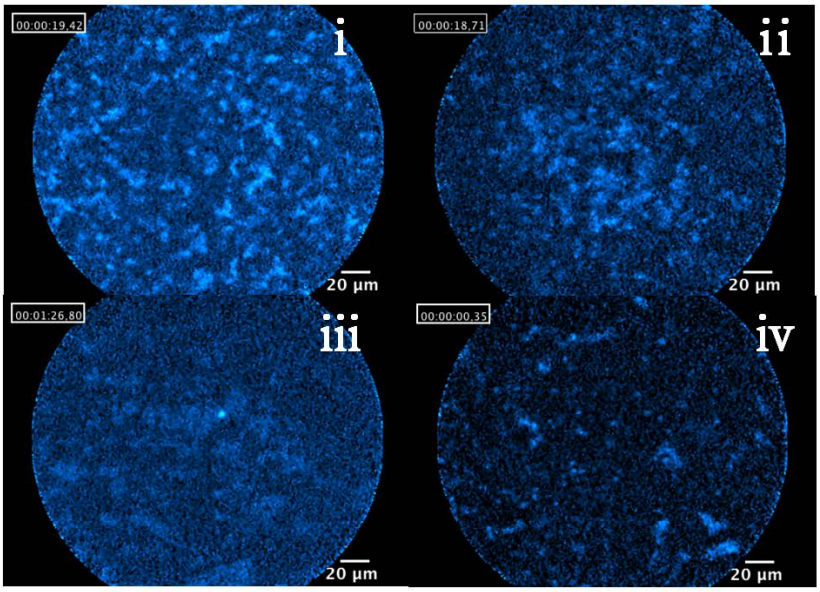
Fluorescence-Raman Endomicroscope Imaging System for Real-time Multiplexed Diagnosis

정신영 강호만[1] 이윤식[2] 정대홍

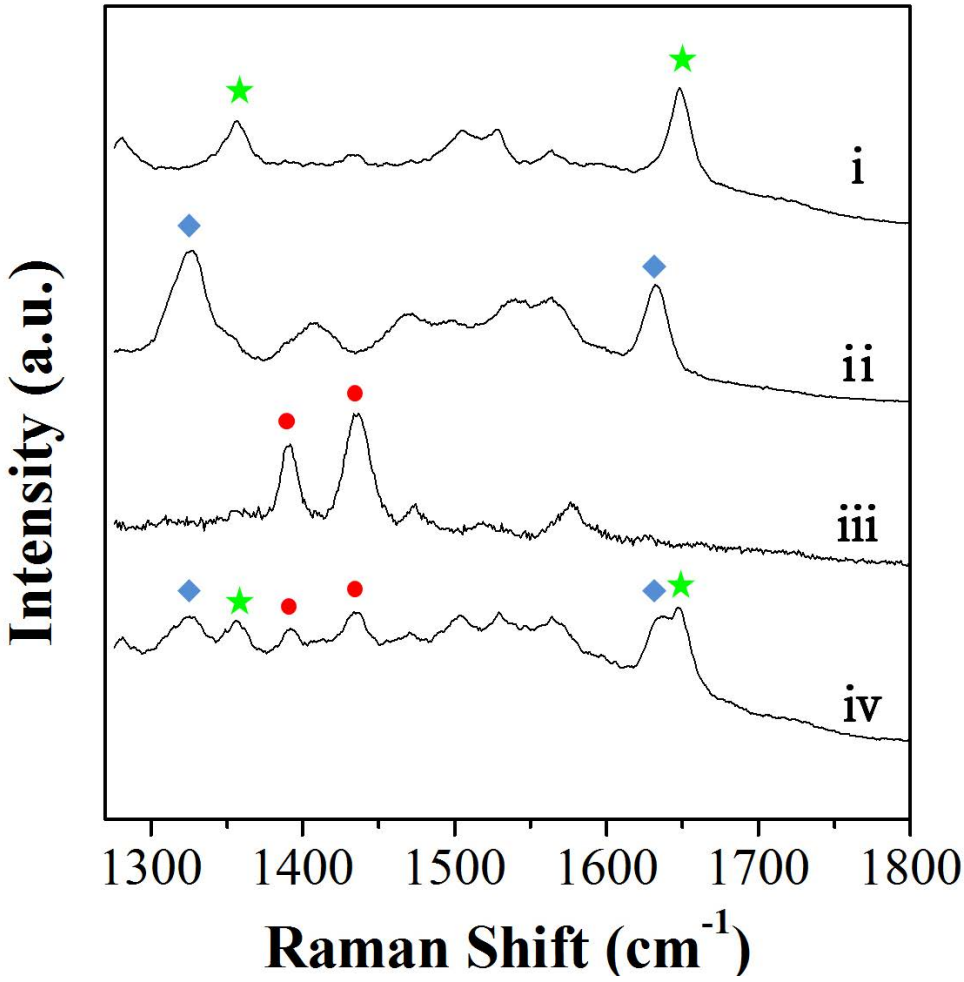
서울대 화학교육과 [1]서울대 협동과정 나노과학기술전공 [2]서울대 화학생물공학부

Recently, optical bio-imaging techniques have received a great interest as the pre-diagnosis method of disease in living animal using fluorescence dye, quantum dots, and Raman spectroscopy. Especially, owing to the intense signal, fluorescence has been widely used to track the distribution and localization of expressed bio-marker for diagnosis of cancer. However, for relatively accurate diagnosis of a specific disease, highly sensitive and multiplex optical bio-imaging technologies are required, because the multiple biomarkers are expressed for a specific disease. In this regard, fluorescence has a limitation in multiplex detection such as broad emission band and less photo-stability. In contrast, Surface Enhanced Raman Scattering (SERS) has great advantages of multiplex detection due to a narrow bandwidth of less than 1 nm. For this reason, we designed the fluorescence-Raman endomicroscopic imaging system (FREIS) with fluorescence-SERS active nanoprobes (F-SERS dots) in order to utilize advantages of intense signal of fluorescence and multiplex capacity of Raman scattering; it was designed to be able to simultaneously detect the fluorescence and Raman signal. Furthermore, FREIS provided the fluorescence images and SERS spectra with real-time; it means this system can be applied for real-time in vivo diagnosis of cancer during clinical endoscopic examinations. Herein, to demonstrate in vivo detection, we investigated the F-SERS dots on the slide glass and the surface of phantom tissue.

(a)


00:00:19.42
i
20 µm
00:00:18.71
ii
20 µm
00:01:26.80
iii
20 µm
00:00:00.35
iv
20 µm

(b)


Intensity (a.u.)
i
ii
iii
iv
1300
1400
1500
1600
1700
1800
Raman Shift (cm-1)

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-485**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Simulation Study of Effects of Crowding Environments and Hydrodynamic Interactions on Dynamics

권계민 성봉준

서강대 화학과

Effects of hydrodynamic interaction(HI) on dynamics of binary colloid mixtures are investigated by comparing Brownian Dynamics(BD) to Fast Lubrication Dynamics(FLD) simulations. Macromolecular crowding affects the dynamics of particles because the movement of the particles is restricted by its neighbor particles. In previous researches on the dynamics of concentrated systems, little attention has been paid to HI because it was presumed that HI might be screened out as the concentration increased. In recent studies, however, it was revealed that HI could affect the dynamics of colloidal particles strongly due to their multi-body and long-range character. Therefore, it is important to systematically investigate the impact of HI in order to properly understand the colloid dynamics in biological and material sciences. In this study, the effects of HI on the colloid dynamics are investigated using coarse-grained spheres. We find that HI reduces the colloid diffusion up to 3 times in crowded environments. We also find that particle displacement with and without HI show similar non-Gaussian distribution but timescales are significantly different.

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장소: 부산BEXCO

발표코드: **PHYS.P-486**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Tynthesis of Size Controlled Silver Nanowires and Their Application

임영록 조용재 김한성 명윤 박정희

고려대 소재화학과

Silver nanoparticles and nanowires size controlled were synthesized by solvothermal method. The diameter of the silver nanoparticles is controlled in the range 50 ~ 100nm and the length of silver nanowires is controlled in the range 1~40μm.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), and X-ray diffraction (XRD).

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장소: 부산BEXCO

발표코드: **PHYS.P-487**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The effects of asymmetricities either in the Xe location or in the shapes of C_n fullerenes on the confinement resonances in photoionization of enthohedral atoms Xe@C60, Xe@C90

이천우 김영록 S.T. Manson[1]

아주대 화학과 [1]Department of Physics, Georgia State University

Confinement resonances in the photoionization of atomsA encapsulated inside the hollow cage of the fullereneC60,A@C60, termed endohedral atoms, have attracted muchattention in recent years. Here we report our current status in re-examining the effects of asymmetricities either in the Xe location or in the shapes of C_n fullerenes on the photoionization of enthohedral atoms Xe@C60, Xe@C90 studied long ago by Wendin from the current points of view.

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장소: 부산BEXCO

발표코드: **PHYS.P-488**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Adsorption of PPCPs (Pharmaceutical & Personal Care Products) with modified metal-organic frameworks (MOFs) having acidity and basicity

최은정 HASAN ZUBAIR[1] 정성화[2]

OCI-SNF R&D팀 [1]경북대 대학원 화학과 [2]경북대 화학과

Removal of naproxen and clofibric acid, two typical PPCPs (pharmaceuticals and personal care products), has been studied by adsorption using modified metal-organic frameworks (MOFs) for the first time. The used MOFs are MIL-101-Cr, MIL-101-Cr functionalized with -SO_3H(S-MIL-101-Cr) and MIL-101-Cr functionalized with -NH_2(ED-MIL-101-Cr). The highest removal efficiency was observed with ED-MIL-101-Cr both in adsorption rate and adsorption capacity. On the contrary, the performances were very poor with S-MIL-101-Cr. Therefore, the adsorption mechanism may be explained with an acid-base interaction between PPCPs and the adsorbent.References[1] Z. Hasan, J. Jeon and S. H. Jhung, *J. Hazard. Mater.*, 209-210, 151-157, 2012

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장소: 부산BEXCO

발표코드: **PHYS.P-489**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Structure and Electronic Properties of Halo-Substituted Aromatic Thiol Self-Assembled Monolayers on Au(111)

강훈구 이동진 Eisuke Ito[1] Masahiko Hara[2] 노재근

한양대 화학과 [1]RIKEN, Japan [2]TITech, Japan

Self-assembled monolayers (SAMs) prepared by aromatic thiols on gold surfaces have much larger potential for electronic device applications due to their electronic properties.1-2 In this study, the formation and structures of SAMs prepared by benzenethiol (BT), toluenethiol (TT), 4-fluorobenzenethiol (4-FBT), 4-chlorobenzenethiol (4-CBT), 4-fluorobenzenemethanethiol (4-FBMT), 4-chlorobenzenemethanethiol (4-CBMT), pentafluorobenzenthiol (PFBT) and tetrafluorobenzenethiol (TFBT) on Au(111) were examined using scanning tunneling microscopy (STM) and Kelvin Prove (KP). We investigate the surface structure and work function change by adsorption of PFBT and TFBT molecules on Au(111). We report the first molecular-scale adsorption structure of TFBT SAMs with highly ordered structure, which adopts a $(\sqrt{3} \times 8\sqrt{2})R45°$ structure. This result will provide new meaningful information on controlling the structural order and electronic properties of fluorinated thiophenols SAMs, which will be very useful in precisely tailoring the interfacial properties of metal surfaces in electronic devices.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-490**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Total internal reflection fluorescence study of the pH- and sequence-dependent enzymatic rate of 10-23 deoxyribozyme and its mechanism

배소현 정지원 김선영[1] 황지희[1] 김성근

서울대 화학부 [1]서울대 생물물리 및 화학생물학

We employed total internal reflection fluorescence microscopy to track individual reaction steps of 10-23 deoxyribozyme as it undergoes its enzymatic cleavage reaction of RNA. We investigated the pH- and sequence-dependent reaction rate of all reaction steps. We found that the step that was most strongly affected by pH was the cleavage step, which was significantly accelerated at a higher pH, with the deprotonation of 2'-hydroxyl group possibly playing an important role. We found that the cleavage step was also strongly affected by the sequence of the RNA substrate. We suggest that the enzymatic core of 10-23 recognizes the RNA sequence and the interaction between the core and the cleavage site determines the rate of the cleavage step.

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장소: 부산BEXCO

발표코드: **PHYS.P-491**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Surface Morphology and Substrate on Thermal Stability and Desorption Behavior of Octanethiol Self-Assembled Monolayers on Cu, Ag, and Au

황선민 강훈구 **Eisuke Ito[1] Masahiko Hara[2]** 노재근

한양대 화학과 [1]RIKEN, Japan [2]TITech, Japan

The formation and thermal desorption behaviors of octanethiol (OT) SAMs on single crystalline Au(111) and polycrystalline Au, Ag, and Cu substrates were examined by X-ray photoelectron microscopy (XPS), thermal desorption spectroscopy (TDS), and contact angle (CA) measurements. XPS and CA measurements revealed that the adsorption of octanethiol (OT) molecules on these metals led to the formation of chemisorbed self-assembled monolayers (SAMs). Three main desorption fragments for dioctyl disulfide (C8SSC8+, dimer), octanethiolate (C8S+), and octanethiol (C8SH+) were monitored using TDS to understand the effects of surface morphology and the nature of metal substrates on the thermal desorption behavior of alkanethiols. We found that substrate morphology strongly affects the dimerization process of alkanethiolates on Au surfaces. It was also found that desorption intensity of the dimer is in the order of Au>>Ag>Cu, suggesting that the dimerization process occurs efficiently when the sulfur-metal bond has a more covalent character (Au) rather than an ionic character (Ag and Cu).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-492**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single-crystal Structure of $|Li_{50}Na_{25}|[Si_{117}Al_{75}O_{384}]$-FAU

김후식 이석희[1] 임우택

안동대 응용화학과 [1]부산교육대 과학교육과

The single-crystal structure of fully dehydrated partially Li^+-exchanged zeolite Y, $|Li_{50}Na_{25}|[Si_{117}Al_{75}O_{384}]$-FAU, was determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group *Fd*3-*m* at 100 K. Ion exchange was accomplished by flowing stream of 0.1 M aqueous $LiNO_3$ for 2 days at 293 K, followed by vacuum dehydration at 623 K and 1×10^{-6}Torr for 2 days. The structure was refined using all intensities to the final error indices (using only the 801 reflections with ($F_o > 4\sigma(F_o)$) R_1/R_2 = 0.043/0.140. The 50 Li^+ ions per unit cell are found at three different crystallographic sites. The 19 Li^+ ions occupy at site I' in the sodalite cavity: the Li^+ ions are recessed 0.30 ? into the sodalite cavity from their 3-oxygens plane (Li-O = 1.926(5) ? and O-Li-O = 117.7(3)°). The 20 Li^+ ions are found at site II in the supercage, being recessed 0.23 ? into the supercage (Li-O = 2.038(5) ? and O-Li-O = 118.7(3)°). Site III' positions are occupied by 11 Li^+ions: these Li^+ ions bind strongly to one oxygen atom (Li-O = 2.00(8) ?). About 25 Na^+ ions per unit cell are found at four different crystallographic sites: 4 Na^+ ions are at site I, 5 at site I', 12 at site II, and the remaining 4 at site III'.

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발표코드: **PHYS.P-493**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Temperature-dependent study of the enzymatic turnover rate of 10-23 deoxyribozyme by total internal reflection fluorescence microscopy

김선영 정지원[1] 배소현[1] 황지희 김성근[1]

서울대 생물물리 및 화학생물학 [1]서울대 화학부

We investigated the enzymatic reaction of 10-23 deoxyribozyme, a DNA molecule that catalyzes the sequence-specific cleavage of RNA, by total internal reflection fluorescence microscopy and identified the following four enzymatic reaction steps: binding between the substrate and the enzyme, cleavage of the substrate, and two dissociation steps of cleaved substrate from the enzyme. We performed temperature-dependent measurement of the rate for each step to determine the activation energy of individual steps. The rate of reaction steps generally increased at higher temperatures except for the cleavage step, which may have been caused by the temperature-dependent pH change of our buffer solution that offsets the effect of temperature. When one end of the cleaved substrate is dissociated while the other end remains bound to the enzyme, a new substrate can bind to the enzyme's free arm, which sends the complex back to the initial stage of the dissociation step. This erratic process, called "looping", was found to occur more frequently as lower temperatures, thereby increasing the apparent enzymatic turnover rate.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Orbital Study on the Effects of Antioxidant for the Resveratrol

권혁재 송영대[1] 이갑용[2]

대구가톨릭대 화학과 [1]경운대 한방자원학부 [2]대구가톨릭대 생명화학과

To investigate the effects of antioxidant for resveratrol, derivatives, we geometrical isomer, *cis*- and *trans*-resveratrol analyzed frontier electron density for the electrophilic reaction by calculation using the semiempirical PM3 methods, respectively. Resveratrol is polyphenol aromatic organic compound. It was found that the *trans*-resveratrol plays an important role in the formation of an energetically more stable compound than *cis*-resveratrol for the HOMO and LUMO energy gap and formation enthalpy(ΔH_f). It is appeared that the *trans* isomer is primarily more biologically activity than the *cis*-isomer.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Structure and Surface Property of Ethanethiol and Trifluoroethanethiol Self-Assembled Monolayers on Au(111)

임동원 강훈구 Eisuke Ito[1] Masahiko Hara[2] 노재근

한양대 화학과 [1]RIKEN, Japan [2]TITech, Japan

Self-assembled monolayers (SAMs) of fluorinated alkanethiols on metals represent one of most studied subjects of functionalized SAMs because of their potential to produce extremely low energy and highly hydrophobic surface coatings. The formation and structures of SAMs prepared by ethanethiol (ET) and trifluoroethanethiol (TFET) on Au(111) were examined using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV) to explore the structure and electronic interface properties of differently substituted alkanethiol SAMs on Au(111). STM observation showed that the ET and TFET SAMs formed at 70 0C for 10 min and 2 h, respectively, have more uniform surface structure and ordered domains compared to those formed for other immersion temperature and time. In particular, ET SAMs formed after 2 h have unique ordered domains containing well-ordered structures and bright rows. Reductive desorption data show that desorption peak for ET SAMs was observed at around 700 mV, whereas desorption peak for TFET SAMs was observed at around 650 mV, suggesting that ET SAMs have higher structural stability compared to TFET SAMs.

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발표코드: **PHYS.P-496**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Blue photoluminescence of the gold nanoclusters encapsulated inside G4-OH

손소형 한노수 김준명 박승민 김주훈 송재규

경희대 화학과

Blue fluorescence-emitting Au_8 nanoclusters have been synthesized using the dendrimer-based approach. The gold nanoclusters were prepared by dendrimer (G4-OH) and gold precursor ($HAuCl_4$). The emission intensity of gold nanoclusters encapsulated inside G4-OH, which is denoted as G4-OH(Au), was higher than that of G4-OH. In addition, the emission peak of G4-OH(Au) was red-shifted compared to that of G4-OH. These observations were attributed to the presence of luminescent gold nanoclusters, which were protected and stabilized by the dendrimers. The gold nanoclusters for the blue emission were assigned as Au_8 by the spherical jellium approximation, while the UV emission of gold nanoclusters originated from Au_4. When we changed the ratio of [$HAuCl_4$]/[G4-OH] for controlling experiment, the shapes of the emission spectra were similar, suggesting the magic numbers of the gold clusters. In the time-resolved emission spectra, three electronic states were found to be involved in the blue emission.

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발표코드: **PHYS.P-497**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis magnetic nanoparticles for cancer cell seperation

김초롱 Kattel Krishna Xu Wenlong Badrul Alam Bony[1] 허우철 tirusew tegafaw Md. Wasi Ahmad 이강호

경북대 화학과 [1]경북대 Chemistry

We report a simple method for the synthesis of surface modified iron oxide nanoparticles. Fe3O4 nanoparticles with particle diameter >30 nm have been prepared and subsequently coated with PAA (Polyacrylic acid) and PEI (Polyethylenimine). They were characterized with HRTEM, XRD, FT-IR, TGA and SQUID magnetometer. We plan to apply the prepared Fe3O4 nanoparticles for cancer cell separation. The magnetic properties of nanoparticles depend on particle size and large particle diameter is preferred for cancer cell separation.

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장소: 부산BEXCO

발표코드: **PHYS.P-498**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Prediction of Impact Sensitivity of Energetic Molecules

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인하대 화학과 [1]국방과학연구소 국방신기술센터 융복합부

Predicting sensitivity of energetic molecules is an important process in designing novel high energy density materials (HEDM). Among various aspects of sensitivity, impact sensitivity is closely related to many accidents in working places. Experimentally, the impact sensitivity is measures by drop weight impact test, where a height of 50% probability in causing an explosion ($H_{50\%}$) was measured. In this work, we performed extensive QSPR studies on prediction of impact sensitivity of 234 molecules using the van der Waals based MSEP method. Here, logarithmic impact sensitivity, log($H_{50\%}$) was used in the regression because this value can represent the nature of impact sensitivity of molecules. We compared our QSPR results with those published using neural network (NN) results.

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장소: 부산BEXCO

발표코드: **PHYS.P-499**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Luminescent Polymer Nanoballs Incorporated with Eu(III) Complexes with Application to Detection of Some Cations in Water

김종문 정용광 강준길

충남대 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, and quantum yield measurements. In addition, the prepared nanoballs were used to probe some cations dissolved in water by monitoring the red luminescence of the nanoballs. Among the cations used in this work, the Cu^{2+} ion significantly quenched the red luminescence of the nanoballs. The quenching effect of the cations was characterized by the Stern-Volmer equation.

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장소: 부산BEXCO

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Characterization of Water-Soluble CdTe/CdS/ZnS Core-Shell-Shell Quantum Dots

김종엽 김연호 장두전

서울대 화학부

Core-shell-shell quantum dots (QDs) of CdTe/CdS/ZnS having an average diameter of 4.2 nm and exhibiting type-II behaviors have been facilely synthesized in water via a one-pot technique. Waterdispersible CdTe/CdS/ZnS QDs have been prepared simply by injecting Zn^{2+}(aq) into an aqueous colloidal solution of CdTe/CdS core-shell QDs having anaverage diameter of 3.8 nm, which were already synthesized and stabilized in water with assistance of 3-mercaptopropionic acid. The optical properties of CdTe/CdS/ZnS QDs have been controlled by adjusting reaction time as well as pH, reaction temperature, and Zn^{2+} amount. The band-gap energy of CdTe/CdS/ZnS core-shell-shell QDs decreases gradually from 2.25 to 2.07 eV as the reaction time changes from 0 to 720 min. The photoluminescence spectrum of CdTe/CdS/ZnS core-shell-shell QDs shifts to the red steadily from 538 to 613 nm as the reaction time changes from 0 to 720 min. Photoluminescence has been found to be the most efficient when CdTe/CdS/ZnS core-shell-shell QDs were grown for 6 h at pH 10.6 and 100 C with [Zn]/[Cd] of 1/300. The photoluminescence quantum yield of the aqueous colloidal solution of CdTe/CdS/ZnS core-shell-shell QDs has been found to be as large as 15%, whereas that of CdTe/CdS core-shell QDs has been observed as 4%.

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장소: 부산BEXCO

발표코드: **PHYS.P-501**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of stable Pickering emulsions using asymmetrically surface-controlled nanoparticles

이근주 조장우

한양대 응용화학과

Stable Pickering emulsions are typically obtained when the particles are wetted by both immiscible oil-water liquids; in this case, introduction a chemical anisotropy to the particles more favorably brings them to the interface. Such particles are often referred to as “Janus” particles. These particles adsorb to interfaces more easily than isotropic particles due to their amphiphilicity and more strongly than molecular surfactants due to their larger size. Therefore, truly amphiphilic “Janus” particles combine the advantages of particle stabilization of emulsions and the amphiphilicity of molecular surfactants to afford better emulsion stabilization. In this study, we synthesize amphiphilic Janus nanoparticles and demonstrate that they effectively assemble at oil-liquid interfaces to form stable Pickering emulsions. The amphiphilicity is achieved by providing a designated hydrophobic surface area to each hydrophilic silica nanoparticle. For this, we develop techniques that allow us to make a part of the surface of silica nanoparticles hydrophobic either by using silane coupling reaction or by inducing phase separation of a hydrophobic polymer layer from the surface of nanoparticles. These Janus nanoparticles offer the potential for engineering more stable emulsions, since the hydrophilic-lipophilic balance can be exactly tuned in one particle system.

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발표코드: **PHYS.P-502**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold-coated Magnetic Nanoparticles for SERS Based Immunoassay.

신민화 CHEN LEI 이영주 정영미

강원대 화학과

Gold-coated magnetic nanoparticles (AuMNPs) are of particular effective for the separation of proteins via application of an external magnetic field. As an ultrasensitive technique, surface-enhanced Raman scattering (SERS) has been developed into protocol for the detection of immunocomplex system. Separation method using magnetic particles and sandwich immunoassay method are applied to obtain high reproducible and sensitive SERS spectra. In this presentation, characterization of gold-coated magnetic particles and detection of immunocomplex by using magnetic particles will be discussed in details.

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발표코드: **PHYS.P-503**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Folic acid-poly acrylic Acid Coated Iron Oxide Nanoparticles for Cancer Cell Separation

tirusew tegafaw Kattel Krishna Badrul Alam Bony[1] Xu Wenlong 허우철 김초롱 Md. Wasi Ahmad 이강호

경북대 화학과 [1]경북대 Chemistry

Super paramagnetic Iron oxide nanoparticles can be used in a variety of biomedical and biological applications including magnetic separation and detection of cancer cells. Magnetic cell separation relies on the ability to selective chosen cells from a heterogeneous cell suspension via labeling the target cells with magnetic nanoparticles. One important aspect of magnetic cell separation is the degree to which a cell binds paramagnetic material. The process involves polymer coated 30 nm iron oxide that was modified with antibodies. The antibodies labeled magnetic nanoparticles were bound to cancer cell and separate from blood cell. Water-soluble iron oxide nanoparticles with average diameters that range from 20-30 nm were synthesized and coated with Folic acid-poly acrylic Acid. They were characterized with XRD, HRTEM, FT-IR, PL spectrometer, TGA, confocal laser scanning microscope and SQUID magnetometer. The nanoparticles can be used as Cancer cell labeling and separation.

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장소: 부산BEXCO

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발표분야: 물리화학

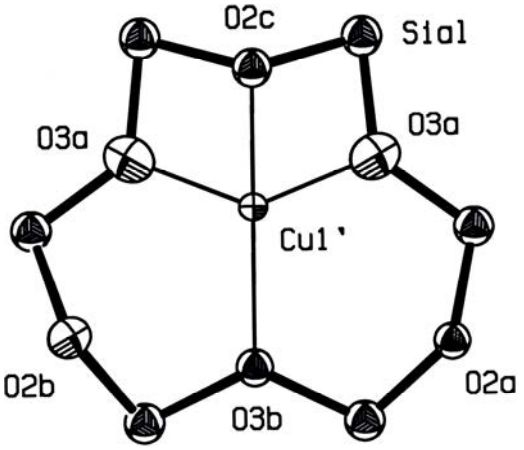
발표종류: 포스터, 발표일시: 수 16:00~19:00

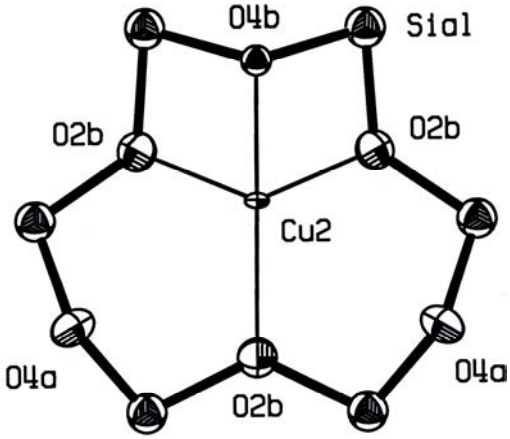
Crystallographic Verification that Copper(II) Coordinates to Four of the Oxygen Atoms of Zeolite 6-Rings. Preparation and Two Single-crystal Structures of Fully Dehydrated, Largely Cu^{2+}-exchanged Zeolite Y (FAU, Si/Al = 1.56)

서성만 임우택

안동대 응용화학과

Two single crystals of fully dehydrated, mostly Cu^{2+}-exchanged zeolite Y were prepared by th eexchange of Na_{75}-Y ($|Na_{75}|[Si_{117}Al_{75}O_{384}]$-FAU, Si/Al = 1.56) with an aqueous stream 0.05 M in $Cu(NO_3)_2$, pH = 4.2, at 294 K for 18 and 24 h, respectively, followed by vacuum dehydration at 673 K and 1×10^{-6} Torr. Their crystal structures were determined by synchrotron X-ray diffraction techniques in the cubic space group *Fd*-3*m* at 100(1) K and were refined to the final error indices R_1/wR_2 = 0.050/0.165 and 0.050/0.163, respectively, for $|Cu_{32.6}Na_{5.3}H_{4.5}|[Si_{117}Al_{75}O_{384}]$-FAU and $|Cu_{33.0}Na_{3.9}H_{5.1}|[Si_{117}Al_{75}O_{384}]$-FAU, respectively. Cu^{2+} ions occupy the 6-ring sites I' and II, preferring I'; Na^+ ions also occupy sites I' and II; neither site is filled. All Cu^{2+} ions in these structures coordinate not only to three trigonally arranged oxygen atoms of their 6-rings, but also to a fourth oxygen atom of those 6-rings to achieve planar, severely distorted square, 4-coordination. This result is in agreement with DFT calculations by Pierloot *et al*. and Berthomieu *et al*. With increasing Cu^{2+}-exchange time, both the Cu^{2+} and H^+ contents of the zeolite increase.





대한화학회
THE KOREAN CHEMICAL SOCIETY

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발표코드: **PHYS.P-505**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SERS-based Immunoassay by Using Au@SiO_2 Core-shell Nanoparticles

사영조 CHEN LEI 정영미

강원대 화학과

Surface enhanced Raman scattering (SERS)-based immunoassay has been developed by using SERS tags which are combining Raman active dyes with metallic nanoparticles. In this study, the SERS tags are functionalized with anti-Immunoglobulin G (anti-IgG) for immunoassay to present a potential application of the core-shell particles in biosensing. Characterization of Au@SiO_2 core-shell nanoparticles SERS tags and application in SERS-based biosensing will be discussed in details.

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발표코드: **PHYS.P-506**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Laser Fabrication of Au@CdS One-Dimensional Nanocomposites

김종엽 이재원 장두전

서울대 화학부

Au@CdS core-shell nanocomposites have been fabricated readily by exciting the surface-plasmon resonances of gold nanospheres, which were connected to each other by 1,5-pentanedithiol (PDT) and then coated with CdS, using picosecond laser pulses at room temperature. Gold nanospheres were cross-linked by PDT molecules to form gold nanostrands, which were then fixated and protected by CdS shells to yield Au@CdS core-shell nanocomposites. The irradiation of the nanocomposites loaded on a grid of transmission electron microscopy with 532 nm pulses of 30 ps has produced Au@CdS core-shell nanowires. The thermalized photon energy of surface-plasmon excitation has induced gold nanospheres to fuse together within CdS shells.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Uniform and Size Controlled Ultrasmall Lanthanide Oxide Nanoparticles for MR Agent Contrast

허우철 Kattel Krishna Badrul Alam Bony[1] Xu Wenlong tirusew tegafaw 김초롱 Md. Wasi Ahmad 이강호

경북대 화학과 [1]경북대 Chemistry

The synthesis of Lanthanide nanoparticles with controlled size has long been of scientific and technological interest. In case of MRI contrast agent, particle size affects contrast enhancement due to different magnetization(?) of nanoparticles. Herein report a facile synthesis of Lanthanide nanoparticles in the presence of stabilizing surfactant, oleylamine and oleylalcohol. They were coated and characterized them with MPXRD, HRTEM, FT-IR, TGA and MRI instrument.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of Sandwich Type Substrate by Using Silver Nanoparticles for SERS-based Immunoassay

이영주 CHEN LEI 신민화 정영미

강원대 화학과

Surface enhanced Raman spectroscopy (SERS) has recently received considerable attention as a powerful analytical tool in ultrasensitive chemical analysis, biological imaging, material studies. A patterned substrate was prepared by using the microcontect printing method in which the polydimethylsiloxane (PDMS) stamp was pressed into the silicon substrate surface, leaving the octadecyltrichlorosilane (OTS) only on the regions defined by the raised structure of the stamp. Herein, antigens which coated on the substrate were selectively capture antibodies that labeled with Raman reporter. In this presentation, characterization and application of SERS-based protein immunoassay for cancer detection will be discussed in more detail.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-509**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Laser-induced fluorescence study of acetaminophen monomer and water cluster

강정석 강혁

아주대 화학과

Acetaminophen (AAP) is a medicine well known as Tylenol, which is widely used mainly as a fever reducer and a pain reliever. In gas phase, two conformers of AAP were found using resonance-enhanced multiphoton ionization (REMPI) and UV-UV hole burning spectroscopy under normal supersonic expansion. We found one obstacle when we get the REMPI spectrum of AAP. The AAP at room temperature easily absorb water. Thus the REMPI spectrum of AAP is masked by broad absorption and dissociative ionization of AAP-water clusters when moist AAP sample is expanded. To solve this problem, instead of measuring ions, we use laser-induced fluorescence (LIF) that measures fluorescence emitted from the excited state. Using the LIF we investigate the electronic spectra of jet-cooled AAP and AAP-water cluster, and compared the results with those obtained by REMPI

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-510**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Crystal Structure of Rhodamine B-Based Sensitive Fluorescent Probe for Nitrite Ion

Muhammad Saleem Razack Abdullah 홍인석 이기환

공주대 화학과

A new rhodamine B-based fluorescent probe for nitrite ion (NO_2^-) has been designed, synthesized, characterized and its properties for recognition of NO_2^- were studied. Nearly non fluorescent probe upon reaction with nitrite ion significantly triggers the fluorescence. Fluorescence response is based on ring opening of spirolactam of the rhodamine B phenyl hydrazide showing absorbance at λ_{max} = 552 nm and emission at λ_{max} = 584 nm. Probe 3 exhibits high sensitivity and extreme selectivity for nitrite ion over other common ions and oxidants (Cl^-, ClO , ClO_2^-, ClO_3^-, ClO_4^-, SO_4^{2-}, SiO_3^{2-}, NO_3^{2-}, CO_3^{2-}) examined in methanol water (1:1, v/v) at pH 7.0. The probe might be a new efficient tool for detection of nitrite ion in natural water and biological system.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of sold-electrolyte interface film on the cathode materials

박연주 신수현 최현철[1] 정영미

강원대 화학과 [1]전남대 화학과

Solid-electrolyte interface (SEI) film plays a key role in the performances of Li-ion-battery. An understanding of components and structure of SEI is important to enhance the battery performance and the safety. We have recently investigated the composition and formation mechanism of SEI on cathode surface under high voltage condition by using XPS, XAS, FTIR, Raman and 2D correlation spectroscopy. Based on this work, chemical additive such as vinylene carbonate (VC) and propylene carbonate (PC) were used in Li-ion battery to enhance the safety problem. We investigated the characterization and formation mechanism of SEI on the cathode surface with and without additive system by using electrochemical and spectroscopic techniques. In this presentation, the effect of electrolyte additives on cathode surface under high voltage condition will be discussed in more detail.

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발표코드: **PHYS.P-512**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aqueous Synthesis of CdS@$Cd_xZn_{1-x}S$ Core@Shell Quantum Dots to Have Controlled Optical Properties

표지영 김연호 장두전

서울대 화학부

Water-soluble CdS@$Cd_xZn_{1-x}S$ core@shell quantum dots (QDs) have been prepared by aqueous synthetic route with 3-mercaptopropionic acid (3-MPA) as a stabilizer. Our obtained CdS@$Cd_xZn_{1-x}S$ QDs have been characterized by UV-vis, photoluminescence (PL) spectroscopy, transmission electron microscopy (TEM), X-ray diffraction (XRD), and energy-dispersive X-ray analysis (EDX). We have found that the alloyed $Cd_xZn_{1-x}S$ shell has been deposited efficiently on the CdS core QDs. As a result, the PL maximum peaks of CdS@$Cd_xZn_{1-x}S$ QDs have shifted to the blue largely compared with the respective ones of the bare CdS QDs. Also, both the PL quantum yield (QY) and the stability against UV irradiation and chemical oxidation of the CdS@$Cd_xZn_{1-x}S$ QDs have been greatly improved as compared with the bare CdS QDs. To understand how the shell thickness affects the optical and photochemical properties, the dependence of PLQY and chemical stability on shell thickness and composition has been discussed. Optimal shell thickness has found to achieve the maximum PLQY. By controlling the diameter of the core and the thickness of each shell, QDs with high PLQY (up to 50%) ranging from the visible to the near IR have been obtained. This facile route to engineering the optical properties of QDs will give new opportunities for applications in bioimaging and biolabeling.

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

Spectroscopic and Computational Study of Acetaminophen

이소영 강혁

아주대 화학과

When small amount of solvent is added to the supersonic expansion of a molecule that has multiple conformers, molecule-solvent clusters are generated and if the binding energy of clusters are larger than the isomerization barrier then the population of less stable conformers is transferred to that of more stable ones. This phenomenon is termed solvent-assisted conformational isomerization (SACI). In our previous studies, we obtained REMPI and UV-UV Hole burning spectra of Acetaminophen (AAP), which has two conformers, and demonstrated that SACI can reduce the number of conformers of AAP to one. REMPI spectrum of AAP expanded with pure helium had broad background when we used commercial sample without pre-treatment process. On the other hand, another REMPI spectrum, which was obtained under the same conditions except that we removed water from AAP before the experiment, did not have broad background. If water is included in AAP, $AAP(H_2O)_n$ clusters are generated in the supersonic expansion, which are ionized by laser and then dissociated immediately because the ionic state is a very unstable dissociative state. The dissociated AAP^+ is detected on the monomer AAP mass channel, therefore the REMPI spectrum of AAP is broadened. We found that the binding site between molecules and solvent was very important to determine the presence or absence of the ionic dissociative state, by using the experimental results of AAP REMPI with THF as a solvent instead of water and quantum chemical calculations.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Living plant cell fluorescence spectra imaging during state transitions

김은철 Shigeichi Kumazaki[1] 안태규

성균관대 에너지과학과 [1]Kyoto Univerisity

Plants have to adapt their environment because they can't move to prefer condition. They regulate protein and gene expression level to against stress (Martin M. et al. Ann. Rev. Plant Physiol. 1986). But light stress is too flexible to be regulated by protein and gene expression system (Kuhlheim et al. Science 2002). Fortunately they have molecule, protein, organism scale protection mechanism which are enough fast to prevent photodamage. Of three photoprotection mechanism, protein level mechanism keep a balance between photosystem I(PSI) and photosystem II(PSII) by moving light harvesting complex protein(LHCP) (Krishna K Niyogi et al. Current Opinion in plant biology 2000). When PSI light is stronger than PSII, LHCP move to PSII. Reversely when PSII light is stronger than PSII, LHCP move to PSI. It's called state 1 and state 2 respectively. But this mechanism is not directly observed in vivo yet. In this study, fluorescence spectra image of living plant cell is observed during state transitions by using near-infrared laser-based fluorescence spectral microscopy.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

X-ray structure of a coordination polymer composed of electron acceptor building blocks.

설창훈 허정석

충남대 화학과

In recently years, many different approaches were tested to make functional MOF materials and seek utilities of coordination polymers. Following this trend, we used a fluorene type of building block to get strongly fluorescent MOF materials which is potentially useful for molecular sensing. We also modified the molecular building block by reacting with malononitrile to attach a electron accepting groups on the moiety. Solvothermal reaction of the new one with Cd ions gave a noble 1-D coordination polymer. Syntheses and X-ray crystal structures of the coordination polymers will be presented.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-516**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

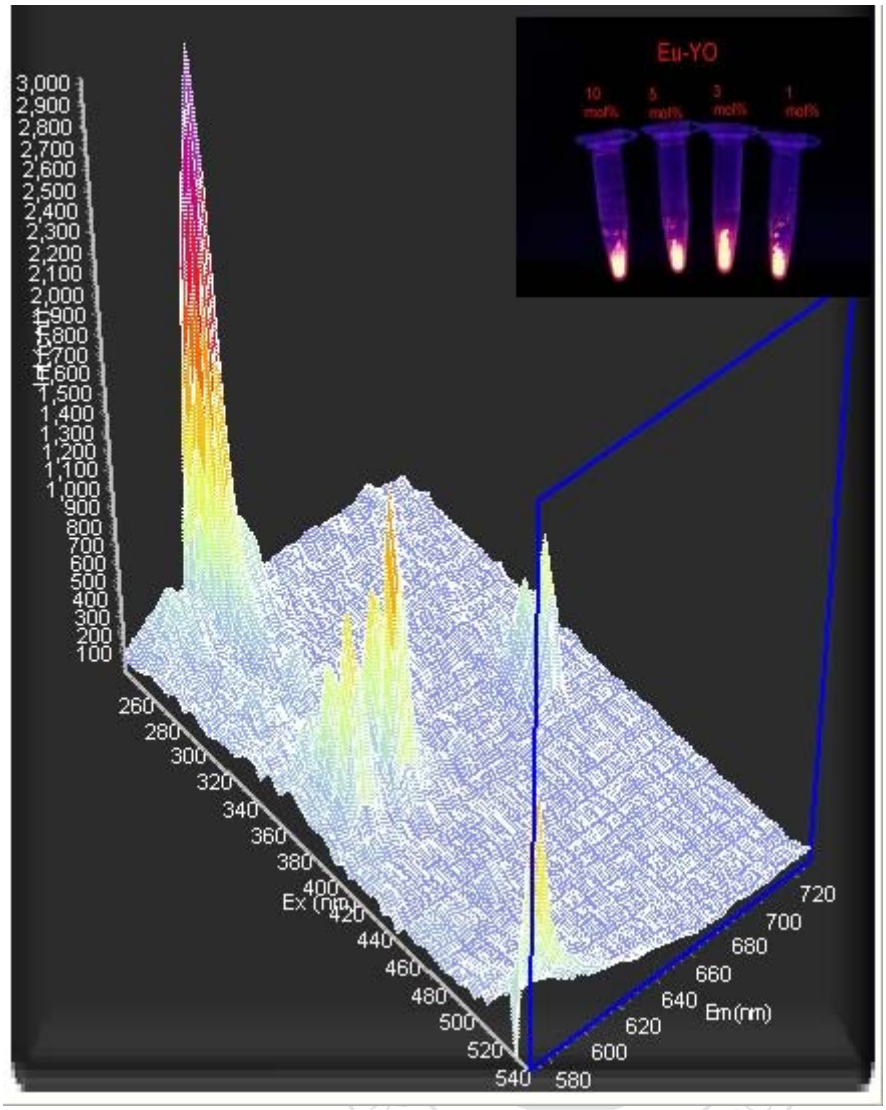
Red,Green emission from Eu,Tb-doped Yttrium Oxides

조인수 손영구

영남대 화학과

Y 산화물을 제조하여 그 물질에 Eu 또는 Tb 등의 원소들을 도핑하여 빛을 조절해 보고자 하였다. 빛의 파장과 강도의 조절함에 있어 다음 변수들이 어떠한 영향이 있는가 관찰해보고자 한다.1) 매트리스 산화물의 구조적인 변화, 2) 도핑되는 원소들의 농도, 3) 도핑물질과 매트리스의 에너지 전이, 4) 도핑되는 두 물질간의 에너지 전이, 5) 내부결함들. 이들 설명들을 뒷받침 해주기 위하여 electron microscopy, UV-vis absorption, X-ray diffraction, photoluminescence 실험을 기본적으로 수행하였다.

THE KOREAN CHEMICAL SOCIETY



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-517**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrogen bond dynamics in concentrated aqueous solutions

김성흔 조민행

고려대 화학과

The vibrational relaxation time and orientational relaxation dynamics of the OD stretching mode of dilute HOD in H2O in concentrated aqueous KSCN solutions at 295 K was investigated using a dispersive femtosecond infrared pump-probe spectroscopy. The OD stretching mode of HOD in aqueous salt solutions is blue-shifted compared with that of HOD in pure water as the salt concentration increases, indicating that the ions partially break the water H-bond network and participate in electrostatic interactions with surrounding water molecules. The transient spectra after excitation of the OD stretching mode reveal two spectral components, which have different decay times, indicating that two spectral features represent two excited species with different vibrational dynamics. We have investigated the vibrational dynamics of these two spectral components and will present the ion effects on the structure and dynamics of water in aqueous solutions.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Assembled Monolayer of Dimethyl Diselenide on Au(111)

이상윤 Eisuke ITO[1] 노재근[2] Masahiko Hara[1]

RIKEN ASI RIKEN-HYU Collaboration Research Center, Japan, 한양대 RIKEN-HYU Collaboration Research Center [1]RIKEN ASI RIKEN-HYU Collaboration Research Center, Japan [2]한양대 화학과

Alkanethiolate self-assembled monolayers (SAMs) on Au(111) surfaces have attracted a great deal of attention because they provide highly ordered structures with tunability of terminal groups, good reproducibility and chemical stability. Alkanethiols usually tend to oxidize to disulfides and other oxidized species during the SAM formation. Thus, as an alternative system for thiolate assemblies, organoselenolates have been investigated against this difficulty. However, there have been no reports on SAMs of organoselenolates with short chains so far. In this study, we investigated structural and thermal desorption behavior of dimethyl diselenide (DMDSe) SAMs and compared with dimethyl disulfide (DMDS) SAMs. We obtained the molecular level STM image of DMDSe for the first time. We also found that their thermal desorption behaviors are different from organosulfur assemblies. We expect that these results will give a good guidance to the fundamental studies and technical applications of organoselenolate assemblies of short chains as an alternative system for thiolated SAMs.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Wavepacket propagation study of the early-time non-adiabatic dissociation dynamics of NH_3X [X=F, Br]

안희선 백경구

강릉원주대 화학과

Adiabatic potential energy surfaces (PESs) of two lowest electronic states of NH_3X [X=F, Br] were constructed within two nuclear degrees of freedom, the stretching of N-H and the H-X bonds by using the CASSCF(16,12)/Aug-cc-pVDZ method. The two-dimensional (2D) diabatic PESs were constructed by using the same procedures used in our NH_3Cl study [*Theor Chem Acc*, 2012, 131, 1212]. By using the 2D diabatic PESs, the early-time dissociation dynamics of the charge-transferred excited electronic state of NH_3X were investigated by time-dependent quantum wavepacket propagations. Our results for NH_3X are compared and analyzed. Especially, we discussed the properties of the proton coupled electron-transfer (PCET) phenomena.

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발표코드: **PHYS.P-520**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Bimetallic on Reductive Dechlorination of m-Dichlorobenzene(m-DCB) using Fe/Pd Nanoparticles Produced by Pulsed Laser Ablation in Liquid (PLAL).

유이슬 최명룡

경상대 화학과

The chlorinated compounds were usually used as solvents in the chemical industry. However, disposal of chlorinated organic wastes in such a way as to minimize the environmental hazards has become an urgent issue nowadays. Organic compounds such as dichlorobenzene cannot be easily and effectively decomposed with currently available biological and chemical treatment methods. The good of this work is the effective dechlorination of m-dichlorination(m-DCB) using Fe 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-DCB. Fe nanoparticle were produced by laser ablating onto the Fe plate immersed in deionized water with a reducing agent, ascorbic acid. By using the Fe nanoparticles generated via PLAL, rapid dechlorination of m-DCB suggests that Pd/Fe bimetallic nanoparticles can be used for remediation of polychlorinated aromatic compounds in the environment. The dechlorination efficiency was increased with on increase of the Pd ratio in Pd/Fe bimetallic systems.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Gd_2O_3 nanoparticle as MRI contrast agents in Cu^{2+} and Zn^{2+} solution

Badrul Alam Bony Kattel Krishna[1] Xu Wenlong[1] 허우철[1] tirusew tegafaw[1] 김초롱[1] Md. Wasi Ahmad[1] 이강호[1]

경북대 Chemistry [1]경북대 화학과

Gadolinium oxide nanoparticle is a well known candidate for magnetic resonance imaging (MRI) contrast agents which shows significant r_1 value. However, doped or hybrid gadolinium oxide nanoparticles may show better contrast than individual one. In this work, biocompatible and hydrophilic D-glucuronic acid coated gadolinium oxide nanoparticle is synthesized with Cu^{2+} and Zn^{2+} which is a novel initiation. The nanoparticles were characterized by XRD, HRTEM and MRI instrument. Paramagnetic gadolinium oxide nanoparticle exhibits a relaxivity value of r_1=19.01 $mM^{-1}s^{-1}$ and r_2= 19.18 mM^{-1} s^{-1}; addition of 5mM Cu^{2+} triggers an enhancement in relaxivity to r_1= 28.46 $mM^{-1}s^{-1}$ and r_2 = 30.55 $mM^{-1}s^{-1}$ and whenever 5mM Zn^{2+} is added, the value of r_1 and r_2 is 47.31 $mM^{-1}s^{-1}$ and 60.58 $mM^{-1}s^{-1}$ respectively.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single-crystal Structures of Li^+-exchanged Zeolite X (FAU, Si/Al = 1.09) from Aqueous Solution Depends on Ion-exchange Temperatures at 293 and 333 K

김후식 이석희[1] 임우택

안동대 응용화학과 [1]부산교육대 과학교육과

Two single crystals of fully dehydrated partially Li^+-exchanged zeolites X were prepared by the exchange of Na-X, $Na_{92}Si_{100}Al_{92}O_{384}$ (Si/Al = 1.09), with Li^+ using aqueous 0.1M $LiNO_3$ at 293 (crystal 1) and 333 K (crystal 2), followed by vacuum dehydration at 623 K and 1×10^{-6} Torr for 2 days. Their structures were determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group *Fd*3- at 100(1) K. Their structures were refined using all intensities to the final error indices (using the 1281 and 883 reflections for which ($F_o > 4\sigma(F_o)$) R_1/R_2 = 0.075/0.244 and 0.074/0.223 for crystals 1 and 2, respectively. Their compositions are seen to be $|Li_{86}Na_6|[Si_{100}Al_{92}O_{384}]$-FAU and $|Li_{87}Na_5|[Si_{100}Al_{92}O_{384}]$-FAU, respectively. In crystal 1, 17 Li^+ ions per unit cell are at site I', 15 another site I', 30 at site II, and the remaining 16 at site III; 2 Na^+ ions are at sites II and the remaining 4 at sites III'. In crystal 2, 32 and 30 Li^+ ions per unit cell fill sites I' and II, respectively, and the remaining 25 at sites III'; 2 and 3 Na^+ ions are found at sites II and III', respectively. The extent of Li^+ exchange increases slightly with increasing ion exchange temperature from 93% to 95%.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper Nanocompound Prepareds with Sodium Hydroxide by Pulsed Laser Ablation in Deionized Water

정현진 최명룡

경상대 화학과

Metal nanocompounds exhibit useful optical or electrical functions as well as catalytic actions for various applications. Owing to the structural variety and stability of the metal oxides, they are currently considered the best supports for heterogeneous catalysts. Cuprous oxide (Cu2O) and cupric oxide (CuO) are well-known materials of p-type semiconductors, and have been employed for gas sensors, CO oxidation catalysts, and various heterogeneous catalysts, owing to their low band-gap energy and high catalytic activity, as well as their nontoxic nature and affordable price. 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, Cu nanocompounds were prepared by PLA in sodium hydroxide solutions. A pulsed Nd : YAG laser (1064 nm, 10 Hz, 7 ns) is used to produce Cu nanocompounds in deionized water; the crystal structures of Cu, Cu2O and CuO were strongly dependent on the sodium hydroxide concentrations. Morphology, size and optical properties of the Cu nanocompounds were characterized by X-ray diffraction (XRD), field emission scanning electronic microscope (FE-SEM), high resolution - transmission electron microscope (HR-TEM) and ultraviolet-visible spectroscopy (UV-vis), Fourier transform Raman scattering spectroscopy (FT-Raman).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot synthesis of Au@SiO_2 core-shell nanochains

손명희 김종엽 장두전

서울대 화학부

Directed self-assembly of gold nanorods into one-dimensional nanostructures through end-to-end linking has been attempted in the recent past. Many groups have reported the potential use of self-assembled gold nanorods in optical devices, sensing applications, electronic circuitry, medical imaging, and cancer thermotherapy. Gold nanorods can be end-to-end assembled using linker molecules such as dithiol molecules, DNA, and antigen-antibody. We present that we have been fabricated facilely end-to-end linked gold nanorods chains and coated them with SiO_2 via a one-pot route. In an isopropanol solution, gold nanorods cann link end-to-end spontaneously with no linker molecules. We here show by means of UV-vis absorption spectroscopy and electron microscopy imaging that gold nanorods can form nanochains through a solvent mediated self-assembly reaction. Coupled longitudinal plasmon resonances between linearly assembled gold nanorods shifted to the red. Then, silica has been coated on self-assembled gold nanorods, implying that end-to-end assembled gold nanorods@SiO_2 core-shell structures have been constructed by a one-pot reaction.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure, Optical, Magnetic and Cellular Toxicity Studies of Biocompatible Ligand Coated $Eu(OH)_3$ Nanorods

Kattel Krishna Xu Wenlong Badrul Alam Bony[1] Md. Wasi Ahmad 허우철 김초롱 tirusew tegafaw 이강호

경북대 화학과 [1]경북대 Chemistry

We report facile one-step synthesis of D-glucuronic acid and L-arginine coated $Eu(OH)_3$ nanorods and characterized with HRTEM, XRD, FT-IR, TGA, SQUID magnetometer, photoluminescent (PL) spectrometer and MRI instrument. The XRD curve of both as-prepared nanorods indicated a single phase pattern attributed to the $Eu(OH)_3$ with hexagonal crystal structure. The (hkl) of the peaks were well indexed and the lattice constants 'a and c' were calculated to be 6.35 and 3.62. The samples possess colloidally stable suspensions of $Eu(OH)_3$ nanorods with an aspect ratio of 13-17 which showed a strong red luminescence with narrow band width. The emission peaks are composed of the characteristic emission of Eu^{3+}, corresponding to $^5D_0$ - ^7F_j (J = 0, 1, 2, 3). The saturation magnetization (M_S) at 5 K and 300 K were calculated to be 1.8137 emu/g and 1.1963 emu/g respectively, and the nanorods are found to be paramagnetic. As observed from in vitro assay, the investigated $Eu(OH)_3$ nanorods exhibited no cellular toxicity. Hence, surface-modified $Eu(OH)_3$ nanorods may render it to be a potential candidate for optical imaging.

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발표코드: **PHYS.P-526**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photoexcitation dynamics of nitric oxide bound ferric myoglobin probed by femtosecond IR spectroscopy

박재홍 이태곤 박재헌[1] 임만호

부산대 화학과 [1]포항공과대 포항가속기연구소/빔라인부

Many NO's biological functions come from its interactions with heme proteins, such as cytochrome c oxidase, hemoglobin, NO synthase enzymes. Recently, it has been revealed that oxymyglobin (MbO_2) plays a role as an NO scavenger, regulating process, ferric myoglobin (Mb(III)) is yielded. Because ferric Mb can bind to NO, it reacts with another NO molecule to yield ferrous MbNO. Other neutral ligand such as CO and O_2 binds only to ferrous Mb and anions can bind to ferric heme but NO can bind both ferrous and ferric heme. We had measured the rebinding dynamics of NO to ferrous Mb and found that most of NO geminately rebinds nonexponentially in 1 ns. Vibrational bands of NO in MbNO revealed two bands and kinetics of the rebinding of both bands are identical, indicating that the dynamics of geminate rebinding to ferrous Mb is conformationally independent. Here we investigated NO rebinding dynamics to ferric Mb and compare it with that of ferrous Mb. Stretching mode of NO has two overlapping bands, main band at 1921 cm^{-1} and minor one at 1904 cm^{-1}, suggesting that ferric MbNO has at least two conformational substates. We observed that 80% of NO dissociated from heme after photo excitation and the rest of them relax to the ground state by vibrational relaxation. The rebinding of NO to ferric Mb in D_2O at 293 K is nonexponential. The decay of the main band is slower than that of ferrous MbNO band but almost ~80% complete in 1 ns, indicating that NO rebinding to the main conformation of ferric Mb is less efficient than ferrous Mb. The minor band shows clearly slower decay than the major one. The minor conformation is suggested to arise from the interaction of the protonated His 64 with NO. Clearly the structure of amino acid residues near the active site of the protein is very critical in controlling protein function (ligand binding).

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Iodine Based Gd2O3 Nanoparticles for MRI Contrast Agents

Md. Wasi Ahmad Kattel Krishna Badrul Alam Bony[1] Xu Wenlong tirusew tegafaw 허우철 김초롱 이강호

경북대 화학과 [1]경북대 Chemistry

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. 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, PL, 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 and the MRI signal of iodine coated Gd2O3 nanoparticles were examined.

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Surface plasmon resonance signals of Au double layers between temperature sensitive layer

TRAN VAN TAN

부산대 나노융합기술

Thermoreversible behavior of surface plasmon resonance (SPR) is reported for various sizes of Au nanoparticles (NPs; 4, 18, and 57 nm) dangled from poly(N-isopropylacrylamide) (PNIPAm) in the solid film regime. The formation and thermal behavior of the polymer layers and NP layers were characterized by SPR spectroscopy. Changes in the thickness of the polymer film depending on temperature are expressed as shifts in the surface plasmon angle. Adsorption of Au NPs with different sizes to form the top layer results in significant amplification of the SPR signal because of the interaction of the propagating and localized SPR. The shapes of the thermal hysteresis curves were observed to be different for adsorption of different sizes of NPs and reveals that the highest sensitivity was found with 4 nm Au NPs for a film coated, where the sensitivity resulted from strong interaction between two Au layers and thermal mobility of the polymer. Therefore, molecular dynamics (MD) simulations were carried out in order to reveal the mechanisms involved in the formation of the Au NP layer on the temperature-sensitive polymer. This research will potentially provide basic fundamental resources for the study of the thermally dependent behavior of optoelectronics and electronics, as well as for further development of platforms for biomedical sensing and actuators.

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Universal Dispersive Correction to Density Functional Theory: Extended application of DFT-*ulg* Method to a variety of GGA functionals

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KAIST 화학과 [1]KAIST EEWS대학원 [2]Materials and Process Simulation Center, California Institute of Technology

Despite the importance of van der Waals (vdW) interactions in biological and energetic systems, it is tricky to accurately predict physical and chemical properties of substances with density functional theory (DFT) whose interactions are dominantly determined by long-range vdW attractions. In general, this is due to dynamic correlation between fluctuating charge distribution. To offset this crucial error, a variety of correction methods has been employed including DFT-D approach in which a pairwise dispersion potential is simply added to the Kohn-Sham DFT energy. In a recent study, Liu *et al*. proposed a DFT-low-gradient model with a proper long-range $1/R^6$ London dispersion interaction at long distances while delivering low gradients at normal valence distances. The successive study by Kim *et al*. removed the restriction of DFT-low-gradient model to hydrocarbons by systematic generalization to the all atom pairs, named as DFT-*ulg*. However, this immediate compensation is only limited to the PBE functional while various breeds of GGA functionals are now available to attain further accuracy in special systems. In this study, we develop a DFT-*ulg* model for various functionals such as RPBE, PBEsol, and PW91, thus allowing us to easily extend the applicable range of the model to the entire periodic table as well as several revised functionals. To support our method, we evidence the accurate prediction for binding energies of other weakly bound molecular crystals based on the parameter optimized only for benzene dimers.

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Novel Shape-Tunable Approach to Fabricate CdSe Crystals under Microwave Irradiation

김형배 장두전

서울대 화학부

We report a unique synthetic approach to fabricate CdSe crystals with tunable morphology and optical properties via a microwave-assisted polyol process. The morphology of CdSe crystals has been controlled by adjusting the relative amounts of two cadmium precursors $CdCl_2$ and CdO in a polyol solvent of ethylene glycol or glycerol; spheres, pebbles, sheets, and tetrapods of CdSe wurtzite structures with their sizes ranged from nanometers to sub-micrometers have been prepared facilely under microwave irradiation. The growth mechanism is discussed in terms of the LaMer theory; the nucleation and growth kinetics of CdSe, which depends decisively on cadmium precursors and polyol solvents, determines the shapes and sizes of diverse CdSe crystals

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Synthesis and CharacterizationStudy of D-Gluocronic acid Coated Single-Phase Mixed $DyEuO_3$ Nanoparticles

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경북대 화학과 [1]경북대 Chemistry

We report a facile synthesis of ultra-small D-Gluocronic acid coated Eu^{3+} doped Dysprosium oxide nanoparticles. They were characterized by XRD, HRTEM, FT-IR, Fluorescence spectrophotometer, TGA, SQUID magnetometer and MRI instrument. The nanoparticles were found monodisperse and average particle diameter is estimated to be ~3 nm. The $DyEuO_3$ nanoparticles were found to be paramagnetic and emitted strong blue fluorescence. The nanoparticles exhibited no appreciable cytotoxicity up to 0.5 mM concentration and in vivo MR experiment showed the negative contrast enhancement on mouse liver and kidneys after the injection of nanocolloid. Hence, it can be used as a MR-optical imaging agent.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Field emission and secondary-electron emission properties of GaAs/MgO on single walled carbon nanotube

박태희 이종택 이휘건

한양대 화학과

We measured the field emission (FE) and secondary-electron emission (SEE) properties of single walled carbon nanotubes (SWNTs) after coating with wide-band-gap and negative electron affinity materials , such as MgO and GaAs including the turn-on field and lifetime stability. The FE was increased successively after MgO coating and subsequent GaAs coating for SWNTs. The turn-on field had a lower value and FE currents were increased by four times compared with pristine SWNTs. A lifetime test revealed that GaAs/MgO/SWNTs protects itself during FE under exposure to O2 gas.The field-enhancement factor, β, was calculated from the Fowler-Nordheim equation of FE results.

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Aggregation and Stabilization of Carboxylic Acid Functionalized Halloysite Nanotubes (HNT-COOH)

주용호 손대원

한양대 화학과

The nanotube structure of halloysite has led to increased interest in its applications as nanoreactors or nanotemplates, catalysts, and capillaries. We modified the functional groups of holloysite nanotubes (HNT) from hydroxyl groups (HNT-OH) to carboxylic acids (HNT-COOH). Aggregation and dispersion properties of HNT-COOH under dry conditions were probed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Moreover, the degree of aggregation and dispersion of HNT-COOH in acidic, basic, and neutral solutions were measured by multiple angle polarized dynamic light scattering (MADLS). HNT-COOH formed aggregates in neutral solution; however, the material was dispersed in basic and acidic solutions. This occurrence is due to hydrogen bonds (HB) between the carboxyl groups of HNT-COOH in neutral solution, which decrease in acidic and basic solution due to charge dispersion.

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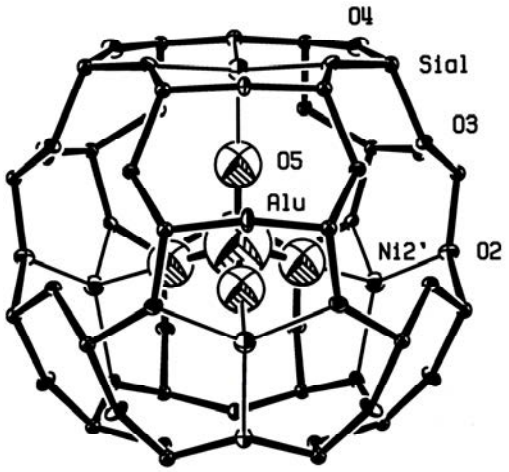
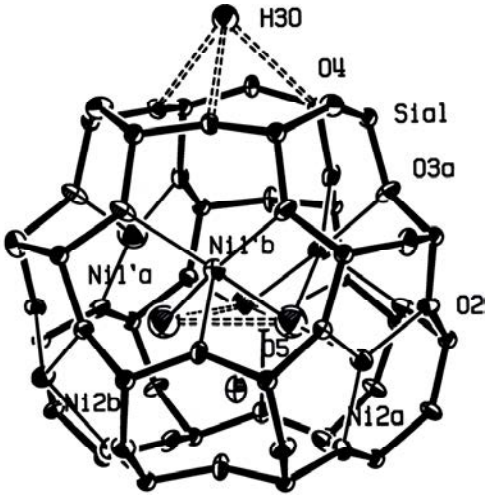
Preparation and Single-crystal Structures of Fully and Partially Dehydrated Zeolite Y (FAU, Si/Al = 1.56) Ni^{2+} Exchanged at a Low pH 4.9

서성만 임우택

안동대 응용화학과

The crystal structures of zeolite Y Ni^{2+} exchanged at pH 4.9, fully dehydrated ($|Ni_{29.7}(Ni_4AlO_4)_{1.1}H_{12.3}|[Si_{117}Al_{75}O_{384}]$-FAU) and partially dehydrated ($|Ni_{14.1}(NiOH_2)_{16.4}(Ni_4AlO_4)_{1.1}(H_3O)_{9.6}|[Si_{117}Al_{75}O_{384}]$-FAU), were determined by single-crystal synchrotron X-ray diffraction techniques. They were refined to the final error indices R_1/wR_2 = 0.044/0.115 and 0.052/0.153, respectively, in the cubic space group *Fd*-3*m*. Some dealumination of the zeolite framework occurred during Ni^{2+} exchange. In the fully dehydrated structure, Ni^{2+} ions primarily occupy sites I and II, with additional Ni^{2+} ions at site I', site II', and a second site II. In the partially dehydrated structure, Ni^{2+} occupies six different sites: I, I', a second site I', II, a second site II, and III'. Because of the low pH of the Ni^{2+} exchange solution, some H_3O^+ ions are observed in partially dehydrated Ni^{2+}-Y; correspondingly some H^+ ions are required for charge balance in fully dehydrated Ni^{2+}-Y. The nonframework oxygen atoms in water and orthoaluminate coordinate to some of the Ni^{2+} ions. Upon full dehydration, a substantial Ni^{2+} migration from I' sites to site I is seen. Unlike the situation at pH 6.2, no hydrolyzed Ni^{2+} ions ($NiOH^+$, Ni_2OH^{3+}, $Ni_4(OH)_4^{4+}$) appear to have exchanged into the zeolite.





대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-535**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Luminescence Properties of Red Oxide Phosphors and characteristic of Coated Red Oxide Phosphors

강봉호 강준길

충남대 화학과

Highly luminescent $(Li_{1-x}Eu_x)_{0.5}(Mo_{1-y}W_y)O_4$ red phosphors were prepared by solid-state reaction under air condition, and their luminescence intensity were investigated as functions of x and y. The phosphor with x = 0.5 and y = 0.4 produced the strongest intensity upon the 396-nm excitation. The excitation spectrum revealed that the direct excitation at 396 and 465 nm was more efficient that the charge-transfer excitation at 320 nm. Oxide-based phosphors were coated with metal oxides (SiO_2, In_2O_3, and MgO), organic compounds (PEG, polystyrene, poly(1-4-phenylene sulfide), and polysulfone) to protect against a moisture. The morphology of uncoated and the coated phosphors were characterized by FE-SEM. The luminescence intensities of uncoated and the coated phosphors were measured at several high temperatures and humidity.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Hollow Platinum Nanoplates via a Galvanic Replacement

이동기 장두전

서울대 화학부

Hollow platinum nanotriangles, which show highly enhanced catalytic properties, have been prepared through a galvanic replacement reaction of silver nanoplates dispersed in Pt^{n+}-added water. Pt^{n+}, prepared in advance by the partial reduction of Pt^{4+} using a weak reducing agent, is readily reduced galvanically to form porous Pt shells, and concomitantly produced Ag^{+} diffuses out to generate hollow Pt/Ag nanocomposites finally. The residual silver has been further eliminated from the nanocomposites using 0.5 M HNO_3(aq) to produce hollow Pt triangular nanoplates. Hollow Pt/Ag nanostructures have been found to catalyze the degradation of rhodamine B efficiently in the presence of KBH_4, although their catalytic performances depend highly on the metals, sizes, and shapes of the nanostructures.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of graphene oxide/poly(acrylic acid) hybrid hydrogel using γ-ray radiation

이성영

한양대 화학과

The graphene oxide/poly(acrylic acid) hybrid hydrogel was synthesized using γ-ray pre-irradiation technique. The γ-ray radiation was used for modifying the functional groups of graphene oxide. The changes of functional groups and structural deformation of graphene oxide by radiation were investigated by spectroscopy. This modified graphene oxide was utilized as initiator for polymerizing acrylic acid monomer to polymeric hydrogel. The analysis of mechanical property confirms the role of graphene oxide in the hydrogel as reinforcing agent. In addition, including more GO hydrogel showed better swelling capacity. The facile synthetic method, mechanical stability and swelling performance of the graphene oxide/poly(acrylic acid) hybrid hydrogel make it an attractive candidate for biomedical material and superabsorbent.

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Calculation of Photoionization Cross Sections of Small Molecules by the R-matrix Method and Multi-channel Quantum Defect Theory

김영록 이천우

아주대 화학과

We implemented UKRmol codes into linux based computer systems, and performed various calculations about several small molecules such as N_2, H_2O, NO.Integrated cross sections, differential cross sections, time delays, multi-channel quantum defects and other properties are calculated, and compared to experimental data.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Ion-Molecule Reactions within $M^+(CH_3SCH_3)_n$ ($M = Cu^+, Ag^+, Au^+$) Heteroclusters

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원광대 생명나노화학과 [1]원광대 생명나노화학부 [2]부산대 화학과 [3]원광대 화학과

In our present study, we have investigated the dynamic insertion of group-11 cation (Cu^+, Ag^+, and Au^+) ion within $M^+(CH_3SCH_3)_n$ heteroclusters ($M = Cu^+, Ag^+, Au^+$) by using laser vaporization combined with supersonic beam expansion in a reflecton time-of-flight mass spectrometer. A number of reaction pathways, including association, dehydrogenation, and elimination, were observed. Computational investigation was carried out to present about the geometrical optimization for all reaction species (reactants, intermediates, transition states, and products) and reaction pathways using density functional theory (DFT). The reaction species were optimized with B3LYP hybrid functional. The computational results are good agreement with the our experimental findings.

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No spin-gap behavior of the triangular spin tube system

구현주 김찬양[1] 강은비

경희대 화학과 [1]경희대 화학교육학과

Magnetic properties of the triangular spin tube system $CsCrF_4$ were examined in terms of the spin exchange interactions evaluated by energy-mapping analysis on the basis of density functional theory calculations. Our results show that the exchange J_1 for the triangular ring and the exchange J_2 along the chain are both antiferromagnetic with the ratio $J_1/J_2 = 0.5$, so the spin gap of $CsCrF_4$ is too small to be experimentally detected. This finding is consistent with the experimental observation and theoretical analysis.

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pH-induced denaturation of ovalbumin studied by SASX and FT-IR spectroscopy

강대훈 유수련 정영미

강원대 화학과

Two-dimensional correlation spectroscopy (2DCOS) has attracted a high level of interest of analytical science community, as it provides considerable utility and benefit in many fields of spectroscopic studies. In the present study, we investigated pH-dependent unfolding of ovalbumin by using FTIR spectra and SAXS in order to monitor the secondary structure of ovalbumin and the global size and shape of the ovalbumin molecule, respectively. To analyze FTIR spectra of pH-dependent of ovalbumin, we have performed 2D COS. Results of FTIR and SAXS. Results of FTIR and SAXS demonstrated the transition from β-sheet to α-helix of ovalbumin.

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Single-step hydrothermal synthesis of ZnS nanorods exhibiting enhanced band-edge emission

김연호 김종엽 장두전

서울대 화학부

One-dimensional semiconductor nanostructures such as nanorods, nanowires, and nanotubes have attracted a great deal of interest due to their distinctive geometries, physical and chemical properties, and enormous potential as fundamental building blocks for nanoscale electronic and photonic devices. ZnS is an important II?VI semiconductor compound with band gap energy of 3.70 eV, and it attracts intense interest due to its excellent luminescent property. Especially, the emission wavelength of ZnS falls in the UV absorption band of most organic compounds and biomolecules, thus it is envisaged that ZnS nanorods based devices may find applications in increasingly important fluorescence sensing. We have developed the facile synthesis of single-crystalline and wurtzite ZnS nanorods via a single-step mild hydrothermal process. The control over the width of the nanorods was achieved by adjusting the reaction time and temperature. Typical nanorods have an average width of 50 nm, perfect-crystalline structure, and show highly enhanced band-edge emission. The photoluminescence spectra of ZnS nanorods exhibit two bands: band-edge luminescence centered at 327 nm and trap-related luminescence centered at 420 nm. As-synthesized our nanorods show strongly enhanced ultraviolet band-edge emission and highly suppressed trap-related emission that would give them potential for optoelectronic devices.

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Preparation of Pd-graphene and CuO-graphene nanocomposites and their catalytic application for C-C and C-N coupling reactions

이경훈 김보현 박준범

전북대 화학교육과

Graphene has been modified with palladium and copper oxide nanoparticles (NPs) to develop high performance catalysts for C-C and C-N coupling reactions. In this research, graphite oxide (GO) sheets were exfoliated and oxidized from graphite powder and GO was impregnated with metal precursors to prepare Pd^{2+}/GO and Cu^{2+}/GO . Their thermal treatments in H_2 flow produced Pd NPs/Graphene (Pd/G) and CuO NPs/G (CuO/G) nanocomposites. TEM images show that the NPs are distributed quite uniformly on the graphene sheet without obvious aggregation. The mean size of Pd and CuO NPs was determined to be ~ 2 nm and ~5 nm, respectively, in diameter. The electronic and chemical structures of the intermediates and final products were investigated using FT-IR, XRD, and XPS. The resulting Pd/G and CuO/G showed excellent catalytic efficiency in C-C and C-N coupling reactions and offer significant advantages over inorganic supported catalysts such as simple recovery and recycling. We believe that the remarkable relativities of graphene based catalysts are attributed to high degree of the dispersions of NPs and thus increased low coordination numbers of the smaller NPs.

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2D Correlation Analysis of cold crystallization of Biodegradable P(HB-*co*-HHx)/PEG Blends

이준희 유수련 Isao Noda[1] 정영미

강원대 화학과 [1]Procter & Gamble Company

Poly(3-hydroxybutyrate-*co*-3-hydroxyhexanoate) (P(HB-*co*-HHx)), which is a new member of the polyhydroxyalkanoate (PHA) family, has been studied extensively. We have recently investigated thermal behavior of spin-coated films of PHB-co-HHx copolymers. It is also important to investigate the thermal behavior of P(HB-co-HHx) in the presence of other polymers like PEG. P(HB-*co*-HHx) is fully miscible with poly(ethylene glycol) (PEG). In this study, P(HB-*co*-HHx) blends with a PEG content of 2, 10, and 20 wt% were prepared from chloroform solution. Crystallization of spin-coated films of P(HB-*co*-HHx)/PEG blends is investigated by 2D correlation spectroscopy. Details of 2D correlation spectra of spin-coated films of P(HB-*co*-HHx)/PEG blends will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-545**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Toxicity of metal nanoparticles in cells

정민주 박승민 신승근 김국기 권혜진

경희대 화학과

The current debate about nanoparticles in liquid phase is used for several applications such as optical and magnetic devices, catalysts, biological processes and life environments. We study about the cell toxicity of metal nanoparticles prepared by laser ablation by a pulsed Nd:YAG laser operated at 1064 in liquid phase. In cell toxicity study, especially in zebrafish study, nanometer sized silver materials are well known as toxic materials to cells. This study discuss toxicity of various metal nanoparticles to zebrafish. The objective of this study is to evaluate the acute toxicity of nanoparticles on adult zebrafish.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-546**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Exchange of Lithium Cations into Zeolite Na-Y from Undried Methanol Solution

김후식 이석희[1] 임우택

안동대 응용화학과 [1]부산교육대 과학교육과

The ion exchange of Li^+ into zeoliteY, $Na_{75}Si_{117}Al_{75}O_{384}$ (FAU, Si/Al = 1.56), was attempted using methanol-water mixed solvents. Four solvents ranging in composition from as-purchased (undried) methanol (water concentration 0.02 M) to pure water were used. Four single crystals of Na-Y were treated with 0.1 M $LiNO_3$ in each of the four solvents at 333 K. Their structures were determined by single-crystal X-ray diffraction techniques in the space group *Fd*3-*m* at 100(1)K. In the four structures, Li^+ and Na^+ fill sites I' and II; the remaining cations, when they can be found, occupy III' sites. The site preference for Li^+ over Na^+ is approximately I' > II > III'. The greatest degree of exchange of Li^+ for Na^+, 96%, was achieved from undried methanol under the conditions employed. The extent of Li^+ exchange decreases with increasing water content and was least, 72%, from pure water. The low water content of the undried methanol appears to play an essential role in the ion exchange process.

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장소: 부산BEXCO

발표코드: **PHYS.P-547**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasensitive Biosensor for Disease Diagnosis Based on Biomarker Coated Three-Dimensional Network of Carbon Nanotubes

이수범 서정은 조석진 조용덕[1] 박미경 안도연 이해원

한양대 화학과 [1]한양대 나노융합과학과

The blood contains the information on the status of human body and the signs of infections. That is the number one reason why the blood test has been conducted to diagnose diseases over many years. However, the blood test has two major vulnerable points: the necessity of highly trained analysts and the time consumption. To solve the problem a new assay method, which guarantees fast, accurate, and low cost analysis, should be developed to replace the currently available commercial methods, such as ELISA, CMIA, and SPR. The new assay method is based on the biomarker coated 3D CNT Network and the saliva test. The saliva test, which provides the similar biological information, has more advantages over the conventional blood test. This noninvasive test does not require professional analysts or expensive analytical instruments to operate. The biomarker coated 3D CNTs Network has larger surface areas than conventional 2D CNT Network and creates trillions of multiple pathways for analytes to take. Larger surface areas and multiple pathways enhance the sensitivities of the biosensor and increase the performance of the biosensor remarkably at extremely low concentration.

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장소: 부산BEXCO

발표코드: **PHYS.P-548**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Anodic TiO_2 Nanotube Arrays Coated with Crystalline TiO_2 Particles at Room Temperature

이대기 이완인[1] 장두전

서울대 화학부 [1]인하대 화학과

In recent years, it is highly desired to synthesize well-aligned crystalline TiO_2 nanotubes arrays (TNTs) without employing an additional thermal annealing process, which may lead to cracks and aggravate sample integrity. In this work, we have fabricated TNTs employing an electrochemical anodization method and coated them with crystalline TiO_2 nanoparticles through direct deposition of TiO_2 precipitate synthesized in the initial electrolyte solution containing TiF_4. TNTs were fabricated through electrochemical anodization of pure titanium foil in an NH_4F-contained ethylene glycol electrolyte solution at room temperature. The appropriate amount of H_2SO_4 was also added in the electrolyte solution to adjust pH. And then, as-fabricated TNTs were soaked in the electrolyte solution for 1-60 h. Then, crystalline TiO_2 particles were synthesized in a TiF_4-contained acidic solution and deposited onto the as-fabricated TNTs substrate. The resulting arrays have a highly ordered, vertically aligned, and one side-opened structure. The crystalline TiO_2 particles were deposited on the nanotubes clearly well. The photo-oxidation ability of the coated TNTs has also been compared with that of other TiO_2 structures.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-549**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aggregation of laser-generated gold nanoparticles mediated by formalin

MD.ALAUDDIN 김국기 송재규 박승민 **Madhusudan Roy**

경희대 화학과

We have investigated the effects of formalin (F) on the assembly of colloidal gold nanoparticles (AuNPs) prepared by laser ablation of a solid gold target in deionized water. The surface plasmon resonance (SPR) band appeared at 519 nm for pure AuNPs, while it decreased and shifted to red upon addition of formalin. On the other hand, a new broad SPR band appeared at ~700 nm, of which red-shift was prominent with increase in the incubation time. The average size of initial AuNPs was around 12 nm while it increased to 23 nm after addition of formalin. It turned that formalin acts as a cationic surfactant for AuNPs with negative surface charge in the colloidal solutions. Furthermore, we elucidated the adsorption properties of formalin on silver nanoparticles by surface enhanced Raman scattering (SERS) along with density functional theory (DFT) calculations and found that formalin is strongly bound to Ag-ion via C-O---Ag bonding.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-550**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study of thermal behavior of spin-coated film of P(HB-*co*-HHx)/PEG blends

박준후 유수련 Isao Noda[1] 정영미

강원대 화학과 [1]The Procter & Gamble Company (U.S.A)

Poly(3-hdroxybutyrate)(PHB)-based copolymers, such as poly(3-hydroxybutyrate-*co*-3-hydrohexanoate)(P(HB-*co*-HHx)) have been studied as environment-friendly polymer. P(HB-*co*-HHx) are fully miscible with biodegradable polyethylene glycol (PEG).In this study, to investigate thermal behavior of P(HB-*co*-HHx)/PEG blends, 2D correlation spectroscopy was applied to the temperature-dependent infrared-reflection absorption spectra of spin-coated films of P(HB-*co*-HHx)/PEG blends. Details of 2D correlation spectra will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-551**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Au nano-prism by laser ablation in liquids

권혜진 김국기 송재규 박승민

경희대 화학과

Gold nanoparticles were synthesized by laser (Nd:YAG, λ = 1064 nm) ablation of a gold target immersed in various concentrations of NaI solutions (0 ? 50 mM). Laser power and ablation time were varied to obtain the optimum ablation condition for the formation of nano-prisms. The shape of nanoparticles were examined by analyzing the surface plasmon peak shape and position, and further confirmed by transmission electron microscopy (TEM) images.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-552**

발표분야: 물리화학

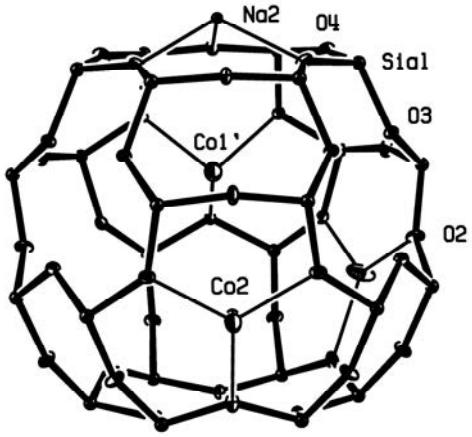
발표종류: 포스터, 발표일시: 수 16:00~19:00

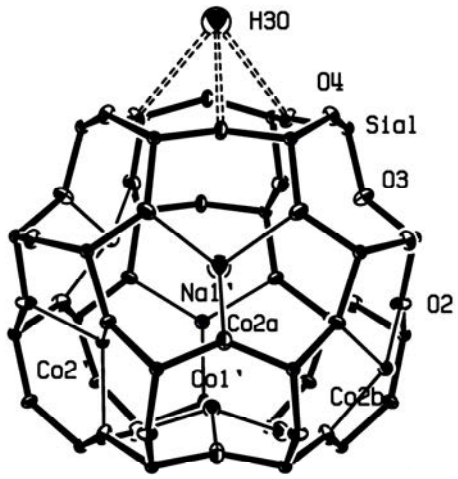
Preparation and Single-crystal Structures of Fully and Partially Dehydrated Zeolite Y (FAU, Si/Al = 1.56) Largely Co^{2+} Exchanged at pH 5.1

서성만 임우택

안동대 응용화학과

The structures of fully and partially dehydrated zeolite Y Co^{2+} exchanged at pH 5.1, were determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group *Fd*-3*m* and were refined to the final error indices R_1/wR_2 = 0.046/0.120 and 0.062/0.191, respectively. Two crystals were used; their unit-cell formulas are approximately $|Co_{31}Na_8H_5|[Si_{117}Al_{75}O_{384}]$-FAU and $|Co_{30.5}Na_6(H_3O)_4(H_2O)_4H_4|[Si_{117}Al_{75}O_{384}]$-FAU, respectively. In the fully dehydrated structure, Co^{2+} ions occupy sites I, I', and II; the Na^+ ions are also at site II. In the partially dehydrated structure, Co^{2+} occupies sites I', II', II, and III'; the Na^+ ions are at site I'. Some H_3O^+ ions are seen in the partially dehydrated structure, and H^+ ions must be present in both crystals for charge balance. Upon dehydration Co^{2+} ions move into the hexagonal prisms and Na^+ ions move from sodalite cavities to supercages. Instead of the H^+ and H_3O^+ found here, zeolite X Co^{2+} exchanged at a higher, less well defined pH, 6-7, had been found to contain OH^- ions.





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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-553**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly single crystalline IrxRu1-xO2 mixed metal oxide nanowires

정하영

이화여대 화학과

The nanostructured Iridium-Ruthenium mixed metal oxide (IrxRu1-xO2) is the most promising candidate as a highly efficient electrode material for electrolysis of water. We present a facile a facile n efficient synthesis and structural characterizations of highly single crystalline IrxRu1-xO2 mixed metal oxide nanowires for the first time via a simple vapor phase transport process by carefully controlling the relative ratios of IrO2 and RuO2 precursors. We also observed that an Eg mode of and IrxRu1-xO2 nanowire measured from Raman scattering is being linearly blue-shifted and its linewidth is asymmetrically broaden with respect to the increase of the Ir contents, indicating that we could quantitatively determine stoichiometry information as well as crystal structure for mixed metal oxide nanowires.

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장소: 부산BEXCO

발표코드: **PHYS.P-554**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Properties of Pt Nanoshells Synthesized via Acid Etching of SiO_2@Pt Nanospheres.

곽진아 이동기 장두전

서울대 화학부

Metal nanostructures attract considerable attention scientifically as well as industrially because they can be possibly used in diverse applications. Among a variety of noble-metallic nanostructures, platinum nanostructures having outstanding catalytic and electrical properties have been widely applied in chemical, petrochemical, electronic, and automotive industries. We have synthesized Pt nanoshells using hard templates of SiO_2 nanospheres. Monodispersive SiO_2 nanospheres have been prepared from the sol-gel process of tetraethylorthosilicate under base catalysis following the Stober method, and the sizes of SiO_2 nanospheres have been controlled by adjusting the amount of NH_4OH. Pt seeds prepared by the citrate reduction of H_2PtCl_6 have been topped on SiO_2 nanospheres through amino groups and transformed into the shells of SiO_2@Pt core/shell nanostructures via a seeded-growth method. Finally, SiO_2 nanocores have been removed by hydrofluoric acid. Pt nanoshells have been found to catalyze the degradation of rhodamine B efficiently in the presence of KBH_4 compared with SiO_2@Pt core/shell nanostructures. We will present the catalytic mechanism of Pt nanoshells with structure-dependent kinetic results measured at various temperatures.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-555**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mode-dependent Vibrational Predissociation of An+(H2O)n (n=1-10): Time-resolved Studies

Madhusudan Roy MD.ALAUDDIN 송재규 박승민

경희대 화학과

Aniline (water)n cluster ions are generated by R2PI and subsequently photodissociated with IR light in a field region. Typical vibrational modes of aniline (water)n cluster ions include N-H (symmetric and anti-symmetric), hydrogen-bonded O-H, and free O-H (symmetric and anti-symmetric) modes. Here, we have selectively excited these modes of vibration with IR photon to liberate one water molecule. Interestingly, the rates of ejection of water were mode-dependent; the ejection of water molecule took shorter time when we excited O-H mode compared to N-H mode. When the cluster ions are vibrationally excited, the energy is redistributed over the whole vibrational modes and ultimately used up to eject water molecule through fission of the hydrogen bonding. In case of N-H mode excitation, the ejection of water molecule takes longer time as it is located far away from the amino group. On the other hand, the excitation of O-H mode facilitates ejection of water due to the relative proximity of water molecule to the energized moiety. Also, we analyzed the ejection rate of water as a function of the cluster size.

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장소: 부산BEXCO

발표코드: **PHYS.P-556**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal nanoparticles (NPs) plasmon coupling for SERS-based immunoassay

CHEN LEI 정영미 **Bing Zhao**[1]

강원대 화학과 [1]*State Key Laboratory of Supramolecular Structure and Materials, Jilin University*

In this presentation, we construct a plasmon coupling structure with reorganization of antigen and antibody which can provide high SERS enhancement. We detect atto610 signal indirectly to achieve protein immunoassay due to the low Raman scattering section of protein itself. For SERS applications, this proposed method will broaden the area of SERS applications, from common protein immunoassay to disease-related proteins; based on SERS of different target proteins, it will provide evidence about selectivity of SERS to different proteins; the most important impact is that it will provide rapid and high-sensitivity SERS-based protocol for protein immunoassay and disease-related proteins, which would be very helpful for early diagnosis of related diseases.

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장소: 부산BEXCO

발표코드: **PHYS.P-557**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of laser ablation in liquid phase

김국기 권혜진 신승근 송재규 박승민

경희대 화학과

We investigated the effect of magnetic field and ion on the plasma plume produced by laser ablation of metal in water. We found that the optical intensity of plasma plume depends on magnetic field. Consequently we also analyzed liquid plasma plume by ICCD and observed that decay time increases in present of magnetic field. Furthermore, we have not only studied plasma plume but also studied laser light scattering for the generation of nanoparticles in liquid phase laser ablation.

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장소: 부산BEXCO

발표코드: **PHYS.P-558**

발표분야: 물리화학

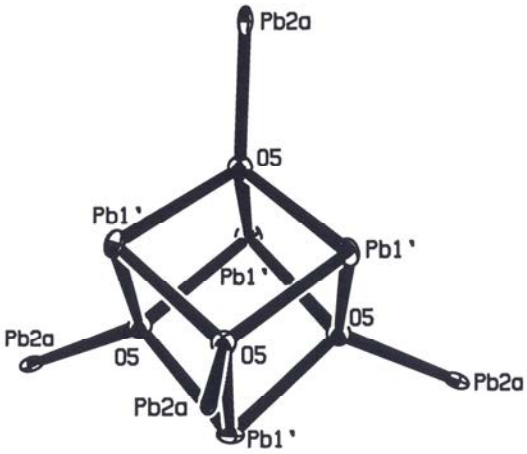
발표종류: 포스터, 발표일시: 수 16:00~19:00

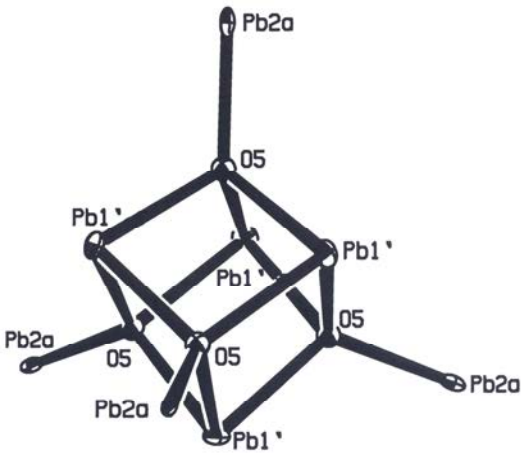
Preparation and Single-crystal Structure of Lead Oxide Nanoclusters in Zeolite Y (Si/Al = 1.56), $|Pb^{2+}_{5.5}(Pb_4O_4(Pb^{2+}_{0.67}Pb^{4+}_{0.33})_4)_6|[Si_{117}Al_{75}O_{384}]$-FAU

서성만 임우택

안동대 응용화학과

The single-crystal structure of excessively Pb^{2+}-exchanged zeolite Y was prepared by the exchange of Na-Y ($|Na_{75}|[Si_{117}Al_{75}O_{384}]$-FAU, Si/Al = 1.56) with an aqueous stream 0.05 M $Pb(C_2H_3O_2)_2$ at 294 K, followed by vacuum dehydration at 1 × 10^{-6} Torr and 723 K. Its single-crystal structure, $|Pb^{2+}_{5.5}(Pb_4O_4(Pb^{2+}_{0.67}Pb^{4+}_{0.33})_4)_6|[Si_{117}Al_{75}O_{384}]$-FAU, was determined by single-crystal synchrotron X-ray diffraction techniques. It was refined to the final error indices R_1/wR_2 = 0.0574/0.1404 in the cubic space group *Fd*-3*m*. In $|Pb^{2+}_{5.5}(Pb_4O_4(Pb^{2+}_{0.67}Pb^{4+}_{0.33})_4)_6|[Si_{117}Al_{75}O_{384}]$-FAU, about 53.5 Pb^{n+} ions per unit cell occupy three different equipoints; 24 are at site I', 24 are at site II, and the remaining 5.5 are at another site II. Eight Pb^{4+} ions in some of the positions must have higher oxidation states due to elevated dehydration temperature; Pb(IIa) is supposed to coexist of Pb^{2+} and Pb^{4+} ions by assumption for the charge balance of zeolite framework. A distorted Pb_4O_4 cube, alternating Pb^{2+} at Pb(I') and O^{2-} at O(5), coordinates with four of Pb^{2+} and/or Pb^{4+} ions through its oxygen atoms to give a $[Pb^{2+}_4O^{2-}_4(Pb^{2+}_{0.67}Pb^{4+}_{0.33})_4]^{32/3+}$ cluster in six of eight sodalite cavities in zeolite Y.





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THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-559**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Metal Oxide Nanowires on Eletrospun TiO2 Nanofibers

조유경 김명화[1]

이화여대 화학나노과학과 [1]이화여대 화학 나노과학과

In this study, we report hierarchically driven single crystalline MoO3 and RuO2 nanostructures directly on TiO2 nanofibers prepared by the electrospinning method toward catalytic applications. Both metal oxide nanostructures were successfully grown via atmospheric pressure chemical vapor deposition method without any catalysts. Particularly, MoO3 and RuO2 1-dimensional nanostructures can be used as the effective catalysts or electrochemical electrode materials. Crystalline Structures of products are confirmed using scanning electron microscopy (FE-SEM), X-ray diffraction (XRD) spectrum, Raman spectroscopy, and high resolution electron microscopy (HRTEM).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-560**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Photophysical Properties of CdS Hollow Submicrospheres Prepared via Microwave Irradiation

김연신 김형배 곽진아 장두전

서울대 화학부

A new fabrication method of hollow nanostructures via microwave irradiation has been explored, resulting in hollow spheres with a shell thickness within the quantum confinement range. CdS, a yellow solid with a band gap of 2.42 eV, is our material of interest due to its direct band gap and its ability to absorb almost all visible light. Thus, CdS has recently shown much interest in solar cells, displays, and optoelectronic devices due to its unique photochemical and photophysical properties. With the assistance of microwave irradiation, we have developed a facile method of preparation of uniform CdS hollow submicrospheres with a shell thickness within the quantum confinement range. Compared to the polystyrene template or the template-free synthetic methods of CdS hollow nanospheres, our method of preparation allows for much more control and results in highly uniform and well-defined hollow structures. Other advantages of this method are that it has very few steps, it gives us control over the size of the nanospheres, it is easily scalable, and that it does not require an inert environment. The physical characteristics of these CdS hollow structures have been studied with data extracted from HRTEM, HRXRD, and XPS, revealing a cubic zinc blende crystal structure with a crystallite sizes ranging from 4.7 to 6.2 nm depending on the size of the overall hollow submicrosphere. The photophysics of the CdS hollow spheres was then characterized with absorption and photoluminescence spectra.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-561**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Helical foldamers of γ-peptide based on 2-(aminomethyl)cyclohaxanecarboxylic acid

변병진 강영기

충북대 화학과

The γ-peptide helical foldamers with different characteristic hydrogen bonding patterns have been designed computationally using di- to octa-$\gamma^{2,3}$-peptides based on 2-(aminomethyl)cyclohexanecarboxylic acid (γAmc_6) with a cyclohexyl constraint on the C^{α}—C^{β} bond. The conformational analyses on the γAmc_6 peptides with homochiral (2*S*,3*S*) or (2*R*,3*R*) configurations reveal that the (*P*/*M*)-2.5_{14}-helices are most preferred in the gas phase, whereas the (*P*/*M*)-2.3_{12}-helices are most stable in water due to larger helix dipole moment and more favorable hydrogen bonds of the 12-helix compared to the 14-helix, as also evidenced by detailed conformational studies of di-γAmc_6-peptides. However, negligible difference in electronic energy between 12-helix and 14-helix for octa-γAmc_6 peptides in water indicates that oligomers of γAmc_6 residues longer than octamer exist as a dynamical ensemble of 12- and 14-helices with quite similar probability each other. As the peptide sequence becomes longer, intrinsic folding propensities of 12- and 14-helices are also found to increase both in the gas phase and in water. The helical parameters of 14-helical foldamer are calculated to be similar to those of 14-helix from γAc_6a oligomers in the solid state. A cyclohexyl constraint on the C^{α}—C^{β} bond is proven to enforce the backbone of γ-peptides into well-ordered conformation by limiting backbone torsional mobility.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-562**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SnO2 nanowire on Nb2O5 nanowire

이지영

이화여대 화학나노과학과

Synthesis of nanostructured metal oxides has been considered important because of its highly effective performance and enhancing capacity of devices. Niobium oxide (Nb2O5) is thermodynamically stable phase and one of the best promising metal oxides. Niobium oxide nanowire can be used photocatalyst, highly effective gas sensor and as electrochromic materials. For fabricating Nb2O5 nanowire, we made niobium hydroxide(Nb(OH)5) solution as precursor and used CVD which simple method to fabricate material of nanoscale. Tin oxide (SnO2) nanowire is already fabricated and characterized as sensing material, for example sensors for highly sensitive detection of toxic gases. Therefore we synthesized SnO2 nanowire on Nb2O5 nanowire which we made by using CVD. Synthesis of SnO2 nanowire on Nb2O5 nanowire means that it exbits advantages of two materials. Hence this experiment is meaningful. We characterized the morphology and structure of SnO2 nanowire on Nb2O5 nanowire by using scanning electromicroscopy (SEM), X-ray diffraction (XRD) and transmission electronmicroscopy (TEM).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-563**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Z-form DNA Specific Binding Geometry of Zn(II)*meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin Probed by Polarized Spectroscopy

김윤화 장윤정 이현미[1] 김석규

영남대 화학과 [1]대구가톨릭대 안경광학과

Zn(II)-*meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin (ZnTMPyP) produced a unique linear dichroism (LD) spectrum when form a complex with Z-form poly[d(G-C)$_2$]. The spectrum was characterized by a large positive wavelength-dependent LD signal in the Soret absorption region. The magnitude of LD in both DNA and Soret band increased as the [porphyrin]/[DNA base] ratio increased and were larger by 20~40 times compared to the negative LD of the ZnTMPyP bound to B-form poly[d(G-C)$_2$] and poly[d(A-T)$_2$]. The angles calculated from LD were 49° and 42° for B_x and B_y transitions of the porphyrin with respect to the local helix axis of Z-form poly[d(G-C)$_2$]. Appearance of unique LD spectrum for the Z-form poly[d(G-C)$_2$] complex was accompanied by bisignate circular dichroism spectrum in the Soret region, whose magnitude was proportional to the square of the porphyrin concentration, suggesting that a strong stacking interaction between the Z-form poly[d(G-C)$_2$] bound ZnTMPyP. From these observations, conceivable binding mode of ZnTMPyP to Z-form poly[d(G-C)$_2$], in which ZnTMPyP binds at the major groove or across the groove, complex was proposed. In contrast with Z-form poly[d(G-C)$_2$], ZnTMPyP binds to poly[d(A-T)$_2$] in the monomeric manner with the angles of 57° and 59° for the two porphyrin's transition moments with respect to the local polynucleotide helix axis. The polarized spectral properties of ZnTMPyP bound to B-form poly[d(G-C)$_2$] coincide with the intercalated non-metallic TMPyP namely, a negative CD signal in the Soret band and a negative wavelength-dependent reduced LD signal with its magnitude large than that in the DNA absorption region in spite of its axial ligands.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-564**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

$BiOCl_xI_{1-x}$ photocatalysts for dye removal under visible light irradiation

김원주 손영구

영남대 화학과

수열합성방법을 이용하여 BiOCl 과 $BiOCl_xI_{1-x}$ 을 합성하였습니다. 이들을 Methyl orange 와 Rhodamine B 를 이용하여 염료분해실험을 실히하였으며, 통해 광촉매로서의 활성을 측정하고, 또한 BET 를 통해 각각의 비표면적을 측정하였습니다. 모든 실험은 Scanning electron microscopy(SEM)과 X-ray diffraction(XRD)과 UV-vis spectrometer 을 이용하였습니다.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **PHYS.P-565**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of VxRu1-xO2 Nanowires via Chemical Vapor Deposition

천성희

이화여대 화학나노과학과

Nanostructure of Vanadium-Ruthenium mixed metal oxide is a promising candidate as a catalytic electrode for electrolysis of water. We show a efficient synthesis method of highly single crystalline VxRu1-xO2 mixed metal oxide nanowires for the first time via a simple vapor phase transport process (chemical vapor deposition) by careful controlling the relative ratios of VO2 and RuO2 precursors. In addition, we present structural characterizations of VxRu1-xO2 nanowires through SEM, XRD, TEM and Raman.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-566**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical behavior of ortho-Carborane Triggered by Aryl Substitution: Carborane-Based Dyads with Phenyl Carbazoles

위경량 김성관 강상욱

고려대 소재화학과

Among three different isomers of carborane (C2B10H12), the 1,2-C2B10H12 (o-Cab) cage was demonstrated to exert unusual effects on the excited-state properties of the aryl substituents. Molecular assemblies formed by linking the carbazolyl group (Cz) with the o-Cab cage through the p-phenylene or p,p'-biphenylene spacer revealed unique excited-state behavior with charge-transfer character which is entirely different from that of the m- and p-counterparts, giving a new type of carborane-based dyads. It was demonstrated that photoexcitation of Cz in bis-1,2-(Cz-phenyl)-o-Cab generates the charge-separated state with the Cz radical cation and o-Cab radical anion ends.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-567**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA sequence dependent binding of non-intercalating chiral binuclear Ru(II) complexes

박종진 프리아 장윤정 이동진[1] 김석규

영남대 화학과 [1]경일대 화학공학과

The binding properties and sequence selectivity of enantiomeric binuclear Ru(II) complexes contains non-intercalative bridged ligand (bip) with poly[d(A-T)$_2$]and poly[d(G-C)$_2$] sequences have been investigated by using biophysical methods. With the polynucleotides the interaction of both enantiomers is shown to be purely non- intercalative and the binding mode is dependent upon the enantiomer (ΔΔ or ΛΛ) and the DNA base sequence as well as the insensitive to concentrations of DNA and metal complex (ratio). The CD experiments performed with poly[d(A-T)$_2$]and poly[d(G-C)$_2$] exhibits sequence dependent properties and established that ΔΔ and ΛΛ-[μ-Ru$_2$(phen)$_4$(bip)]$^{4+}$ presents a pronounced selectivity for AT-base sequence. The binding of enantiomers to poly[d(A-T)$_2$] gives rise to positive ICD signal corresponding to bridged ligand absorption, which confirms the minor groove binding mode to AT-regions. The average angle (α) between the binuclear Ru(II) complexes and the poly[d(A-T)$_2$]helical axis revealed the well-defined binding mode with an orientation of the bridged ligand moiety. The binding specificity can be unambiguously defined from fluorescence measurement, since ΔΔ and ΛΛ-[μ-Ru$_2$(phen)$_4$(bip)]$^{4+}$ were able to provide selective fluorescence response towards poly[d(A-T)$_2$] base sequence.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-568**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ruthenium oxide nanowires on Rhodium oxide nanofibers

김유림 김명화[1]

이화여대 자연과학대학 화학나노과학과 [1]이화여대 화학 나노과학과

Ruthenium oxide (RuO_2) has remarkable chemical and thermal stability and its nanostructures have been prepared for many applications such as high energy density capacitors, hydrogenation and the oxidation of CO. Also, rhodium oxide is interesting material which has been used in catalysis especially the conversion of CO or NO gases. Generally nanostructures have more improved catalytic ability than large scale structure. Thus it is a task of great significance to synthesize rhodium oxide nanofibers in nanoscale. Electrospinning as the synthesis of rhodium oxide nanofibers is a facile method to make uniform fibers of nano and microscale. We have first prepared rhodium oxide nanofibers by electrospinning and then grown highly crystalline RuO_2 nanowires directly on rhodium oxide nanofibers successfully. Additionally, we characterized the morphology and structure of RuO_2 nanowires on rhodium oxide nanofibers by scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectrum and transmission electron microscopy (TEM).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-569**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photo-induced DNA cleavage by Cu(II)-*meso-tetrakis*(*n-N*-methylpyridiniumyl)porphyrins (n = 2,3,4) and their binding mode to supercoiled DNA

김래영 프리아 이길준[1] 김석규

영남대 화학과 [1]경운대 한방자원학부

The DNA cleavage activity of well known CuTMPyP complexes was investigated under irradiation in the absence of reducing agent. *m*-CuTMPyP was most efficient in cleavage than *o*- and *p*-CuTMPyP isomers. The conversion of supercoiled form (SC) to the nicked circular form (NC) depends on the duration of irradiation of the complex with DNA. Mechanistic investigations revealed that hydroxyl radicals and singlet oxygen contribute to the photo-induced DNA cleavage activity. Reduced linear dichroism spectroscopy showed angles of *o*-CuTMPyP's electric transition moments, in which the periphery pyridinium ring was prevented from free rotation, of 59˚ and 61˚ with respect to the local DNA helix axis. The spectra of *m*- and *p*- CuTMPyP complexed with DNA were characterized by large signals in the Soret band, coincident with those of known intercalated porphyrins.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-570**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Fe2O3-, NiO- and Cu2O-TiO2 Tube by Electrodeposition Photoelectrode and Their Photoresponsive Behavior

김창우 서상필 **Zheng jin you** 강영수

서강대 화학과

The solar energy has been recognized as the most promising resource for sustainable energy development.1,2 The hydrogen and oxygen evolution from solar energy resource is one of the facile approaches using a water splitting process. One of the primary challenges is improvement of the energy conversion efficiency and economical production cost in the field of photo-electrochemical cells (PEC). Until now, TiO2 nanoparticles a photocatalytic material have been widely employed in a PEC system. However, their visible light absorption are still challenging because of their wide bandgap (3.0 ~ 3.2 eV). Therefore coupling of the lower energy band gap semiconductors such as SnO2, CdS, and CdSe with large band gap semiconductors such as TiO2 has been applied for the improvement of charge separation. The doping with other elements on the TiO2 or ZnO for the harvesting of visible light was also carried out to increase their photoelectrochemical performance.In this work, we report Fe2O3-, NiO- and Cu2O-TiO2 tube as a photoelectrode. The electro-deposited Fe2O3 and Cu2O in anodized TiO2 tube can improve the photocatalytic activities and result in the enhancement of solar energy conversion. The energy-band between TiO2 tube and Fe2O3, NiO and Cu2O is energetically favorable. We prepared successfully heterostructure with visible light activity using a two-step electrochemical process of anodization and an electrodeposition method. The structure and optical properties of the TiO2 nanotubes and their heterostrucute have been well characterized and displayed a strong photo-response in the visible region and low recombination rate of the electron-hole pairs.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-571**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Time-resolved Fluorescence of Highly Single Crystalline Structures of Thioflavin T

석지수 이유민 이민영[1] 김명화[2]

이화여대 화학나노과학과 [1]이화여대 화학나노과학부 [2]이화여대 화학 나노과학과

Thioflavin T is widely used to detect the amyloids which are insoluble fibrous protein aggregates. There has been studied regarding thioflavin T binding to amyloid structure using fluorescence spectroscopy. However, there is a little information about its own fluorescence properties in the crystalline state. In this study, we synthesized single crystals of thioflavin T using chemical vapor deposition (CVD), and then measured its fluorescence lifetime using fluorescence-lifetime imaging microscopy (FLIM). The crystal morphology and structure of the single crystals were investigated by scanning electron microscope (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD). The crystalline length scale varies from nanometers to micrometers. The single crystals are shaped like a sword. The results show that the fluorescence lifetime of thioflavin T crystal is greatly increased in the crystalline state.References[1]Jee, A.-Y.; Lee, Y.; Kim, M. H. The Journal of Chemical Physics 2012, 136.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-572**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photodynamic Behavior of Heteroleptic Ir(III) Complexes with Carbazole-Functionalized Dendrons Associated with Efficient Electron Transfer Processes

위경량 김성관 강상욱

고려대 소재화학과

We prepared dendrimers of heteroleptic iridium(III) complexes, [(dfppy?Cz1)2Ir(dpq)]+ (G1) and [(dfppy?Cz2)2Ir(dpq)]+ (G2), which have the dfppy ligand connected to carbazole-functionalized dendron Czn (n = 1, 2). While parent complex [(dfppy)2Ir(dpq)]+ (G0) shows an intense emission at 635 nm with a lifetime of 1 μs assigned to dpq-based metal-to-ligand charge-transfer (MLCT) phosphorescence, excitation of the dendrimers at either carbazole (309 nm) or MLCT band (355 nm) resulted in markedly weaker and much shorter-lived MLCT emission (τp = 44 ns for G1 and 115 ns for G2) at room temperature. Upon exciting the carbazole chromophore of G1 and G2 at 309 nm, furthermore, both the carbazole fluorescence and the MLCT emission were very weak at room temperature. It was found that the lifetime of carbazole fluorescence is 20 ps for G1 and 62 ps for G2, shorter by 2-orders of magnitude than that of free carbazole dendron Czn′?OH (τF = 6.1 ns). These observations demonstrate that both the excited-singlet state of carbazole and the triplet MLCT state of the Ir(dpq) core are efficiently quenched in the dendrimers. Since the apparent quenching of either carbazole fluorescence or MLCT emission observed at room temperature does not occur at 77 K, the temperature-dependent emission behavior of G1 and G2 for both the carbazole fluorescence and the MLCT phosphorescence was attributed to the participation of activated processes, that is, electron transfer from excited-singlet carbazole to the Ir(dpq) core as well as from the ground-state carbazole unit to the triplet MLCT Ir(dpq) core. This mechanism was supported by transient-absorption spectroscopic experiments that demonstrate the generation of the carbazole radical cation after exciting G1 and G2 by laser pulses.

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장소: 부산BEXCO

발표코드: **PHYS.P-573**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conformational properties of genotoxic benzo[a]pyrene-7,8-dione and cytosine base studied using Quantum mechanics

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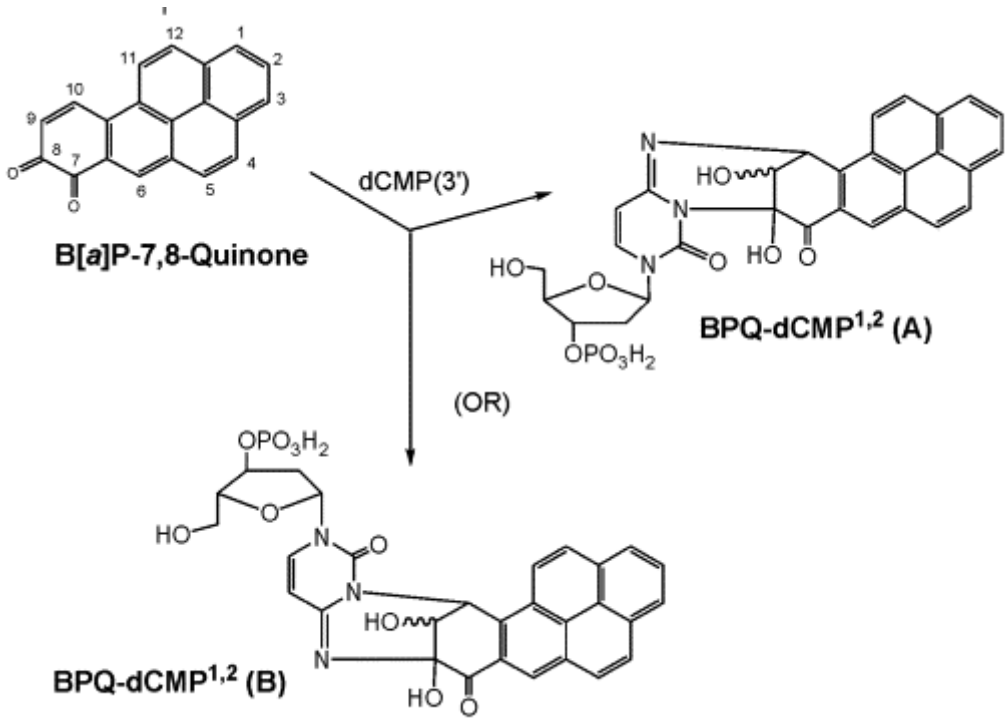
영남대 화학과 [1]대구가톨릭대 안경광학과

Benzo[a]pyrene-7,8-quinone (BPQ) is a family of polycyclic aromatic hydrocarbons(PAH) and is a widely distributed environmental pollutant from the incomplete combustion process of fossil fuel and variety of sources. DNA damage associated with benzo[a]pyrene (B[a]P) metabolites generated by the aldo-keto-reductase family of enzymes (AKR) pathway, including the formation of DNA adducts. We have investigated the conformational characteristics and electrostatic potential of the cyclic BPQ?dCMP(A) and ?dCMP(B) adducts using density functional theory. In the case of the BPQ-dCMP adducts, eight possible structures, each of which consists of two isomers included cis and trans forms, were identified. The shape of BPQ-dCMP adducts is L-shaped conformation. Considering the conformation of the BPQ relative to the nucleotides, BPQ may be located along the minor groove of DNA with BPQ?cytosine adduct.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-574**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Incorporation of ruthenium oxide nanoparticles into polyaniline hollow nanospheres and its application to supercapacitors.

이진호 임상규

국민대 생명나노화학과

Development of the redox supercapacitors with extraordinarily high capability for energy storage is growing attention for their application in a high capacitance battery of cellular phones or hybrid electric vehicles. Among the transition metal oxides used on an electrode material, ruthenium oxide (RuO_2) was reported to show excellent cycle performance and highest specific capacitance. However, only a very thin surface layer of RuO_2 contributes the charge storage process due to its inherently dense morphology. The dissolution and detachment of RuO_2 from the electrode during the cycling is also problematic. To overcome this problem, we incorporated RuO_2 nanoparticles into the polyaniline (PANi) hollow nanospheres. The synergetic effect of highly enhanced surface area of the PANi electrode and incorporation of RuO_2 nanoparticles on the specific capacitance is investigated.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-575**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Direction of insertion of *bis*-intercalated Ru(II)complex in DNA probed by DAPI

김경원 김현정 장윤정 김종문 한성욱[1] 김석규

영남대 화학과 [1]경운대 환경공학과

Binding mode of a *bis*-Ru(II) complex, in which two [Ru(1,10-phenanthroline)H_2dipyrido[3,2-a:2',3'-c]phenazine]H^{2+} were tethered by a 1,3-bis(4-pyridyl)propane linker (refered to Ru-bpp), to DNA has been reported as intercalation. Direction of intercalation of Ru-bpp complex in DNA was investigated using fluorescence probes, 4',6-diamidino-2-phenylindole (minor groove binder) and methyl green (major groove binder), with optical spectroscopy including linear dichroism (LD), circular dichroism (CD) and fluorescence intensity measurement. The absence of the positive induced CD and LD signal of DNA bound DAPI (0.1 ratio) confirms the extrusion of DAPI from DNA by the Ru-bpp at 0.18 ratio and removal of methyl green from DNA. This observance insists the intercalation of Ru-bpp complex through the major groove of DNA.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-576**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of SrTiO3 - TiO2 Hybirdstructure Nanotube for improved Photoelectrochemical Properties via TiO2 Tube with Extended Pore Widening and Application in Dye-Sensitized Solar Cells

서상필 김창우 강영수

서강대 화학과

SrTiO3 and TiO2 heterostructured tubes were fabricated using anodized TiO2 tubes on Ti substrate for dye sensitized solar cell. The pore size of as-anodized TiO2 nanotubes was controlled for TiO2 nanotubes using tetraethylene glycol solvent and morphology of SrTiO3 for inside and outside surfaces of TiO2 nanotubes by Sr under hydrothermal condition. Formations of their hetero-structures are proposed and their photocatalytic acivity is compared with various SrTiO3 morphology[1]. Compared with TiO2 anatase tubes, the enhanced photoelectrochemical property of SrTiO3 - TiO2 tubes of enlarged pore diameter could be attributed to the enhanced of charge separation by TiO2 tubes / SrTiO3.References[1]J. Zhang, J. H. Bang, C. Tang and P. V. Kamat ACS Nano, 2010, 4, 387.Keywords : Hybirdstructure, TiO2 Tube with Extended Pore Widening, SrTiO3

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-577**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Titanium phosphate의 합성과 광촉매 활성 연구

김영용 권기영

경상대 화학과

Titanium 과 Phosphate 의 비율을 조절하므로써 다양한 형태의 Titanium Phosphate (TiP) 를 수열합성법 (Hydrothermal method) 으로 합성하였다. 이런한 화합물들의 형태를 SEM 과 TEM 으로 관찰하였으며 특히 P/Ti = 2 인 조성에서 섬유 형태의 결정을 얻었다. Phosphate 의 양이 줄어듬에 따라서 TiP 와 TiO2 가 함께 혼합물의 형태로 존재하는 것을 확인하였다. 이들을 가지고 Chlorophenol (4-CP), Trichlorophenol (TCP), 와 Bisphenol A (BA) 의 광촉매 분해 반응에 응용하였을 때 Phosphate 의 조성이 줄어듬에 따라 광활성이 증가함을 확인하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-578**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

β-Turn Foldamers of γ-PeptidesBased on 2-(Aminomethyl)cyclobutanecarboxylic Acid and 2-Aminocyclobutylacetic Acid

유재익 강영기

충북대 화학과

We have designed computationally the γ-peptide β-turn structures through the combinations of chirospecific $\gamma^{2,3}$-residues of 2-(aminomethyl)cyclobutanecarboxylic acid (γAmc_4) and chirospecific $\gamma^{3,4}$-residues of 2-aminocyclobutylacetic acid (γAc_4a) with cyclobutyl constraints on the C^{α}-C^{β} bond and the C^{β}-C^{γ} bond, respectively. To check the capability of each β-turn structure to be incorporated into the β-hairpin of α-peptides, the structures of the Ala-based tetrapeptides, hexapeptides, and octapeptides such as Ac-Ala_n-X_2-Ala_n-NHMe (X = γAmc_4 and γAc_4a; n = 1, 2, and 3) were optimized and their relative Gibbs free energies were calculated at the M06-2X/cc-pVTZ//M06-2X/6-31+G(d) level of theory with the implicit solvation model SMD in water. The chirospecific di-γ-peptide of γAc_4a with the (3*S*,4*R*)-(3*S*,4*S*) configurations are found to form the most stable β-turn structure in the gas phase and in water. However, the β-turn structures of chirospecific di-γ-peptides of γAmc_4 are more similar to a type II′ turn of α-peptides than those of γAc_4a dipeptides in the gas phase and in water. Therefore, the γ-peptide β-turn structure of γAc_4a residues with the (3*S*,4*R*)-(3*S*,4*S*) configurations can be used as a β-turn motif in β-hairpins of Ala-based α-peptides.

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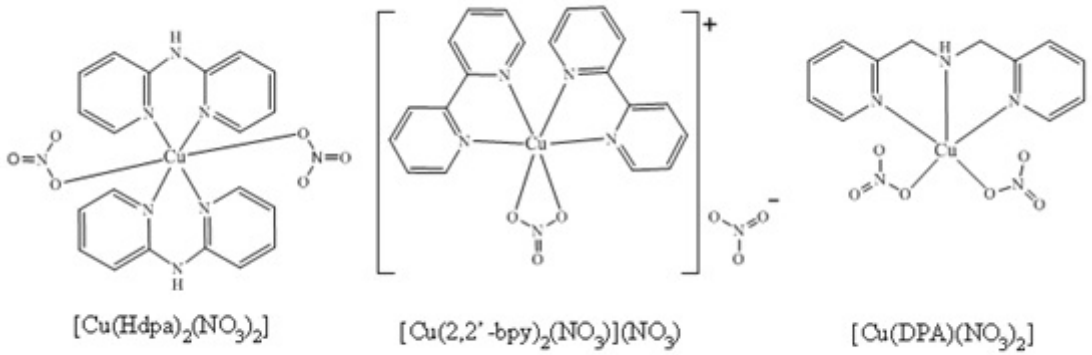
장소: 부산BEXCO
발표코드: **PHYS.P-579**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Real-time detection of DNA cleavage induced by $[Cu(L)_2(NO_3)_2]$ (L=2, 2'-dipyridylamine, 2, 2'-bpy, DPA)

권지혜 박희진 김철[1] 김석규 조태섭

영남대 화학과 [1]서울과학기술대 정밀화학과 친환경소재제품센터

$[Cu(L)_2(NO_3)_2]$ (L=2,2'-Hdpa, 2,2'-bpy, DPA) complexes were synthesized, and their activity as catalyst for DNA cleavage reactions were investigated using electrophoresis and linear dichroism technique (LD). The magnitude of LD signal in the DNA absorption region reflects the flexibility or the length of DNA when the reaction conditions are properly adjusted. Hence, the tracking of the LD intensity change allows a real-time detection of DNA cleavage reaction. The cleavage reaction efficiency with respect to the ligand structure was followed the order of 2,2'-bpy > 2,2'-Hdpa > DPA, where 2,2'-bpy was the most effective.



• Hdpa : dipyridylamine, bpy : 2,2'-bipyridine, DPA : dipicolylamine

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-580**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantum Chemical Calculations of Electronically Excited States :Methacetin(MC), Phenacetin(PC) and Its Solvent-Molecule Clusters

안아름 최명룡

경상대 화학과

Quantum computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. It has played an important role in interpretation and prediction of experimental results. Also it is widely used in the design of new drugs and materials. In this study, theoretical calculations of methacetin(MC), phenacetin(PC) and its solvent-molecule clusters to analyse the spectroscopic data obtained in this laboratory are reported. We calculated the two lowest energy conformers, cis- and trans- MC and PC using density functional theory (DFT) with a 6-311+G(d) basis set and obtained the cis-MC and PC as a global minimum molecule. We further carried out calculations on MC, PC and its solvent-molecule clusters using time dependent-DFT (TD-DFT) to predict excited state molecular information.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **PHYS.P-581**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of axial ligand on the binding mode of M-*meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin to DNA probed by Polarized Spectroscopy

이창윤 정맹준[1] 김석규

영남대 화학과 [1]경북대 나노소재공학부

The binding modes of cationic porphyrins, namely M-*meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin (MTMPyP, where M=free base, Cu(II), Ni(II), Co(III), Mn(III), V(IV)=O and Ti(IV)=O), to native DNA were systematically investigated by polarized light spectroscopies, *viz.* circular and linear dichroism spectroscopy (CD and LD, respectively). At low [porphyrin]/[DNA] ratio, planar porphyrins including TMPyP, CuTMPyP and NiTMPyP exhibited a negative CD signal in the Soret region and large negative, wavelength-dependent LD^r signal which is characteristics of their intercalative binding mode. In the intercalation pocket, the molecular plane of porphyrin is declined to a large extent. As the mixing ratio was increased, a bisignate CD spectrum became apparent for all of the planar porphyrins, while the shape of LD^r remained the same, indicating the coupling of the electric transition moments of the intercalated porphyrins. Thus, coupling can occur between the porphyrins when they are separated at least two DNA base-pairs according to the nearest neighbouring site exclusion model. This coupling interaction was the weakest for NiTMPyP. The porphyrins with axial ligands, namely VOTMPyP, TiOTMPyP, MnTMPyP and CoTMPyP bind to the exterior of the DNA at a low [porphyrin]/[DNA] ratio, which is indicated by the positive CD signal in the Soret region. The absorption and LD spectra in the Soret region were treated as the sum of two transitions to calculate the angle between each of the electric transition moments of the porphyrin, i.e., the B_x and B_y transitions relative to the local DNA helix axis. The angle of one the two electric transitions of the porphyrin is in the range of 56°~59°, while the other is in the range of 59°~65°. Increasing the porphyrin density resulted in the appearance of an interaction between the bound porphyrins, which was indicated by the distorted CD spectra. In contrast with the planar porphyrins, which are parallel to each other in the intercalation pocket when they interact by themselves, the

molecular plane of the porphyrin with the axial ligand tilts more toward the local DNA helix axis as the population of porphyrins was increased. CoTMPyP exhibited complicated CD and LD spectra that were impossible to explain by the presence of two porphyrin species: those with a monomeric external binding and electric coupling. Since the CoTMPyP-DNA complex started to aggregate at relatively low [porphyrin]/[DNA] ratios, the complication may due to the involvement of extensive porphyrin assembly.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-582**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Y2O3:Eu3+ Nanostructures: An Optical Study for Highly Efficient Wavelength Conversion Nanoparticles

Abhijit Pandurang Jadhav Amol Uttam Pawar 강영수

서강대 화학과

Synthesizing phosphor nanoparticles with controlled shape, size and doping of sensitizing elements is the key factor for their efficient wavelength conversion applications. In the present article we report an optical study of red emitting Y2O3:Eu3+ nanostructures with homogeneous size distribution and different dopant concentrations through chemical co-precipitation process. An effect of reaction temperature on the particle size and dopant incorporation in the host crystal is reported in this work. Higher reaction temperature produced phosphor nanoparticles of bigger average size, lower size dispersion and higher dopant contents. Maximum percentage quantum efficiency of as synthesized nanoparticles was found to be around 86.49%. Effect of dopant concentration on the photoluminescence (PL) emission characteristics and PL quenching in the nanophosphors is reported. These nanoparticles have great potential for its application in wavelength converting devices.Keywords: Europium doped yttrium oxide, concentration quenching, wavelength conversion applications, quantum efficiency.References: -1.A. P. Jadhav, C. W. Kim, H. G. Cha, A. U. Pawar, N. A. Jadhav, U. Pal and Y. S. Kang, J. Phys. Chem. C, 2009, 13, 136002.A. P. Jadhav, A. Pawar, C. W. Kim, H. G. Cha, U. Pal and Y. S. Kang, J. Phys. Chem. C, 2009, 113, 16652.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-583**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electronic Spectroscopic Studies of Jet-cooled n-Cyanoindole (n=3, 4, and 5) and Its Water Clusters

민아름 문철주 안아름 최명룡 김성근[1]

경상대 화학과 [1]서울대 화학부

n-Cyanoindole (n=3,4,and 5) as a derivative of indole has an important intrinsic property for its enormous biological activities in biological systems. We measured the excitation spectra of n-Cyanoindole (n=3,4,and 5) monomer using resonance-enhanced multiphoton ionization (REMPI) in the gas phase. In these spectra, we show that vibronic bands are consisted of very simple and sharp peaks at low frequency but very congested and broad bands at high frequency. Then, we obtained UV-UV hole-burning spectra to identify the number of conformers in the cyanoindole system. We also calculated the optimized structures of n-Cyanoindole (n=3,4,and 5) by time-dependent density functional theory (TD-DFT) with a 6-311++G** basis set. For the their water clusters, its three (n=3,4,and 5) REMPI specta have a red-shifted origin band compared to that of the monomer. And we show a clear identification of the two conformers of 3-Cyanoindole-water clusters and single conformer of 4,5-cyanoindole water clusters.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-584**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

β-Sheet foldamers of γ-peptides based on 2-(aminomethyl)cyclopropanecarboxylic acid and 2-aminocyclopropanylacetic acid

이지향 강영기

충북대 화학과

The β-sheet structures of γ-peptides have been designed computationally by the chirospecific γ-residues of 2-(aminomethyl)cyclopropanecarboxylic acid (γAmc$_3$) and 2-aminocyclopropanylacetic acid (γAc$_3$a) with cyclopropanyl constraints on the C$^{\alpha}$—C$^{\beta}$ and the C$^{\beta}$—C$^{\gamma}$ bonds, respectively, using the meta-hybrid M06-2X density functionals in the gas phase and in water. Solvation free energies were calculated using the Solvation Model based on Density (SMD) method. The double-strands of di- and tetra-peptides of chirospecific (2*R*,3*R*)-γAmc$_3$ and (3*S*,4*R*)-γAc$_3$a residues are found to form the stable β-sheet structures in the gas phase and in water. It is found that the parallel β-sheet structures for tetrapeptides of γAmc$_3$ and γAc$_3$a residues are more stable than their antiparallel ones in the gas phase and in water. In the case of dipeptides, the parallel β-sheet structure of γAmc$_3$ residue is more stable than its antiparallel one, whereas the parallel β-sheet structure of γAc$_3$a residue is less stable than its antiparallel one in the gas phase. In particular, the parallel β-sheet structures are found to be stabilized by intermolecular C—H···O and N—H···O hydrogen bonds, which is consistent with the X-ray structures.

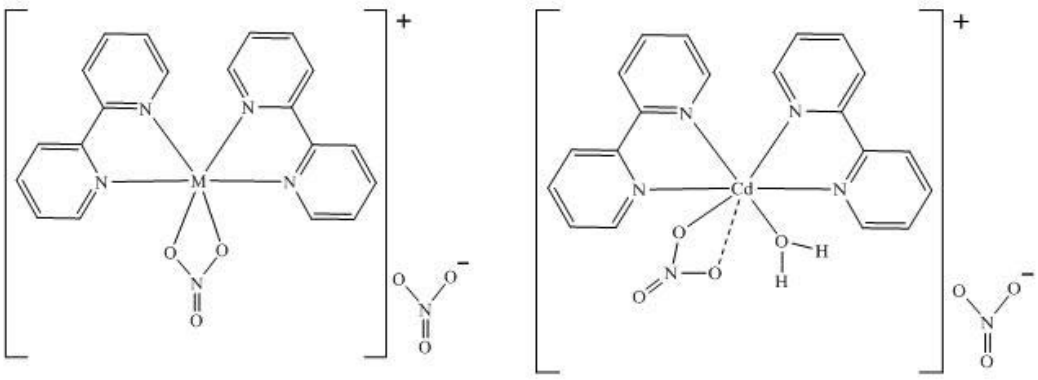
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **PHYS.P-585**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Real-time detection of DNA cleavage induced by [M (2, 2'-bpy)$_2$ (NO$_3$)](NO$_3$) Divalent Cations: M = Cu, Zn, and Cd

박희진 권지혜 김철[1] 김석규 조태섭

영남대 화학과 [1]서울과학기술대 정밀화학과 친환경소재제품센터

[M(2,2'-bpy)$_2$(NO$_3$)](NO$_3$) (M = Cu, Zn, Cd) complexes were synthesized, and their activities as catalysts in the DNA cleavage reactions were investigated using electrophoresis and linear dichroism (LD) techniques. The magnitude of linear dichroism (LD) intensity of DNA decreased by the nicking of one of the strand of double helical DNA or cleaving of both strands, since the magnitude of LD signal in the DNA absorption region is directly proportional to the flexibility or the length of DNA when the reaction conditions are properly adjusted. Thus, the profile of LD signal change upon reaction time demonstrates real-time kinetic aspects of DNA cleavage reaction. [Cu(2,2'-bpy)$_2$(NO$_3$)](NO$_3$) complex exhibited the best efficiency.



[M(2,2'-bpy)$_2$(NO$_3$)](NO$_3$) (M=Cu, Zn) [Cd(2,2'-bpy)$_2$(NO$_3$)](NO$_3$)

❖ bpy : 2,2'-Bipyridine

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **PHYS.P-586**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

REMPI and UV-UV Hole-burning Spectroscopic Studies of Jet-cooled Methacetin and Phenacetin

문철주 민아름 안아름 최명룡 김성근[1]

경상대 화학과 [1]서울대 화학부

Methacetin (MC) and phenacetin (PC) are both one of the typical synthetic fever reducers as similar to acetaminophen (AAP), a major ingredient of Tylenol?. AAP, MC, and PC are derivatives of acetanilide. They are substituted by hydroxyl, methoxyl, ethoxyl group in the para position of acetanilide, respectively. In our previous work, we investigated the conformational structures of jet-cooled AAP. In this work, we present the conformational investigations of MC and PC using one color resonant two-photon ionization (REMPI) and UV-UV hole-burning spectroscopy. Continuously, we investigate conformational information of respective water clusters. In addition, the contribution of the methyl internal rotation of MC and PC was investigated.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-587**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Method development for the prediction of long-term stress relaxation behaviors of absorbable PLLA stent from accelerated aging techniques

고석연 고영주 최동훈[1]

(주)삼양바이오팜 의약연구소 [1]연세대 내과학교실/심장내과

In the medical device industry, it is important to predict the shelf life of polymer-based devices from accelerated aging techniques because real-time testing is ver time-consuming in most cases. In this work, test method for predicting stress relaxation behavior of PLLA stent, which is one of the bioabsorbable polymeric stents, has been developed by adjusting two kinds of well-known shelf life prediction methods, variable Q_{10} method and D&A method.Stress relaxation results were evaluated by measuring normal force pressed on the stent to its half diameter. And tests were performed at room temperature to 55℃. As a result, it took about 3~4 days for PLLA stents to be relaxed to 40% of its maximum stress at 37℃. And we could predict that after 6 months later only about 28% stress will remain at the same temperature.Though these methods couldn't be directly applied on the long-term behavior of PLLA stent in blood vessels, we could make a new step forward improving prediction method by introducing shelf life predicting methods for medical device to predict stress relaxation behavior of PLLA stent.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-588**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chiral Separation of Basic Compounds on Sulfated β-Cyclodextrin-Coated Zirconia Monolith by Capillary Electrochromatography

박정학 김은주 박진명 정정애

영남대 화학과

Sulfated β-cyclodextrin (SCD)-coated zirconia monolith was used as the chiral stationary phase in capillary electrochromatography for chiral separation. Adsorbed Lewis basic SCD moieties on Lewis acid sites of the zirconia surface provided a stable chiral stationary phase in reversed-phase eluents. Retention, chiral selectivity and resolution of a set of six basic chiral compounds were measured in eluents of varying pH, composition of methanol and buffer. Optimum mobile phase condition for the separation of the compounds was found to be methanol content of 30%, buffer concentration of 30mM and pH of 4.0.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-589**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoarray Chip for High-Sensitive Immunodiagnosis of Human Thyrotropin

이승아 강성호

경희대 응용화학과

The gold nanoarray chip as a key component of a biosensor platform was feasible for accurate and highly sensitive detection of human thyroid-stimulating hormone (TSH) known as thyrotropin. Optimum condition was successfully determined using a gold nano-patterned sandwich immunoassay chip to detect human TSH (hTSH). A 100 nm gold array chip could make use of smaller sample volumes and achieve higher sensitivities due to the small size of the entire array. The total internal reflection microscopy enabled quantification of the biomarker protein (hTSH) over a wide dynamic range from the zM to the pM level. The detection limit was about 12,000 times lower compared with those obtained by traditional chemiluminescence immunoassays technique applied to the evaluation of TSH in human serum. The TSH-nanoarray chip method based on a single-molecule sandwich immunoassay produced an improved detection sensitivity of TSH and demonstrated the possibility of this assay's use for diagnosing disease.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-590**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Combination of Palm PCR and Portable Capillary Electrophoresis for Fast On-site Analysis of Influenza A Virus

임서연 강성호

경희대 응용화학과

It is critical to establish on-site analysis providing efficiency by disregarding from place and time constraints in detection of pathogens. We developed a fast combined method of Palm polymerase chain reaction (PCR) and portable capillary electrophoresis (CE). Being a united diagnosis system enables us to diagnose a disease without exposure to chemical changes or pollutions while transferring a sample. In addition, our system is appropriate for rapid diagnostics, in the way that 'Palm PCR' which performs high-speed nucleic acid amplification and portable CE facilitating sensitive DNA analysis with high precision and detection sensitivity allows five times or more improvement in the time-to-results over individual commercial PCR and CE. This is because, the total time-required to complete the accurate diagnosis takes within 30 min. Herein, the combined method was used to identify two influenza A-associated genes (the HA and NP genes of the novel H1N1 influenza). Separation was achieved with a sieving matrix of poly(vinyl pyrrolidone) (M_r = 1 300 000) in 1× TBE Buffer. Therefore, the combined Palm PCR-portable CE system should be an improved fast diagnostic method in molecular gene diagnostics.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-591**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study about Stability of Co-hydrotalcite Synthesis from co-precipitation process

김빛내리 권수한

충북대 화학과

층상 이중 수산화물인 하이드로탈사이트는 두 층 사이로 음이온을 포획하는 우수한 기능을 가지고 있다. 다양한 종류의 수지에 여러 다른 첨가제와 함께 사용되어 수지의 물성의 개선 및 안정성을 향상시킬 수 있다. 본 연구는 공침법을 이용하여 하이드로탈사이트에 코발트이온을 침착시키는 것을 목적으로 한다. 코발트화합물에서 코발트이온을 얻어 하이드로탈사이트에 침착시킨 후 반응시간, 온도, pH, 전압을 변화시켜 반응성을 알아보고 나타난 결과를 통해 최적조건을 찾고, 첨가제로서 고효율적인 성질이 나타나는지 알아본다.
본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-592**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The determination of methylene chloride(MC) in aqueous drug solutions by headspace-GC-FID using standard addition method

경규진

(주)삼양바이오팜 의약연구소/분석센터

In this work, the quantitative analytical method of methylene chloride(MC) in aqueous drug solutions has been developed by HS-GC-FID(Headspace-Gas chromatography-Flame ionization detector). A number of analytical methods such as direct aqueous injection and liquid-liquid extraction direct injection were tried to determine MC in aqueous drug solutions. But these methods couldn't be applied because of some limitations of low column stability(direct aqueous injection) and solvent contamination risk(liquid-liquid extraction). Finally the quantitative analytical method has been developed using headspace technique, but only if samples are diluted into dimethylacetamide(DMA). The chromatographic analysis was performed on Supelco OVI-G43 column and samples were diluted 10-fold into dimethylacetamide(DMA). Because these samples have complex matrices such as drug substance(API), biodegradable polymers and salts(calcium chloride, sodium succinate), we evaluated the matrix effect through a comparison of external standard and standard addition method. And it showed a decrease of the analyte signals in the presence of matrix components. Thus, considering this matrix effect, the standard addition method was adopted for a reliable quantitative analysis of MC in aqueous drug solutions and this standard addition method demonstrated good specificity, linearity, accuracy and precision.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Resolution of Chiral Oxazolidinones and some important chiral compounds on Recently Prepared Four π-Acidic Chiral Stationary Phases

유정재

경북대 대학원 화학과

Oxazolidinones are mainly used as antimicrobials. The antibacterial effect of oxazolidinones is by working as protein synthesis inhibitors, targeting an early step involving the binding of N-formylmethionyl-tRNA to the ribosome.[1] In chemistry, they are useful as Evans auxiliaries, which are used for chiral synthesis. Four 3,5-dinitrobenzoyl derivative Pirkle type chiral stationary phases(CSPs) were used for resolution of eleven chiral oxazolidinones. In addition to the chiral oxazolidinones, Some important chiral compounds, 2,2,2-trifluoro-1- (9-anthryl)ethanol, 1,1'-bi-2-naphthol, 6,6'-dibromo-1,1'-bi-2-naphthol, 1,1'-binaphthyl-2,2'-dihydrogen phosphate, naproxen, N-benzoyl-DL-valine, 5-phenyldihydrofuran-2(3H)-one, N-(3,5-Dinitrobenzoyl)-DL-phenylglycine, were used as analytes for the resolution on the four CSPs.[1] Shinabarger, D. (1999). "Mechanism of action of the oxazolidinone antibacterial agents". Expert Opinion on Investigational Drugs 8 (8): 1195?1202.

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Deamination reaction between histidine and glutamine in APCI negative ion mode

김여울 최성신

세종대 화학과

Amino acids are organic compounds which consist of a basic amino group ($-NH_2$), an acidic carboxyl group (-COOH), and an organic R group (or side chain). Deamination is the process in which amino groups are removed from amino acids, and it is important reaction in biological systems to convert excess amino acids into usable resources such as hydrogen and carbon. Liquid chromatography/mass spectrometry (LC/MS) is one of useful tools for the analysis of amino acids. Atmospheric pressure chemical ionization (APCI) is widely used for analyzing polar and relatively non-polar compounds. In this study, a mixture of twenty protein amino acids was analyzed using APCI-MS and the heterocluster anion of histidine and glutamine ($[His + Gln - H]^-$ and $[His + Gln - 18]^-$) was observed. Formation mechanism of $[His + Gln - 18]^-$ was examined using deuterated amino acids.

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Influence of 1,2-unit on pyrolysis behaviors of SBR

권혁민 최성신

세종대 화학과

Styrene-butadiene rubber (SBR) is a copolymer consisting of styrene and butadiene. Butadiene has three microstructures of 1,2-unit, *cis*-1,4-unit, and *trans*-1,4-unit. Grades of SBR are determined by contents of the four components. SBR has good abrasion resistance and good aging stability when protected by additives, and is widely used in car tires. Microstructural analysis of SBR is going on in many ways such as Fourier transformation infrared spectroscopy (FTIR), matrix assisted laser desortion/ionization-mass spectrometry (MALDI-MS), nuclear magnetic resonance spectroscopy (NMR), and pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS). In particular, Py-GC and Py-GC/MS are useful for obtaining information of the chemical structures of polymeric materials and their compositions. In this study, SBRs with different microstructures were pyrolyzed and the pyrolysis products were analyzed using GC/MS. Major pyrolysis products of SBR were butadiene, benzene, toluene, 4-vinylcyclohexene, ethylbenzene, styrene, 2-phenylpropene, indene, azulene, 3-phenylcyclopentene, 4-phenylcyclohexene, and biphenyl. The relative abundances of pyrolysis products differed according to the kinds of SBRs.

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Comparative study of corrosion inhibition of aluminum in acidic and neutral chloride media by some amino acids

윤종화 김연규

한국외국어대 화학과

Cl-가 포함된 용액에서 일어나는 Al 의 부식에 대하여 methionine 과 histidine 의 부식 억제 효과를 조사하였다. Methionine 은 낮은 덮힘율로 Al 표면에 Langmuir adsorption isotherm 에 따른 흡착이 일어나며, histidine 은 상대적으로 높은 덮힘율로 10-4 M 이하 농도에서 Al 표면에 Langmuir isotherm, 10-4M 이상 농도에서 Temkin adsorption isotherm 에 따른 흡착이 일어나는 것으로 보인다.

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Method Development and Validation for Ascorbic acid in Human Plasma using High Performance Liquid Chromatography

김윤정 하나[1] 한송희[1]

전북대 병원 임상시험센터 분석팀 [1]전북대병원 임상시험센터

A high performance liquid chromatography (HPLC) method for the determination of ascorbic acid in human plasma was developed. The ascorbic acid in human plasma was extracted and stabilized using 10% m-phosphoric acid. The method was followed by analysis of ascorbic acid in Symmetry (C_{18}, 4.6 × 250 mm, particle size, 5 μm, 100 Å) with mobile phase of 5 mM Hexadecyltrimethylammonium bromide and 50 mM KH_2PO_4 solution at a flow rate of 1.0 mL/min. The analyte was determined using HPLC with UV-vis detector (254 nm and 265 nm) and isoascorbic acid as an internal standard. Method validation was performed in human plasma, including parameters of specificity, precision, accuracy, linearity, limit of detection, and quantification during intra- and inter-day. The standard calibration curves for ascorbic acid in human plasma were linear over the concentration range of 1 ~ 100 μg/mL. This HPLC method for ascorbic acid is useful in the pharmacokinetic study of ascorbic acid in human plasma after oral administration of food or drugs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of melanoma using antibody-conjugated quantum dots in coculture model for high through-put screening system

최영선

한국파스퇴르연구소 Nano/Bio Chemistry

We proposed an effective strategy for evaluating targeting specificity of antibody-conjugated QD nanoprobe in coculture system mimicking in vivo-like tumor microenvironment in which cancer cells grow with normal cells. Analysis of the images was performed with automated confocal microscopy. We have employed melanoma-melanocyte coculture model to assess the specific binding of QDs conjugated with melanoma antibodies. Conjugation of antibodies to QD significantly improved the melanoma specificity, while unconjugated antibody alone suffered from non-specific binding to melanocytes. Concentration-dependent binding and competitive inhibition studies with QD-antibody conjugate reproducibly proved the specificity to melanoma cells against melanocytes. Specificity and targeting efficiency of nanoprobes evaluated in a simple coculture model may provide a reasonable assessment for in vitro diagnosis of early stage melanoma development before in vivo studies. Further, a rapid and sensitive cancer cell detection system demonstrated herein may allow for development of high through-put screening platforms for early cancer diagnosis and anti-cancer therapeutics.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural investigations of $xLi_2MnO_3 \cdot (1\text{-}x)Li(Mn_aNi_bCo_c)O_2$(x = 0.35, 0.40, 0.50) cathode materials for lithium-ion battery

서가영 이영일

울산대 화학과

Recently, a family of structurally integrated $xLi_2M'O_3 \cdot (1\text{-}x)\ LiMO_2$ electrode materials (M′= Mn, Ti and M = Mn, Ni, Co) have been received a great deal of attention owing to their high capacity over 200 mAh/g when electrochemically activated above 4.4 V by the removal of Li and oxygen from their structure on charge. Such structurally integrated electrode materials are expected to replace the present $LiCoO_2$ cathode material in lithium ion batteries due to their high energy density and low cost. In this work, structural investigations of manganese-rich $xLi_2MnO_3 \cdot (1\text{-}x)Li(Mn_aNi_bCo_c)O_2$(x = 0.35, 0.40, 0.50) cathode materials has been performed by ^{7}Li MAS NMR.

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발표코드: **ANAL.P-600**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The study of structural properties for soft carbon treated with H_3PO_4 as an anode material of Li ion batteries

이경은 권영민 이영일

울산대 화학과

Lithium ion batteries have been widely used as power sources for portable electronic devices, electronic vehicles, and energy storage systems for renewable energy. The soft carbon materials have been recently received much attention as an anode for the large scale of Li ion battery. Soft carbon has graphene layers neatly stacked but less-long order. Generally, it has excellent high performance, but low discharge capacity and low crystallinity than that achieved with the conventional carbonaceous materials. Recently researchers have been studied addition of various atoms into soft carbon for improving both high capacity and high performance. Herein, the soft carbon anode materials treated with phosphoric acid to achieve high electrochemical properties have been characterized by using ^{31}P magic angle spinning (MAS) NMR and SAXS. ^{31}P MAS NMR spectra are shown that the two types of P are encapsulated. With SAXS profiles, interlayer distance and inter-domain distance in the soft carbon have been calculated.

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발표분야: 분석화학

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Synthesis, characterization and evaluation of pentacyanoferrate-conjugated small molecules using for homogeneous electrochemical immunoassay.

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단국대 첨단과학대학 화학과 [1]단국대 화학과

A homogeneous electrochemical immunoassay based on pyridyl-N coordination to pentacyanoferrate for the detecting small organic antigens is presented. The unique point in this paper is the direct conjugation of pyridyl-N in small organic antigen to pentacyanoferrate. The use of pentacyanoferrate as an electrochemical label is promising means owing to its good electrochemical property, which is utilized for the electrical signal for the electrochemical immunoassays. As a redox mediator and small antigen, pentacyanoferrate-(4-aminomethylpyridine-hippuric acid) (Fe-HA), was synthesized and electrochemically characterized onto the ITO electrodes. The synthesized Fe-HA shows well-reversible redox peaks at $E_{1/2}$= 0.2 V vs. Ag/AgCl. The ultraviolet-visible spectrum of Fe-HA solution also suggested the direct coordination between pyridyl-N and the iron ions. The competitively on the interaction Fe-HA and free HA to anti-hippuric acid antibody (anti-HA), which can generate the electrical signals linearly proportional to the HA monitored by differential pulse voltammetry (DPV), with the detection limit of 1 μg/mL of HA. While pentacyanoferrate-based immunoassay is in its simplicity, the proposed immunoassay offers attractive opportunities for detecting small antigens in the health care area.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Heterogeneous electrochemical immunoassay for detection of Tuberculosis using cationic polymer-modified electrodes

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단국대 나노바이오의과학과 [1]단국대 화학과

Heterogeneous electrochemical immunoassay for rapid and quantitative detection of Tuberculosis in human serum was proposed in this work. We report the determination of antibody-Tuberculosis (*anti*-TB) using the ionic charge-selective electron transfer on the polyelectrolytes-modified indium-tin oxide(ITO) electrode. The surface morphology of the modified polyethyleneimine (PEI) immobilized ITO electrode was examined by scanning electron microscopy (SEM). Antigen-Tuberculosis(Ag-TB) was immobilized via EDC/NHS bioconjugation onto the PEI modified ITO electrode. After the interaction between Ag-TB and (*anti*-TB) on ITO electrode. the electrical signals proportional to the Ag-TB was monitored by cyclic voltammetry (CV) and differential pulse voltammetry (DPV).Because of blocking effect of heavy molecule, electron transfer is slowly than absence anti-TB, and then current was decreased.The resulting currents were linearly related with the concentration of anti-TB. The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different antigens in the health care area.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of an efficient polystyrene stationary phase by the modification of silica monolith particles of improved characteristics via RAFT polymerization

Faiz Ali 정원조

인하대 화학과

Small sized (ca 2 um) silica monolith particles with better particle and pore size distribution were prepared by an improved and simplified procedure. The silica monolith particles were reacted with 4-chloromethylphenylisocynate followed by diethyldithiocarbamate to yield initiator attached silica particles. Radical addition fragmentation transfer (RAFT) polymerization of styrene upon them was carried out to give polystyrene attached stationary phase whose separation efficiency was well above 30,000 when packed in a column of 30 cm length.

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Comparison of different columns in the analysis of dextrin using High-performance liquid chromatography electrospray ionization-mass spectrometry (HPLC ESI-MS)

박세환 권진주[1] 김정권

충남대 화학과 [1]국방과학연구소

Dextrin is actually a name for a type of low molecular weight carbohydrates, where dextrin is produced by enacting the process of hydrolysis on starches. In this study, the analysis of dextrin was performed by reversed phase high performance liquid chromatography with ultraviolet (UV) and refractive index (RI) detectors. The performances of two different columns (ODS C_{18} and amine) which are frequently used in the analysis were compared in the analysis of dextrin. Isocratic elution was used to elute out sample using 10~100 % acetonitrile. The absorbance of dextrin was detected at 191 nm. The UV detector wavelength was using of 191 nm. The dextrin solution was prepared in a concentration of 10 mg/ml (10000 ppm) in 1 mM sodium acetate. Adjusted retention time, retention time of unretained solute, retention time of solute of interest, intensity, W1/2, number of plates, and capacity factors were calculated based on the LC chromatograms. Each column has shown unique properties. In case of SiO_2-based amine column, 60% ACN has to be used to elute out the dextrin in similar time scale from the other ODS C_{18} column using 75% ACN. Overall, ODS C_{18} column showed the better performance. The experimental condition for the LC-ESI-MS analysis of the dextrin sample was optimized. In HPLC, a SiO_2-based amine column is used to separate dextrin where isocratic elution using 10% ACN was used to elute out the dextrin from the amine column. The LC-ESI-MS analysis of the diluted dextrin sample provided adduct ions of $(C_6H_{10}O_5)nNH_4^+.H_2O$ at m/z 684.2 for n= 4, m/z 846.3 for n= 5, m/z 1008.2 for n= 6, m/z 1170.4 for n= 7, m/z 1332.4 for n= 8, and m/z 1494.4 for n=9 and $(C_6H_{10}O_5)nNH_4^+$ at m/z 666.3 for n= 4, m/z 828.4 for n= 5, m/z 990.4 for n= 6, and m/z 1152.4 for n= 7. The detailed experimental procedures and results will be provided during the presentation.

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A substitution effect in the TEMPO-Bz-Peptide free radical initiated peptidesequencing mass spectrometry

오한빈 문봉진

서강대 화학과

A variety of radical-based peptide sequencing mass spectrometry methods have been developed in recent years, whose examples include electron capture dissociation, electron transfer dissociation, photodissociation of photolabile group, UV photodissociation, collisional homolytic cleavage of radical precursor, and so on. Among these methodologies, the collisional homolytic cleavage of radical precursor molecule, for example, o-TEMPO-Bz-NHS, is the focus of the present study. When collisional activation is applied to o-TEMPO-Bz-peptides, facile homolytic cleavage occurs between the benzyl carbon and the oxygen of TEMPO moiety, thus producing benzyl radical peptide cations. Upon the additional collisional activation on these benzyl radical peptide cations, this localized radical site further induces peptide backbone fragmentations. These processes are referred to as 'free radical initiated peptide sequencing (FRIPS)'. In the current study, we added a functional group to the benzene ring in order to shed light on how a functional group substitution affects the radical induced peptide sequencing. The added functional group included NO2, Br, OMe, and CN. Interestingly, the substituted o-TEMPO-benzyl group affected the FRIPS process, yielding MS3 spectra with different fragmentation patterns. The precursor survival yields were also obtained as a function of the applied collision energy in order to shed light on the mechanistic aspect of the substitution effect on the FRIPS process. In the conference, the details of the observed mass spectra will be presented.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Au/Ag Hollow-Shell Embedded Silica Nanoparticles as SERS Probes for Multiplex Detection

강호만 임준혁[1] 경산[1] 김종호[2] 정대홍[3] 이윤식[1]

서울대 협동과정 나노과학기술전공 [1]서울대 화학생물공학부 [2]한양대 화학공학과 [3]서울대 화학교육과

Optical imaging has emerged as a promising techniques due to several advantages such as little harmful radioactivity, high sensitivity and spatial resolution, high-throughput capabilities, and low costs [Nat. Rev. Drug Discovery 2008, 7, 591-607]. However, it has the limited penetration depth due to light scattering and absorption of the hemoglobin and water in animal tissues. Therefore, near-infrared (NIR) window (~700-900 nm) region has been recently considered to be an alternative region to improve the penetration depth of the tissues [Nat. Biotechnol. 2001, 19, 316-317]. Here, we report an approach to modulate optical properties of plasmonic Au/Ag hollow-shell (HS) assemblies on silica nano sphere template by using galvanic replacement reaction to generate reproducible signal intensity and high sensitivity at NIR laser source (785 nm). The plasmonic Au/Ag HS can exhibit single-particle SERS signal with high signal-to-noise ratio. Furthermore, we obtained the SERS signals from deep tissue phantom up to 7 mm depth at NIR excitation laser, and demonstrated the capability of NIR-sensitive SERS nanoprobes for in vivo multiplex detection in a live animal model, and furthermore, for in vivo multiplex imaging, diagnosis and screening of antibody drugs.

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Simultaneous Multiple Biomarker Detection for the Early Diagnosis of Acute Myocardial Infarction (AMI) using Surface-Enhanced Raman Scattering (SERS)

박경아 김기형[1] 주재범

한양대 생명나노공학과 [1]한양대 바이오나노공학과

A simultaneous immunoassay technique using surface-enhanced Raman scattering (SERS) has been developed for the multiplex detection of cardiac markers. Three biomarkers, troponin I, CK-MB, and myoglobin, were selected as target markers in this work. Here, the detection of single biomarker cannot provide a definitive information about the disease because its sensitivity is very low due to the possibility of the false positive result, different duration and peak elevation time of each biomarker in the blood. To solve this problem, it is necessary to monitor three biomarkers simultaneously. For this purpose, hollow gold nanosphere (HGN) was used as a detection probe and magnetic bead as a capturing substrate. The sandwich immunocomplex format using monoclonal antibody-antigen-monoclonal antibody set has been adopted for this assay. Here we report a preminary result for the multiplex detection of three cardiac markers.

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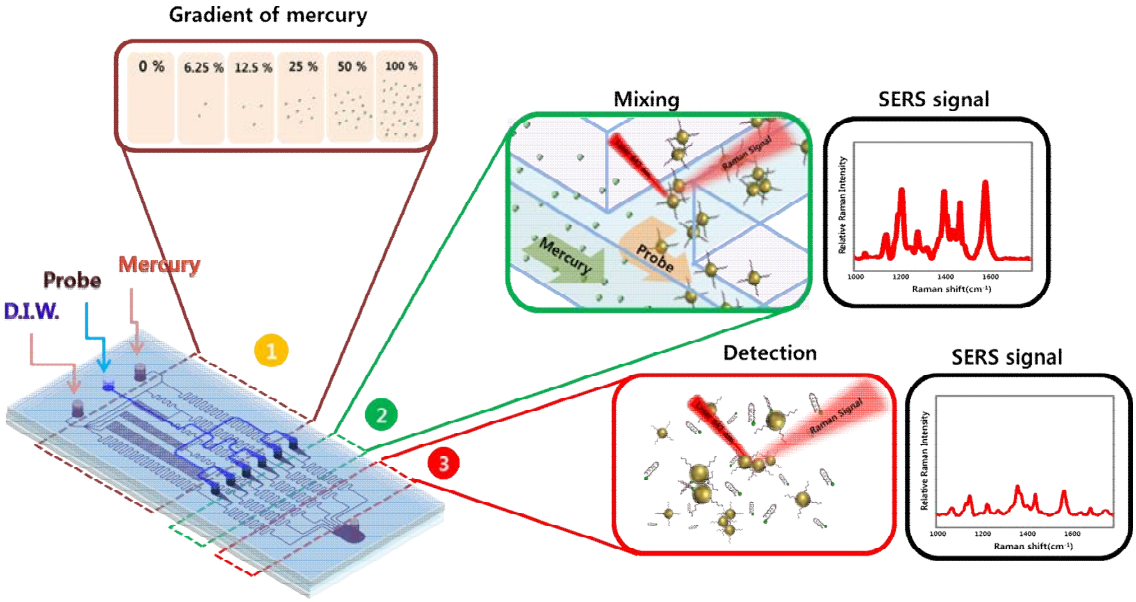
Sensitive mercury detection using SERS-based microfluidic sensor

박세휘 김기형 주재범[1]

한양대 바이오나노공학과 [1]한양대 생명나노공학과

The accumulation of mercury in human body causes various harmful effects such as brain and neurological damage and myocardial infarction. In this study, we report a novel method for tracing the mercury (II) ions in water using a surface-enhanced Raman scattering (SERS)-based microfluidic gradient chip. This gradient chip is made of a programmable and fully automatic channel for generating different concentration for mercury (II) ions and therefore obtains a standard curve directly from the chip. In addition, aptamer-conjugated Au_{core}/Ag_{shell} nanoparticles have been used as efficient SERS probes. The reason for this selection is that gold colloid is superior to other colloids in long-term stability, and silver colloid has 100-1000 times greater Raman signal enhancement effect than gold colloid. Thus, gold nanoparticles were coated with silver for maximum Raman enhancement. The SERS detection together with microfluidic gradient chip using aptamer-conjugated Au_{core}/Ag_{shell} nanoparticles provides a selective detection of mercury (II) ion in drinking water. In the presence of mercury (II) ions, Cy3-labeled DNA aptamers were belived to be released from the metal surface causing a decrease in the observed SERS signal intensity. Quantitative analysis of mercury (II) ions was performed by monitoring Raman peak intensity of Cy3 at 1,590 $cm^{?1}$ and its LOD was estimate to be 0.312 μM. The proposed microfluidic gradient chip shows its capability for obtaining a standard curve for mercury ions in simple and accurate manner.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Fast and sensitive recognition of various explosive compounds using Raman spectroscopy and principal component analysis

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Recently, the development of methods for the identification of explosive materials that are faster, more sensitive, easier to use, and more cost-effective has become a very important issue for homeland security and counter-terrorism applications. However, limited applicability of several analytical methods such as, the incapability of detecting explosives in a sealed container, the limited portability of instruments, and false alarms due to the inherent lack of selectivity, have motivated the increased interest in the application of Raman spectroscopy for the rapid detection and identification of explosive materials. Raman spectroscopy has received a growing interest due to its stand-off capacity, which allows samples to be analyzed at distance from the instrument. In addition, Raman spectroscopy has the capability to detect explosives in sealed containers such as glass or plastic bottles. We report a rapid and sensitive recognition technique for explosive compounds using Raman spectroscopy and principal component analysis (PCA). Seven hundreds of Raman spectra (50 measurements per sample) for 14 selected explosives were collected, and were pretreated with noise suppression and baseline elimination methods. PCA, a well-known multivariate statistical method, was applied for the proper evaluation, feature extraction, and identification of measured spectra. Here, a broad wavenumber range (200-3500 cm^{-1}) on the collected spectra set was used for the classification of the explosive samples into separate classes. It was found that three principal components achieved 99.3 % classification rates in the sample set. The results show that Raman spectroscopy in combination with PCA is well suited for the identification and differentiation of explosives in the field.

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Detection of *Escherichia coli* Bacteria Using Surface-Enhanced Raman Scattering

고주희 주재범[1]

한양대 바이오나노공학과 [1]한양대 생명나노공학과

The development of rapid, simple, cost effective, highly sensitive and robust methods for bacteria detection still remains a challenge. Although rapid bioanalytical methods shorten assay times from days to few hours, in most of cases they require a pre-analytical cultivation enrichment to reach necessary detectability as well as to remove interferences. Cultivation enrichment can be substituted by biospecific purification procedures such as immunomagnetic separations. In this paper, we demonstrate a fast and highly sensitive assay for E. coli bacteria detection using antibody-conjugated gold nanoprobes and surface-enhanced Raman scattering technique. Here, the gold nanoparticle was used as a detection probe, and the magnetic bead as a capturing substrate, respectively. We performed this novel bacteria assay by conjugating the *E. coli*-recognizing LPS on the gold nanoprobe surface, thereby enabling targeted binding and detection of *E. coli* cells. The sandwich format is employed, in which the whole bacteria cell is captured by an antibody-immobilized magnetic bead and detected upon binding to Raman-reporter tagged gold nanoprobes. Various intensity changes of Raman spectra obtained in the presence of different concentrations of *E. coli* will be shown in this presentation. This novel SERS-based bacteria detection is a simple and fast sensing technique which can be applied to early pathogenic bacteria diagnosis.

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Quantitative Fluorescent-free Detection of Troponin by Differential Interference Contrast Microscopy *via* Rapidly Making Nanoarray Protein Chip

He Nan 강성호

경희대 응용화학과

Quantitative label-free detection method of troponin based on a single-molecule sandwich immunoassay nanoarray chip has been investigated by differential interference contrast (DIC) microscopy. Nanoarray biotin-probes were patterned onto 3-mecaptopropyl trimethoxysilane-coated glass surface with a spot diameter of ~500 nm within 1 min using Nano-eNabler^{TM} system-based surface patterning tool. The nanopatterning method was ~2,000 times faster on the chip manufacturing process than conventional atomic force microscopy based dip-pen nanolithography. The 200 nm nanoparticles, carboxylate-modified FluoShere^{TM}, conjugated with troponin specific antibody were detected for the immunoassay. Total internal reflection fluorescence microscopy confirmed the accuracy and precision of DIC microscopy. Using DIC detection method, the detection limit of troponin was fM level. It shows the DIC technique can be used as a fluorescent-free detection method for the single-molecule sandwich immunoassay nanoarray chip.

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Ultra-Fast Detection of *Feline Infectious Peritonitis* Virus Based on Single- and Multi-channel Microchip Electrophoresis

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경희대 응용화학과

Feline infectious peritonitis virus (FIPV) is one of the feline coronavirus, which causes most severe devastating diseases of Felidae. We developed single- and multi-channel microchip electrophoresis (ME) with a laser-induced fluorescence (LIF) detector for ultra-fast detection of FIPV. The programmed field strength gradient (PFSG) method at 1.3 cm-effective channel length was used for the detection of FIPV via a reverse transcript polymerase chain reaction. The optimum sieving gel concentration was 0.3% PEO (M_r = 8,000,000). The FIPV was detected within 9.6±0.2 s under a PFSG (470.56 V/cm for 9 s, 294.11 V/cm 1.5 s, and 470.59 V/cm for 9.5 s) by single-channel ME, which was 50 times faster than that obtained with conventional slab gel electrophoresis. The method was applied in multi-channel ME system to identify high-throughput detection of FIPV with high speed. The ME methods showed an excellent precision with less than 0.5 of standard deviations for migration time and peak area. This assay technique should be a simple and powerful diagnostic method for ultra-fast analysis of disease-related specific DNAs with high speed, precision and accuracy.

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Separation and Characterization of Oxidized Phospholipids in Oxidatively Modified Low Density Lipoprotein by Nanoflow Liquid Chromatography-Tandem Mass Spectrometry

이주용 임상수 문명희

연세대 화학과

Oxidized low density lipoprotein (oxLDL) has been reported as critical biomarkers of coronary artery disease (CAD). OxLDL is oxidatively modified form of LDL, altered in size and composition of lipids, fatty acids, apolipoproteins. When OxLDL is accumulated, an increased amount of plaque is produced in blood vessels causing serious problems in human body. Studies on oxLDL and oxidized phospholipids (OxPLs) have been conducted and published, but most of them are generally limited in terms of a comprehensive profiling of lipids because they are focused on phosphatidylcholine (PC) species in most cases without a comprehensive examination on oxidized PLs in LDL. In this study, profiling of modified PLs including phosphatidylglycerol (PG), phosphatidic acid (PA), phosphatidylinositol (PI), phosphatidylserine (PS) in oxLDL, in addition to PC, were carried by nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS-MS). To study the oxidized PLs in standard LDL, bilayer vesicles made up of PC, PG, and PA standards individually, were oxidized by $CuSO_4$ solution and patterns of structural change in OxPLs were studied by examining collision induced dissociation (CID) spectra of OxPLsusing nLC-ESI-MS-MS. The patterns of molecular structure of OxPLs were included in a database library for the structural determination using LiPilot, a software program written in our laboratory for the identification of PL species as well as OxPLs based on CID patterns, in order to investigate the oxidized PLs from oxidized LDL.

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Simultaneous Analysis of All Classes of Phospholipids by Nanoflow Liquid Chromatography/Tandem Mass Spectrometry in Negative Ion Mode : An optimization of Ionization Modifier

방대영 임상수 문명희

연세대 화학과

In this study, a total of 13 different Lyso-phospholipids (LPLs) and phospholipids (PLs) standards were utilized to develop an analytical condition for simultaneous separation and characterization using nLC-ESI-MS-MS. By using ammonium formate and ammonium hydroxide as ionization modifier in mobile phase, all classes of LPLs and PLs were simultaneously detected in the negative ion mode of MS analysis. While MS analysis of most PL classes is carried out in negative ion mode, analysis of neutral polar (polar but electrically neutral) lipids like phosphatidylcholine (PC) and sphingomyelin (SM) is highly efficient in positive ion mode. Therefore, analysis of PL mixture samples often requires two separate runs in both positive and negative ion mode. In order to establish run conditions to carry out a single nLC-ESI-MS-MS for all PLs, the ionization efficiency of 13 different types of PL molecules in nLC-ESI-MS has been evaluated in negative ion mode by varying the modifiers and their concentrations. Experiments demonstrated that a mixed modifier (0.05% ammonium hydroxide plus 1 mM ammonium formate) was found to be effective in the analysis of PL mixtures without losing ionization efficiency. The optimized condition was applied for the analysis of a phospholipid mixture extracted from a human urine sample, yielding the identification of a total of 85 PL species. Analysis of the same sample with dual nLC-ESI-MS2 runs in both positive and negative ion mode confirmed that nLC-ESI-MS3 with the mixed modifier run only in negative ion mode gave comparable results.

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Observation of Protein aggregation Induced by Focusing/Relaxation Procedure in Asymmetrical Flow Field-Flow Fractionation

양이슬 김기훈 문명희

연세대 화학과

This study was aimed to examine an artifact in which protein aggregation can be generated during focusing/relaxation procedure, an essential step to assure sample relaxation prior to separation in asymmetrical flow field-flow fractionation (AF4). In order to examine the effect of inducing aggregation in AF4 channel, frit-inlet asymmetrical flow FFF (FI-AF4) channel was utilized together with AF4 for comparison FI-AF4 channel utilizes hydrodynamic relaxation in which sample relaxation is achieved automatically during sample injection, thus there is no need of stoppage of migration flow. For comparison, a chip-type miniaturized channel was constructed by assembling an acryl block inserted with a ceramic frit as an accumulation wall while two acryl plate (2.0 mm thick) for depletion wall were utilized: one as plain plate for AF4 channel and the other plate embedded with a small inlet stainless frit at the beginning of the channel for FI-AF4. By replacing the acyl plate, channel setup for both AF4 and FI-AF4 can be readily obtained. Aggregation of protein can be induced by utilizing a special carrier solution. For instance, α-Casein can be aggregated into spherical micelles (50~600 nm) under a Ca2+ containing buffer. When using AF4, it was observed that the ratio of retention time of α-Casein aggregates to void time was shifted more than that observed by FI-AF4, which supported that size of aggregates during AF4 separation was larger than that in FI-AF4. Thus, it can be concluded that focusing/relaxation may contribute to induce protein aggregation.

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Discovery of Potential Phospholipid Biomarkers of Coronary Artery Disease by Flow Field-Flow Fractionation and Nanoflow Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry

변슬기 이주용 문명희

연세대 화학과

Advanced technologies in mass spectrometry (MS) has expanded its capability to analyze lipid molecules at a molecular level and it has been applied in chemical and medical fields to identify lipids as potential biomarkers of various human diseases. Biomarker studies in lipidomics have attracted an increased attention over the past years as they were developed as quick assessment tests for certain diseases. By coupling liquid chromatography (LC) to MS, lipids can be separated and identified, enabling a detection of lipids that exist in trace or ultra-trace amounts. Coronary artery disease (CAD) refers to a vascular heart disease in which thick arterial walls reduce the amount of blood flow delivered from or to heart and slow down blood supply. In order to identify biomarkers of CAD, plasma phospholipids (PL) and lysophospholipids (LPL) from high density lipoprotein (HDL) and low density lipoprotein (LDL) of patients with CAD and controls were identified. HDL and LDL of plasma were separated and collected by employing a size separation method, flow field-flow fractionation (FlFFF). Twenty two lipid species that showed greater than a five fold change in average concentration between ten CAD patients and ten controls were defined as candidate biomarkers.

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Development of Novel Algorithm for Automated Identification of Phospholipids from Nanoflow Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry

임상수 변슬기 이주용 문명희

연세대 화학과

Lipidomics is a comprehensive study of structural and functional characteristics of various kinds of lipids. Great advance in mass spectrometry related techniques have been accelerating lipidomic studies with its own specific advantages. However, unlike proteomic analysis, conventional analysis of tandem mass spectra of several lipid classes is severely laborious. Currently, various sophisticated algorithms are being utilized in proteome analysis for facile comprehension of raw mass spectra, programmed analysis of mass spectra of lipidome still remains to be developed. LiPilot, a novel computer software program for the structural characterization of phospholipids (PLs) including lysophospholipids (LPLs) from tandem MS spectra is introduced. The algorithm utilizes raw mass spectra produced from nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS-MS) experiments accompanying both retention time and m/z values of precursor and fragment ions from data?dependent, collision-induced dissociation(CID). Moreover, structure of library files presenting the typical fragmentation patterns of PLs from an LTQ-Velos ion trap mass spectrometer to identify PL or LPL molecular species were also introduced. Characterization procedure is processed by the calculation of a ‘confidence score’ to optimize identification efficiency which covers the effect of total peak intensities of matched and unmatched fragment ions, the difference in m/z values between observed and theoretical fragment ions, and a weighting factor to differentiate regioisomers. This new tool was validated using a mixture of 24 PL and LPL standards and was further evaluated with a human urinary PL mixture sample, which yielded the identification of 93 PLs and 22 LPLs.

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Development of a Microbore Hollow Fiber Enzyme Reactor (mHFER) for Global Shotgun Proteomics

김진용 문명희

연세대 화학과

With well-established protocols, the shotgun proteomic method is widely used for identification of proteolytic peptides and their various post-translational modifications. The shotgun proteomic method is based on the digestion of proteins in advance, followed by the separation of proteolytic peptides and the identification of proteins by tandem mass spectrometry. Although there is no doubt that the digestion of proteins is indispensable for bottom-up approach based proteomics, the typical protocols for protein digestion have some critical shortcomings, such as low efficiency, long incubation time, and manual operation. In this study, we developed a microbore hollow fiber enzyme reactor (mHFER), which is a simple, highly reproducible, inexpensive, and user friendly device for global shotgun proteomics. In addition to improve the digestion efficiency, mHFER could be easily coupled with nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS-MS) for a full automation and a high throughput analysis. mHFER module is simply constructed with a microbore hollow fiber (mHF, a MW cutoff of 10 kDa) in which one end of mHF is blocked by an epoxy and in inserted in a PEEK tubing connected with capillary tubings on both sides. Because mHF is porous and its one end is closed, injected protein samples is concentrated and simultaneously digested inside mHF by pump flow when enzyme is loaded in sequence. To examine the usefulness of mHFER as a proteolytic reactor, experiments were conducted by varying temperature and injection amount of bovine serum albumin (BSA). Consequentially, the proteolytic peptides eluted after digestion through membrane pore of mHF leave toward nLC-ESI-MS-MS system, showing the unprecedented depth of proteome coverage with high reproducibility.

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The reaction monitoring of TDI cross-linking with H_2O using MALDI-MS and FT-IR

김지석 오무현 노희윤 하승호 김성호

순천향대 화학과

H_2O 는 TDI 경화반응에 불순물로 작용하여 side 반응을 일으킴 으로써, 우레탄반응의 물성에 영향을 준다.TDI 와 H_2O 경계면 에서 일어나는 두 물질간의 반응을 FTIR 과 MALDI-MS 를 이용하여 고찰 하였다.H_2O 의 농도, 반응시간 등의 변화에 따라 달라지는 반응생성물을 분석을 통하여 TDI/H_2O 반응을 체계 있게 모니터링 하였다.

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The reaction monitoring of TDI cross-linking with EG using MALDI-MS and FT-IR

이연정 김초롱 이빛나 이정선 김성호

순천향대 화학과

우레탄반응의경화제로 사용되는 TDI 는 생성되는 우레탄 폴리머의 물리적 성질을 조절하기 위하여 EG 등의 OH 작용기를 가진 화합물을 함유하고 있다. 본 연구에서는 TDI 와 EG 의 반응비율에 따라 변화하는 반응생성물을 MALDI-MS 와 FTIR 을 이용하여 분석함으로써 TDI/EG 반응을 체계 있게 모니터링 하였다.

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Ground organic monolith particles of improved separation efficiency in HPLC

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인하대 화학과

Ground organic monolith particles were prepared and packed in a glass-lined stainless steel column under high pressure and the separation performance was examined with a test mix composed of polar and nonpolar aromatic organic solutes. Methacrylic acid (functional monomrer), ethylene glycol dimethacryalte (EDMA, crosslinker), AIBN (initiator), and polyethylene glycol (PEG, porogen) were dissolved in toluene and heated at 60 oC for 24 h. The product was briefly smashed and washed with a series of solvents with stirring and dried. Choice of molecular weight of PEG was very critical to optimize separation performance. The number of theoretical plates of the column (1.0 X 300 mm) packed with this phase were over 10,000. Cheap production of ground organic monolith particles and their use as low cost separation media have been demonstrated in this study.

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Gold nanoparticles modified polydopamine and multiple nonenzymatic labels-based electrochemical thrombin aptamer sensor

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An electrochemical thrombin (TB) aptamer sensor was fabricated by immobilizing a thiolated TB binding aptamer onto the poly-dopamine/AuNPs surface for the competitive detection of TB. The poly-dopamine/AuNPs surface was characterized using AFM, SEM and electrochemical impedance techniques and the conjugate was characterized by TEM, DLS, and UV/Vis. The TB detection was based on the competition between multiple methylene blue-labeled-TB and free TB for the aptamer binding sites. Square wave voltammetric (SWV) responses before and after competition suggested that TB can be successfully detected with the poly-dopamine/AuNPs based-TB aptamer sensor. Under the optimized condition, the linear dynamic range and the detection limit were determined to be 2 pM ~ 10 nM and 1 pM, respectively.

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Amplified Electrochemical Detection of a Cancer Biomarker by Enhanced Precipitation Using Horseradish Peroxidase Attached on Carbon Nanotubes

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An electrochemical nanoimmunosensor based on multiwall carbon nanotubes (MWCNTs)/gold nanoparticles (AuNPs) was developed for the amplified detection of prostate specific antigen (PSA). The amplified detection was achieved by the enhanced precipitation of 4-chloro-1-naphthol (CN) using a higher number of horseradish peroxidase (HRP) molecules attached on multiwall carbon nanotubes (MWCNTs). Cyclic and square wave voltammetric techniques were used to monitor the enhanced precipitation of CN that accumulated on the electrode surface and subsequent decrement in the electrode surface area by monitoring the reduction process of the $Fe(CN)_6^{3-}/Fe(CN)_6^{4-}$ redox couple. The linear range and the detection limit of PSA immunosensor were determined to be 1.0 pg/mL-10.0 ng/mL and 0.40 ± 0.03 pg/mL respectively. The validity of the proposed method was compared with an enzyme-linked immunosorbent assay method.

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Sensitivity Enhancement through Multiple Non Enzymatic Labels-Catalyzed Reaction: A Competitive Electrochemical Immunosensor for a Cancer Biomarker

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We developed a non-enzymatic labels-catalyzed competitive electrochemical immunosensor for a protein biomarker, carcinoembryonic antigen (CEA). The CEA immunosensor was fabricated by immobilizing a monoclonal CEA antibody on a gold nanoparticles (AuNPs) deposited biopolymer (polydopamine) film. The multiple 3,3′,5,5′-tetramethylbenzidine (TMB) conjugates were prepared using CEA and magnetic beads. The CEA detection was based on the competition between the free CEA and (TMB) conjugated CEA through the catalytic oxidation of ascorbic acid by multiple TMB. The linear range and the detection limit were determined to be 10-1000 pg/mL and 3 pg/mL, respectively. The immunosensor was tested in CEA spiked human serum samples and satisfactory results were obtained.

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발표코드: **ANAL.P-625**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantiomeric separation of 3-substituted 1,4-benzodiazepin-2-one derivatives on (1R,2R)-(+)-1,2-diphenylethylenediamine-based chiral stationary phase

성지영 탁경미 현명호

부산대 화학과

Some synthesized drugs have a property of chirality which can show different pharmaceutical effect on a living organism. If enantiomeric drugs are not completely separated, it can cause negative problems on our body. The tragic of thalidomide is a well known example, which shows the importance of resolving chiral compounds. Some kind of 3-substituted 1,4-benzodiazepin-2-one derivatives are effective treatments that can relieve a anxiety or nervous disease. Therefore, it is worthwhile to resolve these derivatives accurately. Among various method, HPLC chiral stationary phase(CSP) is known as a powerful method which can analyze enantiomers effectively. In this study, we resolved 3-substituted 1,4-benzodiazepin-2-one derivatives on a CSP developed in our laboratory. This CSP was synthesized starting from (1R,2R)-(+)-1,2-diphenylethylenediamine. We found out 3-substituted-1,4-benzodiazepin-2-one derivatives are highly recognizable on (1R,2R)-(+)-1,2-diphenylethylenediamine-based CSP.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-626**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Virus-tethered Magnetic Gold Microspheres with Biomimetic Architectures for Enhanced Immunoassay

전창수 황인성[1] 정택동[1]

서울대 자연과학대학/화학부 [1]서울대 화학부

In immunoassays, nonspecific bindings to biosensing surfaces can be effectively prevented by formation of biocompatible and hydrophilic self-assembled monolayer (SAM) on the surfaces. A thin gold layer on magnetic microspheres enables facile SAM formation and thereby accepts second layer of virus scaffolds for the immobilization of functional proteins. The merger of the virus and SAM-Au protected microspheres not only provides exceptionlly dense functional groups for the antibody loading, but also resembles biological cellular structures and thus harnesses enhancement factors originating from the unique morphology. The bead-based immunoassays for the detection of cardiac marker proteins exhibit increased sensitivity of virus-Au microspheres, as low as 20 pg/mL of cardiac troponin I in serum, and extremely low nonspecific adsorption when compared with bare polymer beads. This increased sensitivity due to virus filaments and SAM-Au layer demonstrates the feasibility of merging viruses with non-biological materials to yield biomimetic tools for the enhanced immunoassay with quantitative manner.

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발표코드: **ANAL.P-627**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

남조류 cell 안의 조류독소와 cell 밖으로 용출된 조류독소를 동시에 측정하는 측정법 개발

임미연 김어진 표동진

강원대 화학과

국내 상수원의 부영양화된 호수나 유속이 느린 하천에서는 여름이면 녹조류, 남조류, 규조류, 와편조류 등의 대량 번식에 의해 녹조현상이 나타나게 된다. 특히 남조류 중에서 마이크로시스티스에서 발생되는 마이크로시스틴-LR 은 간독소 물질로 조류독소 중 강한 독성을 나타내는 물질 중 하나이다. 우리나라는 거의 매년 반복적으로 녹조가 발생하여 피해를 입지만 남조류의 독성을 측정 가능한 상수원이 매우 한정적이어서 녹조가 발생하였을 때 즉각적인 측정에 어려움이 있다. 본 연구에서는 남조류 cell 밖의 물에 녹아 있는 조류 독소와 남조류 cell 안의 조류독소를 동시에 측정할 수 있는 방법으로 산 처리, 얼림, sonication 등의 방법을 이용해 가장 효과적으로 cell 을 파괴하여 물 밖으로 독소가 나오게 하여서 정확한 양의 조류독소의 측정할 수 있도록 하였다. 조류 독소를 측정하는 방법으로는 본 실험실에서 개발한 스트립 형광법으로 조류독소를 정량 분석하였다. 이 방법은 기존의 측정방법에 비해 간편하고 신속하게 측정이 가능하여 실제로 하천이나 호수의 조류독소를 측정하기에도 매우 편리하다.

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장소: 부산BEXCO

발표코드: **ANAL.P-628**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

남조류 대량 수거를 위한 필터 및 수거장치 개발

김어진 임미연 표동진

강원대 화학과

하천이나 호수로부터 남조류를 대량 수거하는 방법에는 응집제를 사용한 침전법과 필터를 사용하는 여과법이 가장 널리 사용되는 방법이다. 본 연구는 남조류를 대량 수거 한 후 남조류로부터 바이오 에탄올을 생산하고자 하기 때문에 필터가 장착된 수거 장치에 남조류가 포함되어 있는 시료를 흘려주게 되고 필터에 남조류가 걸러지게 되어 남조류를 모을 수 있는 여과법을 사용하고자 하였다. 남조류의 한 종류인 마이크로시스티스의 size 는 4~7μm 이지만 자연상태에서는 증식한 다수의 세포가 공통의 점질 수분에 매재하기 때문에 군체는 육안적인 크기가 되기 때문에 사이즈가 커 필터에 걸러지게 된다. 이러한 남조류를 대량수거하기 위해 가장 적당한 pore size 의 필터를 찾고자 종이, 면, 폴리에스테르, 면과 폴리에스테르의 혼방섬유 등을 필터로 사용해 보았다. 또한 가장 적절한 필터를 찾은 후 필터를 효과적으로 사용할 수 있도록 하는 장치를 개발하였다. 남조류를 걸러낼 때 가장 문제가 되는 남조류에 의한 필터 막힘 현상이 발생하므로 한 개의 장치만으로는 많은 양의 남조류를 수거할 수 없으므로 Multi-bay 시스템을 개발하고자 하였다.

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장소: 부산BEXCO

발표코드: **ANAL.P-629**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

초임계유체를 이용한 아시아산 생강으로부터 커큐미노이드 추출

김어진 임미연 표동진

강원대 화학과

최근 소비자의 의식이 향상되고 합성살충제의 문제점이 나타나면서 인체와 환경에 무해한 살충제의 수요가 급증하고 있다. 이로 인하여 천연물에서 살충 효과가 있는 물질을 추출해서 친환경적인 살충제로 사용하는 연구가 이루어지고 있다. 본 과제에서는 초임계유체를 이용하여 아시아산 생강으로부터 살충 효과가 있는 커큐미노이드를 추출하는 방법을 개발하였다. 초임계유체는 CO2 를 사용하였고, 유속은 3ml/min 을 사용하였다. 추출 효율을 비교하기 위하여 압력과 온도, 추출시간을 변화시켜 주었다. 압력은 200atm, 250atm, 300atm 로 변화시켜 주었고, 온도는 40℃, 50℃, 60℃로 변화시켜 주었다. 추출시간은 1 시간 30 분, 2 시간, 2 시간 30 분으로 변화시켜 주었다. 마지막으로 modifier 의 유무에 따른 효율을 비교하여 최적의 추출조건을 확립하였다. 초임계유체를 이용하여 추출한 커큐미노이드의 양은 HPLC 를 이용하여 정량하였다. column 은 Waters spherisorb? ODS column(4.6 x 250mm, 5μm)을 사용하였고 이동상은 methanol(70%), water(30%)를 0.8ml/min 의 유속으로 사용하였다.

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발표코드: **ANAL.P-630**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new nano-composite carbon ink for disposable dopamine biosensors

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부산대 IBST [1]부산대 바이오센서연구소/분자과학기술 [2]부산대 분자과학기술협동과정 [3]부산대 바이오피지오연구소 [4]부산대 나노소재공학과 [5]부산대 바이오피지오센서연구소

A new method for the development of disposable dopamine sensors based on screen printed carbon electrode (SPCE) will be introduced. The method developed uses SPCEs coupled with immobilized enzyme, tyrosinase. SPCEs were prepared by using a nano-composite carbon ink which was manufactured by an 'in-house' procedure with reduced graphene oxide (rGO) fragments, Pt nanoparticles (Pt) and carbon materials. The rGO-Pt-carbon composite ink was used to print the working electrodes of the SPCEs and a commercial Ag/AgCl ink was used to print electrodes' tracks, reference and counter electrodes. After the construction of nano-composite SPCEs, tyrosinase was immobilized onto the working electrodes by using a biocompatible matrix, chitosan. The response of the nano-composite biosensors to dopamine was based on the amperometric detection of the enzymatically generated dopamine-quinone at -0.3 V vs. Ag/AgCl. The performance of the biosensors was characterized by comparison with the composition of nano-material embedded and enzyme contents. The results indicated that the rGO and Pt embedded carbon inks provided significant improvement in an electro-catalytic activity and sensitivity compared with the results obtained from bare or Pt embedded carbon inks. Experimental parameters such as pH, operation potential and storage stability are optimized and will be presented in the poster. This disposable biosensor exhibits great potential for rapid, simple, cost-effective and on-site analysis of dopamine.

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Block-Copolymer-Templated Gold Nanoparticles Array for Sensitivity Enhancement of Surface Plasmon Resonance Biosensing

정경화 장윤희[1] 김동하[1]

이화여대 화학나노학과 [1]이화여대 화학나노과학과

Surface plasmon resonance (SPR) is a resonantly coupled electromagnetic field between the incident light and the conduction band electrons of metal, which shows amplified electromagnetic field propagating at dielectric/metal interface. This field is subceptible to the change in the refractive index, allowing for label-free optical biosensing. To increase the SPR sensitivity, many strategies were developed for detecting trace amount of small biomolecules. Utilization of gold nanoparticles (AuNPs) is one of the most promising platforms for that purpose, mostly used as a label. While AuNP-based labeling can enhance 10~1000 fold of sensitivity enhancement for the recognition of a sandwich-type target in a Kretschmann setup, detection of the analyte onto AuNPs array in the same setup was also reported with 1~10 fold enhancement. Here, we demonstrate unique strategies for enhancing the sensitivity of label-free SPR biosensor by inducing the coupling between propagating SPR (PSPR) of Au film and localized SPR (LSPR) of Au NPs array using block copolymer (BCP) template.Au NPs array was integrated onto flat Au film via PS-b-P2VP block copolymer (BCP) template. By varying the loading protocol of AuNPs, we could control the degree of regularity of Au NPs. In addition to the electric field enhancement by the coupling effect, Au NPs provide larger surface area than neat Au film, which also contribute to better sensing performance.

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Carbon nanofibers grown on Co and Cu catalysts by Chemical Vapor Deposition

박은실 이창섭

계명대 화학과

본 연구에서는 CVD 법을 이용하여 Co 와 Cu 계 촉매를 탄소나노섬유 합성에 이용하였다. 탄소나노섬유 성장에 적합한 촉매의 활성을 알아보기 위해 Cobalt nitrate($Co(NO_3)_2 6H_2O$)와 Copper nitrate($Cu(NO_3)_3 9H_2O$)를 농도 별로 제조하여 최적 농도의 촉매를 찾았고, 이를 Aluminum nitrate($Al\ (NO_3)_3 9H_2O$)와 Ammonium Molybdate($(NH_4)_6Mo_7O_{24}$)를 함께 반응시켜 필터링하여 침전물이 생성되도록 하였다. 이렇게 얻은 침전물은 110℃로 건조시켜 촉매 분말을 제조하였다. 이 촉매를 석영관 보트에 넓고 얇게 펴서 열분해 화학 증착법을 이용하여 탄소나노섬유를 합성하였다. 이때 가장 반응성이 좋은 특정 농도의 물질을 선택하여 각각 합성온도(600~900℃), 합성 시간, 촉매열처리 조건 변경, 반응 가스의 종류 등의 합성조건을 변화하여 최적의 조건을 찾았으며, 결과물은 SEM, EDS 및 XRD 를 사용하여 물성을 분석하였다. 탄소나노섬유는 다양한 산업분야의 구조재 소재로서 본 연구의 결과는 탄소섬유의 응용·산업화 발전에 큰 기여를 할 것이라 기대한다.

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발표코드: **ANAL.P-633**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Deposition-Precipitation of Fe compound on C-fiber textiles

이상원 이창섭

계명대 화학과

In this study, Fe oxide compounds were homogeneously deposited on C-fiber textiles by the method of deposition-precipitation. 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 deposition of Iron, we changed the concentration of Iron solution before heating and then Urea hydrolysis was done. Hydrolysis helps to deposit Fe(III) on C-fiber. In the process of deposition-precipitation, appropriate time, temperature, change of the color were checked. In reduction process, H_2/N_2 mixture gas was used. Then the change state of sample was studied. The resultant samples were characterized by Scanning Electron Microscopy(SEM), Energy Dispersive Spectroscopy(EDS), and X-Ray Diffraction(XRD).

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Synthesis of Carbon nanofibers on Iron and Copper Catalysts by Chemical Vapor Deposition

현유라 이창섭

계명대 화학과

In this study, Carbon nanofibers have been synthesized using iron catalyst and ethylene as a carbon source. The fiber thickness and surface area have been studied from the influence of both iron and copper concentration. The catalysts were prepared by dissolving the calculated amounts of iron nitrate and copper nitrate in water. The precipitate of catalysts obtained through filtering after drying at 110℃. The CVD process in a high-temperature furnace by the following steps: 1) heating up to 700℃ at a rate of 10℃/min a N_2 for 1h 10min to reduce the Fe^{3+} to Fe; 2) stabilized by temperature flow H_2/N_2 for 30min; 3) CVD process in mixture of 20.1% ethylene and H_2/N_2 at 700℃ for 1h. Finally the structural characterization of the CNFs was performed by SEM and TEM. Also, the composition analysis was carried out using EDS.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Tris(2,2'-bipyridyl)ruthenium(II) Eletrogenerated Chemiluminescence Sensor Based on Graphene-Titania-Nafion Composite Films.

이상정 강창훈 이원용

연세대 화학과

Graphene has excellent electronic, thermal and mechanical properties. Its physical properties have been extensively studied, however, its analytical applications remain largely unexplored. $Ru(bpy)_3^{2+}$ electrogenerated chemiluminescence (ECL) has been given much concern in chemical analysis because of its wide applications, good electrochemical stability, and high ECL efficiency in aqueous media. In this study, $Ru(bpy)_3^{2+}$ was incorporated into the graphene-titania-Nafion composite film. The introduction of conductive graphene into titania-Nafion greatly facilitates the electron transfer of $Ru(bpy)_3^{2+}$ in the matrix. As a result, the modification improves the ECL efficiency for detection of analytes, such as tripropylamine (TPA). In a practical experiment, the $Ru(bpy)_3^{2+}$ immobilized graphene-titania-Nafion modified electrode showed wide linear range and low detection limit for the ECL determination of TPA, comparable to the ECL sensor based on CNT-titania-Nafion composite. The study shows that graphene holds great promise for ECL application.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Optimized Method to Produce the Biodiesel from the Algae and its Quantitative Evaluation by GC

정지은 김성환

경북대 화학과

The existence of modern society has been heavily dependent on fossil fuels but it is well known that fossil fuels are limited resources. Therefore a variety of renewable energy resources such as biomass, hydro, wind, solar, and geothermal energy that can replace fossil fuels are currently being developed. Among them, algae can be the attractive replacement for oil based fuels because they are the fastest growing plants in the world and contain oil component at least 50% of their total weight. In a previously published paper, a procedure to generate biodiesel from algae based on Bligh and Dyer method has been reported. However, the procedure requires usage of a large volume of chloroform which is known to be toxic. Additionally, the procedure contains several extraction and conversion step and hence it is difficult for automation. Therefore, in this study, an improved procedure that does not include chloroform and has fewer steps to produce biodiesel from the algae has been developed. The procedure has been quantitatively evaluated by use of GC-FID.

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장소: 부산BEXCO

발표코드: **ANAL.P-637**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimization of comprehensive 2D GC-MS for improved characterization of heavy crude oils

조윤주 김성환

경북대 화학과

Complete chemical characterization of heavy crude oils is challenging due to their complexity. Chemical compounds with large molecular weight and polar composition have been studied by Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). Gas chromatography mass spectrometry (GC-MS) is another excellent technique that is very effective in studying smaller and less polar hydrocarbon compounds. However, the conventional GC-MS has limitation for the analysis of complex mixture which includes polar and non-polar compounds. To overcome the limitation, two dimensional (2D) GC-MS has been developed and applied to study mixture samples. This study presents the advantages of 2D GC-MS to separate, characterize, and classify the chemical composition of heavy crude oils based on quadrupole mass spectrometry coupled to a thermal modulator. The obtained 2D GC-MS spectra showed that chemical compositions of the heavy crude oils were quite different from each other. For example, a series of hopanes were observed in oil shale extracts that were not observed in the Arabian heavy crude oil sample. Therefore, the 2D GC-MS is shown to be a powerful technical to evaluate and compare key chemical differences of crude oils originated from various geographic regions.

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발표코드: **ANAL.P-638**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of polyphenol component *Ceramium kondoi* using liquid chromatography coupled with tandem mass spectrometry.

송이 신성철 정성우[1] 박세민 서온누리 이지은 옥세윤

경상대 화학과 [1]경상대 원예학과

Ceramium kondoi has been a folk medicine for the treatment of cancer, inflammation, diabetes, headache, nephropathy. The principal objective of the present study was to characterize in detail the polyphenols of *C. kondoi* using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) in the negative and positive mode with selected ion monitoring (SIM). Ten phenolic compounds were characterized.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Characterization of the extracellular metabolic changes regulated by Aquaporin3/TGF-β

이주은

성균관대 화학

Aquaporin3 (AQP3) is known to be involved in human skin fibroblasts cell migration. There was a trend for AQP3 to increase its expression and have a cell mobility when the human mesotheial cell was treated with TGF-β (transforming growth factor β), which mediates cell proliferation and cellular differentiation. We investigated how the extracellular metabolism was changed by expression level of AQP3. It was also discovered that cell metabolism related to migration can be affected by modulating AQP3 expression with TGF-β. Metabolite profiling was performed to analyse the response of human mesothelial cell cultures using 1H NMR coupled with multivariate analysis. The level of dimethylamine increased in high expressed AQP3 group, whereas formate and pyroglutamate were down-regulated. TGF-β induced extracellular metabolic changes such as organic acids and amino acids. These results indicated that metabolisms of organic acid and some of amino acids were related to expression level of AQP3 and mediated by TGF-β. To investigate the fatty acid metabolism, following study was performed using GC-MS. Although this study showed less significant results than NMR analysis, it can be also related to NMR study and used to trace the migration phenomena. In this study, we showed that metabolomics using NMR and GC-MS can be a potential to get the responses of cell phenotypes exposed to different cellular environments.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of arsenic speciation in sea food using HPLC-ICP-MS

전병권 이경준[1]

충남대 화학과 [1]한국분석기술연구소

비소는 독성을 가진 유해 중금속 원소로서 자연적 또는 인위적인 원인에 의해 여러 형태의 비소 화학종으로 존재한다. 토양이나 공기, 물, 음식 등 어디에나 존재하고 있고 식용수나 식료품, 대기 등에 의해서 우리 인체에 쉽게 노출이 되고 있다. 비소는 크게 두 가지로 나눌 수 있는데 As(Ⅲ), As(Ⅴ)와 같은 무기비소와 DMA, MMA, AsB 등과 같은 유기비소가 있다. 일반적으로 무기비소가 유기비소보다 독성이 훨씬 강하며, As(Ⅲ)가 As(Ⅴ)에 비해 독성이 더 강하다. 유기비소는 독성이 매우 약하거나, 없는 것도 있다. 사람은 특히 해양식품을 섭취함으로서 비소를 과량 흡수하게 되는데, 해양 식품 중 비소는 주로 유기비소 상태로 많이 존재하고 있다. 현재까지 비소의 오염도에 대한 평가는 총 비소 함량을 기준으로 평가되고 있어 해양 식품 중 비소 분석은 정확한 판단이 이루어지지 않고 있다. 본 연구에서는 정확한 비소 분석을 위한 방법을 제시하였다. 최근 사용 중인 분석법은 유기비소인 AsB 와 무기비소인 As(Ⅲ)의 피크가 잘 분리되지 않아 정량이 힘들다. 또한 완충용액을 이동상으로 사용하기 때문에 분석 장비에 손상을 줄 수 있다. 이에 본 연구에서는 이러한 단점을 보완할 수 있는 방법을 연구하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Metabolic profiling of chronic renal failure in rats by 1H NMR spectroscopy

김주애

성균관대 화학과

Chronic renal failure (CRF) is the progressive loss of the kidney's ability to filter waste over a period of months or years. In this study, we applied a 1H NMR based metabolomics approach to investigate the altered metabolic pattern in tissue from CRF model rats induced by surgical reduction in renal mass. Tissue metabolite profiling was applied to identify the change in the level of metabolites in CRF rat models compared to sham control rats. Partial least squares discriminant analysis (PLS-DA) and orthogonal partial least-squares (OPLS) score plots showed significant separation in rats. A t-test was performed to statistically verify the difference of the identified tissue metabolites between two groups. The quantitative results showed that the tissue of CRF rats had higher levels of metabolites for β-hydroxybutyrate, lactate, glutamate, glutamine, methionine as well as lower levels of choline, O-phosphocholine, compared with control. In addition, levels of uremic toxins such as creatinine, dimethylamine, urea were increased in CRF model. In conclusion, this study suggests that NMR-based metabolomic approach is useful for identifying potential biomarkers for CRF and understanding their biological pathways.

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1H NMR-based metabolomic analysis after oral administrationof Poly-γ-Glutamic Acid in rats

배현희

한국기초과학지원연구원 분석연구부/서울센터

Poly-γ-glutamic acid (γ-PGA) is a mucilaginous and biodegradable compound produced by Bacilus subtilis from fermented soybeans, and is found in the traditional Korean soy product, Cheongkukjang. Recently, it was identified that oral administration of γ-PGA induced antitumor immunity. For this reason, this study was carried out to research metabolic changes to the spleen in rats after oral administration of γ-PGA form food source. Six-week old male Sprague-Dawley rats (n=30) were used and were divided into three groups of ten each dose (High 100 mg/kg, Low 25mg/kg, and Control). Each group were orally administrated four times for two days (post 4, 12, 24, and 48 hour). Spleen samples were sacrificed after 48h. We applied 1H-NMR based metabolomics approach to profile of metabolic changes after oraladministration of γ-PGA in rats. Partial least square discriminant analysis (PLS-DA) showed distinct separation between the three groups of ten each dose. Creatinine, Glucose, Glutamate, Hypoxanthine, Lactate and Xanthine in the spleen were showed significant variation depending on the groups. Creatinine, Glucose, Glutamate, Hypoxanthine, and Lactate concentrations decreased ($P \leq 0.05$) after oral administration, while Xanthine concentrations increased. The final objective of this work is that identify altered metabolism and propose a metabolic pathway after oral administration of γ-PGA.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly sensitive microgravimetric glycated hemoglobin detection method based on boronic acid functionalized nanoparticles

안광수 임경래 김동환 이원용

연세대 화학과

In terms of caring diabetes patients, long-term glucose monitoring is important because diabetes is a chronic disease. Unlike fasting and post-meal glucose monitoring, long-term glucose monitoring targets glycated Hemoglobin (Hb). Hb A1c, which is one of the Hb family that forms a conjugate through addition of glucose to N-terminal valine residue of the β-chain of Hb A. The concentration of Hb A1c in human blood presents glucose concentration of the previous 1~3 months. Thus, Hb A1c concentration monitoring is recommended to diagnose diabetes with cutoff value of 6.5% of total Hb concentration. It is known that Hb A1c has two cis-diol groups at surface can make binding to boronic acid with high specificity.There are several methods were reported to determine Hb A1c; cation-exchange high-performance liquid chromatography, electrophoresis, immunoassays, mass spectrometry and boronate affinity chromatography. To overcome limitations of previously reported methods, we bring a non-enzymatic microgravimetric method using quartz crystal microbalance (QCM). Despite the QCM sensor ensures good performance, it still requires lower detection limit and higher sensitivity in diabetes diagnose. This study aims more sensitive microgravimetric detection using QCM by using boronic acid functionalized nanoparticles as signal amplifier.

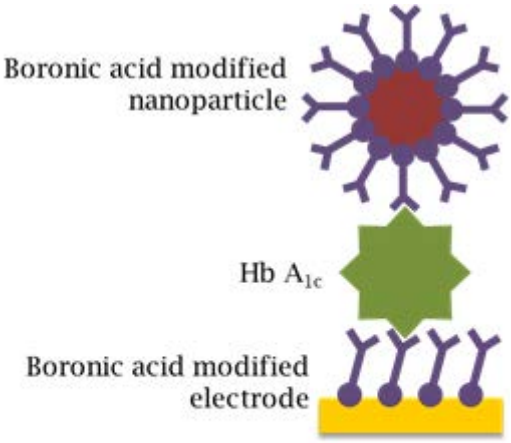

Fig. 1. A Schematic diagram of signal amplification of microgravimetric diabetes diagnosis.

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Highly Sensitive, Ion Selective Sensor Detection of Maleate(II) in Aqueous Media by Tripodal Ligand

이은빈 김재상 김동완 김관겸 박세빈

경상대 화학과

The ion selective electrode, which was selective and sensitive to Maleate ions, was developed using tripodal receptors L1,L2 and L3 as carrier. The electrode(E3) exhibits a good potentiometric response for maleate(II) over a wide concentration range (5.0×10^{-5} to 1.0×10^{-2} M) with a slope 30.70mV/decade. The proposed electrode has a response time 20s. The electrode is suitable for use in aqueous solutions in a wide pH range of 4.0 to 10.0. The proposed sensor revealed comparatively good selectivity with respect to various organic ions and inorganic anions.

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Silver nanomaterials for detection and recovery of Hg2+ in aqueous solution

LI DAN 양성익[1]

경희대 화학과 [1]경희대 응용화학과

The silver nanoplate and snow-like star structure have been successfully synthesized and examined for potential application in detection and remediation of Hg2+ in aqueous solution. The prepared silver nanomaterials were with an average diameter of 50 - 500 nm. Hg2+ can be detected by using the spectroscopic properties of silver nanoplates and the detection limit of Hg2+ was as low as 10 ppb. The concentration of Hg2+ ions can be decreased to less than 0.05 ppm. The results suggest that silver nanomaterials are potentially useful materials for simultaneously rapidly detecting and recovering of Hg2+ pollutants in aqueous solution.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly sensitive and selective beryllium colorimetric sensor based onSchiff-base ligand-functionalized gold nanoparticles

김동완 이은빈 김관겸 박세빈 김재상

경상대 화학과

This presentation reports a novel colorimetric sensor for beryllium (II) based on ligand-functionalized gold nanoparticles (L/AuNPs) which were characterized by UV-vis spectroscopy, and transmission electron microscopy (TEM). The sensor exhibited a high sensitivity, low detection limits that could be achieved by UV-vis spectroscopy. The gold nanoparticles showed high selectivity toward Be^{2+} with binding-induced blue shift in the absorption spectra. In the presence of beryllium, the olive L/AuNP solution turns to light blue. However, other alkali and alkaline earth metal ions did not interfere with the detection of Be^{2+}. The method was successfully applied to detect Be^{2+} in aqueous sample. And also, it was simple, rapid and cost-effective without and modifying procedure.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An Integrated Analytical Approach for Determining the Geographical Origin of Medical herbs Using Mutielement and Metabolome Analysis

권용국

충남대 분석과학기술대학원

Determining geographical origin of crops is becoming important, according to increase import of crops. ICP-MS and ^{1}H NMR are commonly used to determine the geographical origin of crops. In this study, Multielement analysis data detected in ICP-MS and metabolomic data detected in 1H NMR were integrated to improve reliability for determining the geographical origin of medical herbs. Astragalus membranaceus Bunge and Paeonia albiflora Pallas were analyzed by ^{1}H NMR and ICP-MS and integrated multivariate analysis was carried out to characterize the differences between origins. Four classification methods, linear discriminant analysis (LDA), k-nearest neighbor classification (KNN), support vector machines (SVM), and partial least squares discriminant analysis (PLSDA), were applied an validated using double check validation as leave-one-out cross-validation and external validation. The classification results for two medical herbs were more accurate in integrated statistical analysis of ^{1}H NMR and ICP-MS data than typical analysis by either ^{1}H NMR or ICP-MS. This integrated analytical approach is able to reflect diverse environmental factors such as climate and soil. Therefore, our study suggests that a suitable integration of different type of analytical data is useful for determining geographical origin of food and crops with high reliability

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Amperometric sensor for glucose based on covalent attachment of glucose oxidase to an Au electrode modified with gold nanoparticles

김동완 이은빈 김관겸 박세빈 김재상

경상대 화학과

In the present work, a simple technique to fabricate glucose biosensor was described by covalent attachment of glucose oxidase (GOx) to a gold nanoparticle monolayer modified Au electrode. The surface morphology of GOx on Au electrodes was investigated by atomic force microscopy (AFM). Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) were employed to study the electrochemical behavior of adsorbed GOx on Au. The analytical performance of this biosensor was investigated by amperometry. The sensor provided good linear ranges to glucose with a high sensitivity. In addition, the sensor has good reproducibility, and can remain stable over 1 month.

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A highly selective colorimetric and fluorescent chemosensor for Fe(III) ion based on Coumarin derivate

유재성 양성익[1]

경희대 화학과 [1]경희대 응용화학과

Iron ion plays an indispensable role in structural, catalytic and regulatory aspects such as electron and oxygen transport, synthesis of hemoglobin in red blood cell and myoglobin in muscle cell, many co-factor in enzymes and proteins. However, the excess or deficiency concentration of Fe3+ can induce potential health hazard. Thus, fluorescent sensors for Fe3+ are meaningful to develop in environment and living system. We found that optical and fluorescent sensor C14 exhibits a good selectivity and sensitivity toward Fe3+ over other metals. The Fluorescent sensors are remarkable method to detect metal ions because of their possibility to on-site and real-time detection with low concentration.

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Use of copper nanoparticles to remove mercury from contaminated water

LI BIAO 양성익[1]

경희대 화학과 [1]경희대 응용화학과

Mercury contamination from the gold mining and the burning processing of mercury-rich ores is one of the major environmental problems. Mercury can cause serious health problems because it easily passes through the skin, respiratory, and gastrointestinal tissues into the human body, where it will damage the central nervous and endocrine systems. Herein, we report a facile route to synthesize copper nanoparticles in an aqueous solution and their application in removal of Hg2+ in water. The Hg2+ remediation mechanism can be explained in terms of amalgamation process, which is demonstrated by XRD and EDX data.

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An Advanced Electrogenerated Chemiluminescence Sensor Based on Tris(2,2'-bipyridyl)ruthenium(II) Immobilized in the Composite Film of Ionic Liquid/Sol-Gel Ceramics/Nafion

장준호 최한님 김병건 이원용

연세대 화학과

An advanced electrogenerated chemiluminescence (ECL) sensor was fabricated based on ionic liquid(1-ethyl-3-methylimidazolium hexafluorophosphate)/sol-gel ceramics/Nafion composite film. Ionic liquid can be easily mixed in the sol-gel ceramics/Nafion composite solution. The presence of sol-gel in the Nafion increased the pore size of the composite films and thus led to faster diffusion of the immobilized tris(2,2'-bipyridyl)ruthenium(II) ($Ru(bpy)_3^{2+}$) and ECL co-reactant within the composite films. Further incorporation of ionic liquid within the sol-gel ceramics/Nafion composite films increased the ECL response of the resulting ECL sensor because of the decreased charge transfer resistance in the composite modified electrode owing to the conducting and electrocatalytic features of ionic liquid. Therefore, the present ECL sensor based on the ionic liquid/sol-gel ceramics/Nafion composite film showed improved ECL sensitivity for tripropylamine (TPA) compared to the ECL sensors based on both sol-gel ceramics/Nafion composite films and pure Nafion films. The present $Ru(bpy)_3^{2+}$ ECL sensor based on the ionic liquid/sol-gel ceramics/Nafion composite gave a remarkable detection limit (S/N = 3) of 0.48 nM while the ECL sensors based on sol-gel ceramics/Nafion composite and pure Nafion films gave a detection limit of 50 nM and 1.0 μM, respectively. The present ECL sensor showed outstanding long-term storage stability. Furthermore, the selectivity of the present ECL sensor could be readily controlled by selecting appropriate ionic liquids in the composite film. Therefore, it is expected that the composite films with hydrophobic ionic liquid could be easily applied for the determination of hydrophobic alkylamine drugs such as phenothiazine derivatives and erythromycin in human urine samples.

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Spectroscopic Analyses for Concerted Rotations in Tertiary Aromatic Amides

원다은

중앙대 화학과

The rotational barriers about the C-N and Ar-CO bonds in N,N-diethylpyrene-1-carboxamide, N,N-diethyl-1-naphthamide, N,N-diethyl-2-naphthamide and N,N-diethylbenzamide were investigated by variable temperature (VT) NMR spectroscopy and computational study with the GAUSSIAN 09W. From VT-NMR data, the barriers for C-N and Ar-CO rotations have been determined with Gibbs energy by line-shape and coalescence temperature (TC) analyses. The calculated Gibbs energy changes obtained at the B3LYP DFT level of theory with the 6-311G (d) basis set were in good agreement with NMR results. The rotational dynamics in tertiary aromatic amides is a complex process involving rotation around C-N and Ar-CO bond. The conjugation with aromatic rings induced concerted rotations around chiral plane and amide bond. It seems that the rotational barriers in tertiary aromatic amides are determined by competitive delocalization between two bonds.

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High-temperature gas chromatography-mass spectrometric analysis of cholesterols reveals pathogenesis in cardiovascular events

손현화 문주연[1] 정봉철 최만호[2]

KIST [1]연세대 화학과 [2]KIST 미래융합기술연구본부

Cholesterol and its derivatives are associated with cellular functions and their abnormalities are responsible for hormone-dependent disease such as cardiovascular events. Bioactive cholesterol derivatives including cholesterol, 7 cholesteryl esters (CEs), 9 oxysterols, and 4 cholesterol precursors were analyzed using a hybrid SPE purification coupled to high-temperature gas chromatography-mass spectrometry (HTGC-MS). Methanol-based hybrid SPE could increase extraction efficiency and minimize the matrix interference. The overall recoveries of CEs were ranged from 26.1 to 64.0% and other cholesterol derivatives were ranged from 82.1 to 129.3%. The limit of quantification of cholesterol and CEs ranged from 0.2 to 20.0 μg/mL except for cholesteryl arachidonate (100 μg/mL), oxysterols and cholesterol precursors were 0.01 ~ 0.2 μg/mL. Linearity as correlation coefficient was higher than 0.99 with the exception of cholesteryl palmitate, oleate, and linoleate ($r^2 > 0.98$), while precision (% CV) and accuracy (% bias) ranged from 1.9 to 11.9% and from 73.9 to 160.8%, respectively. This technique was then applied to serum samples obtained from acute myocardial infarction patients and model rabbits with hypercholesterolemia to evaluate their metabolic changes.

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발표분야: 분석화학

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Investigation on the Restricted Rotational Dynamics around Coordinated Amide Bond

민지은

중앙대 화학과

The rotational barrier about the C-N bonds in the complex of 2-(bis(pyridin-2-ylmethyl) amino)-N,N-diethylacetamaide and N,N-diethyl-2-(1,4,10,13-tetraoxa-7-azacyclopentadecan-7-yl)acetamide with metal ions were investigated by variable temperature (VT) NMR spectroscopy and computational calculations with the GAUSSIAN 09W. From the VT-NMR data, the rotation barriers about C-N bonds have been determined with Gibbs energy by the line-shape and coalescence temperature (T_C) analyses. By using the Hartree-Fock method with the charge of metallic ion, singlet spin and 6-31G the basis set as the condition, the Gibbs energy was calculated. When analytes form the metal complex, the electrons of nitrogens in pyridine rings and those of amide oxygen make coordinate bonds with metal ions. As a result, we could observe the changes in the chemical shift of N-CH_3 groups in ^{1}H 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 strong. This can be verified from the NMR experiments and computational calculations.

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발표코드: **ANAL.P-655**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct monitoring of ROS response at single cell level using gold nanowire electrode

곽래근 강미정[1]

KAIST(KAIST) 화학과 [1]KAIST 화학과

Reactive oxygen species (ROS) are important biomolecules in cell signaling and homeostasis. Hydrogen peroxide (HP) is one of most studied ROS and it is usually targeted to investigate the cellular oxidative stress. In this report, we used electrochemical method to measure HP response and monitored in real time manner at single cell level. To achieve this goal, we fabricated a nanoelectrode using a single gold nanowire which is ~150 nm in diameter and tens of micrometer in length. To increase selectivity and sensitivity for the detection of HP, we modified the surface of electrode with Prussian blue (PB). PB is known as the most advantageous HP transducer over all existing system. It increases electrochemical reactivity of HP and it also blocks other interfering substances such as ascorbic acid. We located the HP-coated Au nanowire electrode inside or outside a cell and then, we gave chemical or mechanical stimulation to the cell. When a cell experienced oxidative stress, HP was generated so we could measure its reduction current using PB modified electrode. Gold nanowires have high spatial resolution because of its small size, so we could compare the current for HP oxidation at intracellular and extra-cellular space.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of polyphenol level variations in radish sprouts influenced by different light quality using LC-MS/MS and PCA-biplot

정성우 옥세윤[1] 박세민[1] 서온누리[1] 이지은[1] 송이[1] 신성철[1]

경상대 원예학과 [1]경상대 화학과

Among various environmental factors, light is one of the most important variables affecting phytochemical concentrations in vegetables. Polyphenolic phytochemicals are ubiquitous in vegetables, in which they function in various health protective roles. Recently, sprouts vegetables have received a lot of attention as functional foods due to the high nutritional values obtained during their sprouting. Here, we present the results of the effect of different light quality on the accumulation of polyphenols in radish sprouts using LC-MS/MS and discuss the polyphenols variation by PCA-biplot.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of low molecular mass compounds by modified nanoporous gold surface and MALDI-TOF MS

조은지 안미리[1] 김종원[1] 김영환[2] 김성환

경북대 화학과 [1]충북대 화학과 [2]한국기초과학지원연구원 질량분석연구부

Matrix assisted laser desorption inonization time of flight mass spectroemtry (MALDI-TOFMS) has been widely used to study various compounds including peptides, protein, and polymers. Matrix plays a critical role to improve sensitivity of MALDI-TOF MS analysis. However, matrix produces multiple strong peaks at lower molecular weight region of mass spectra and hence it can cause problems when detection of low molecular weight (< 500 dalton) compounds is intended. Therefore, in this study, modified nanoorous Gold (NPG) plate has been combined with LDI TOFMS to study low molecular weight compounds including drugs and hormones. The sensitivity of the LDI MS analysis by use of NPG plate was 4 time or more better than that with stainless steel plate. It is clear that nanostructure can be helpful to improve sensitivity of LDI TOF MS analyses.

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

Quantitative Determination of Sulfathiazole using magnetic nanoparticles and Cy5 doped nanoparticles

김수지 고정아[1] 안정원[2] 임홍빈[1]

단국대 자연과학대 화학과 [1]단국대 화학과 [2]단국대 자연과학대학 화학과

Sulfonamides (SAs) are relatively inexpensive, widely available antibacterials. Residues of these antibacterial drugs in honey are of major concern because of their contribution in development of antibiotic-resistant pathogenic bacteria. Over the years a number of colorimetric, enzyme immuno assay, radio receptor assay, gas chromatographic , thin-layer chromatographic and reversed phase high performance liquid chromatographic methods for the determination of sulfonamides in honey have been developed . However, those methods are time-consuming, require extensive sample clean up and take a lot of time to optimize condition. To solve these problems, we developed a new method using dye-doped silica nanoparticle that involves minimal sample pre-treatment and rapid analysis times. The nanoparticles with uniform shape are modified with several functional groups like amine and carboxylic acid. In this work 46.52(±5.28) nm size of the nanoparticles doped with Cy5 (Eab=650nm, Eem=670nm) were synthesized by microemulsion method. For quantitative detection, we use a lab-built laser induced fluorescence microscope (LIFM) with photomultiplier tube (PMT) and 632.8nm helium?neon laser (with 635nm long wave pass filter). The results showed that the detection limit (LOD) for the compound was 0.048 ng/mL, which was about 10 times lower than that of ELISA method.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantitative determination of Salinomycin in Chicken muscle using Cy5 doped silica nanoparticle& Magnetic nanoparticle.

박지현 최혜원 조희경 임홍빈

단국대 화학과

Salinomycin is an anticoccidial drugs used as feed additives for the prevention and treatment of coccidiosis in poultry farming. Salinomycin, which are polyether ionophorous antibiotics, was primarily used for poultry and this residual could be harmful to human health. In this work, we developed sensitive and selective analytical method to determine Salinomycin using Dye doped silica nanoparticle. Magnetic nanoparticle is also used for sample collection. For quantitative detection, we use a lab-built laser induced fluorescence microscope (LIFM) with Photomultiplier tube(PMT) and 633 nm He/Ne laser (with 672nm~712nm interference filter). As a result, the limit of detection (LOD) for salinomycin was 0.0305 ng/mL, which was about 164 times lower than that of ELISA method.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Size and coverage control of silver nanoparticle coated silica nanocomposite with poly(ethylene glycol) derivatives for efficient surface-enhanced Raman scattering probes

임준혁 강호만[1] 경산 김종호[2] 이윤식

서울대 화학생물공학부 [1]서울대 협동과정 나노과학기술전공 [2]한양대 화학공학과

Surface-enhanced Raman scattering (SERS) technology has shown great potential in high throughput detection of chemical analytes with high sensitivity and selectivity. Several groups have attempted to fabricate SERS active substrate with high signal-to-noise ratio by various methods. We have prepared silver nanoparticles (NPs) coated silica nanocomposite using poly(ethylene glycol) (PEG) derivatives which can act not only as a stabilizer but also as a reducing reagent. By changing the terminal group of the PEG derivatives, we can control the size and coverage of silver NPs on silica nanosphere. And we successfully detected 4-aminothiophenol, as a model compound, with the SERS probes up to 100 fM range.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of capillary electrophoresis inductively coupled plasma mass spectrometry for quantitative analysis of phosphorylated peptide and lab-made interface

방수경 이경석[1] 임용현[1] 김태규

부산대 화학과 [1]한국표준과학연구원 분석화학표준센터

Various inorganic elements play key roles in biological systems as constituents of biomolecules. Especially, phosphorus plays an important role in protein activity by phosphorylation of protein and thus, a quantitative analysis for phosphorylation of protein can be a starting point to unveil its biology. In this study, an inductively-coupled plasma mass spectrometry (ICP-MS) hyphenated to the capillary electrophoresis (CE) was developed for quantitative analysis of phosphorylated peptide. The phosphorylated peptides were separated through electroosmotic flow in CE and quantitative information of phosphorylated peptides were analyzed by counting the number of phosphorus ions in ICP-MS. Since CE and ICP-MS have a considerable difference in flow rate, interface and electrolyte were carefully tested and prepared to achieve both electrical connectivity and fluent sample introduction between CE and ICP-MS. The phosphorus in separated peptide was detected by ICP-MS using medium mass resolution with high sensitivity. The concentration of phosphorylated peptide could be obtained from the peak area in electropherogram obtained by CE-ICP-MS. In addition, metrological traceability to the SI has been introduced to the measurement of phosphorlyated peptide. This work shows the potential of CE interfaced ICP-MS for the quantitative determination of phosphorylation in proteins.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultra-sensitive detection of phenol using antibody functionalized metallic nanoparticles with optical and electrochemical biosensors

장혜리 이혜진

경북대 화학과

In this poster, a ultra-sensitive detection of phenol using antibody-functionalized metallic nanoparticles in conjunction with surface plasmon resonance (SPR) and electrochemical techniques is presented. Since the phenol molecule is known to possess two different epitopes for two different UDP-glucuronosyltrasfreases (UGT) which are active on phenolic substrates, we designed a surface sandwich detection methodology; (i) a mouse anti-phenol (UGT) is first covalently tethered onto the chemically modified gold surface and (ii) phenol is then exposed to the surface followed by the adsorption of rabbit anti-phenol coated Ag nanocubes (NCs). This creates a surface sandwich complex of mouse anti-phenol/phenol/rabbit anti-phenol coated NCs which was then monitored using real-time SPR method. A similar surface sandwich assay was also developed for the electrochemical detection of phenol; phenol molecules were first adsorbed onto the mouse anti-phenol coated metallic nanoparticles(NPs)-modified electrodes followed by the specific interaction of the rabbit anti-phenol tagged with alkaline phosphatase (ALP) conjugated anti-rabbit IgG. The selective electrochemical signal was then achieved by measuring released electrons from the reaction of the substrate, 4-aminophenylphosphate (APP) with the surface formed mouse anti-phenol-NPs/phenol/rabbit anti-phenol/anti-rabbit IgG-ALP complex. The use of anti-phenol coated NPs with the enzymatically amplified sandwich assay facilitated high selective and sensitive detection of phenol.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoparticle-enhanced SPR Biosensor for sub nM Detection of Nickel(II) Ion

김엄지 이혜진

경북대 화학과

In this poster, a highly sensitive nanoparticle-enhanced surface plasmon resonance (SPR) biosensing platform for the detection of Ni(II) ions is described. In order to improve the selectivity of the Ni(II) ion over other divalent cations such as Cu(II), Zn(II), and Pb(II), a surface sandwich assay was designed using two different receptors which are well known to selectively bind to nickel ion, nitrilotriacetic acid (NTA) and polyhistidine; a NTA monolayer coated gold SPR chip was first exposed to interact with Ni(II) ions in water samples followed by the adsorption of polyhistidine coated quasi-spherical gold nanoparticles. The sequential adsorption process of forming the surface sandwich complex of NTA/Ni2+/polyhistidine-gold nanoparticles was monitored using real time SPR. The nanoparticle-enhanced biosensing method using SPR exhibited an superb detectable concentration of 0.2 nM Ni(II) ions. Also the selectivity of Ni(II) ion detection over interfering divalent cations including such as Cu(II), Zn(II), and Pb(II) was investigated and showed remarkable selectivity towards Ni(II). For example, 0.2 nM of Ni(II) could be detected in the 200 times excess of Zn(II) and Pb(II) ions.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Combining experimental results and quantum mechanical calculations to investigate an ionization mechanism of APPI

AHMED ARIF 최철호 김성환

경북대 화학과

Ionization process is a key step for LC-MS analysis because the process can significantly influence the quality of LC-MS data. Atmospheric pressure photo ionization (APPI) is a powerful technique for analysis of polycyclic aromatic compounds (PAH) and analysis of PAH is very important to study environmental substance and crude oils. In a previous study, it has been reported that toluene is the source H+ for APPI when only toluene was used as a solvent. However, what will be the proton source when other common HPLC solvent like methanol, water and acetonitrile co-exist with toluene is not known yet. In this study, the source of H+ during the generation of protonated PAH compounds as well as involved mechanism using APPI were studied for binary solvent mixture of toluene and methanol. Furthermore, quantum mechanical calculations were performed to find ionization mechanisms that agrees with our experimental findings.

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발표분야: 분석화학

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Development of Portable Rotating Disk Electrode System for Heavy Metal Detection

김용훈 강석원[1]

농촌진흥청 농업공학부 [1]농촌진흥청 국립농업과학원

A portable rotating disk electrode system (RDES) equipped with a home-made glassy carbon electrode (GCE) for the determination of Cd and Pb ions is fabricated. The home-made GCE is made of the thick and hard copper alloy rod to minimize the eccentric rotation and shows the proper sensitivity for the redox reaction. Our instrument demonstrates the reliable detection of Cd and Pb ions with good linearity in the concentration range of 100 ~ 500 ug/L.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparison of Shale oils collected from different locations by high resolution mass spectrometry

심아름 조윤주 김성환

경북대 화학과

The modern society is still heavily dependent on fossil fuels, although fossil fuels are known to the limited resources. However, there are many different forms of restricted resources such as oil shale and oil sand. Among those, oil shale is getting a lot of interest because it has huge deposit approximately 290 million barrels. In this study, shale oil samples extracted from 3 different areas of Green River Formation in Colorado ; Garden Gulch Member(GGM), Parachute Creek Member(PCM), Anvil Points Member(APM) were compared. Oil samples were prepared from oil shales by Fisher Assay method. The oil samples were seperated by SARA fraction and analyzed by APPI coupled to Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy (FT-ICR MS). The obtained spectra were analyzed and carbon number, double bond equivalence (DBE) and chemical class distributions were compared. It was found that aromatic, resin and asphaltene generally had large percentage of N1 class except saturate which was mostly composed of HC class. In case of carbon number and DBE, PCM generally had the larger carbon number but the smaller DBE distribution.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Laser Desorption/Ionization and Postsource Decay of Peptide Molecules Produced from the Surfaces of Silicon-On-Insulator (SOI) Wafers

김신혜 김정권[1] 문대원[2] 한상윤[3]

한국표준과학연구원 및 충남대 화학과 [1]충남대 화학과 [2]한국표준과학연구원 표면분석그룹 [3] 한국표준과학연구원 나노바이오융합연구단

We report the generation of intact ions of peptide molecules by laser desorption/ionization (LDI) from the bare surfaces of Silicon-On-Insulator (SOI) wafers. It was demonstrated for soft ionization of various peptides covering a mass range up to 2000 Da. Furthermore, with the addition of citric acid the LDI-on-SOI method extends its detection range as high as up to insulin. The LDI mechanism is discussed to be thermal, which is due to the rapid surface heating caused by the two dimensional thermal confinement in the thin Si surface layer of the SOI wafers. The thermal nature of the LDI process was shown to be further exploited to create postsource decay (PSD) of resulting LDI ions, which was well suited to peptide sequencing using TOF/TOF mass spectrometry.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of Gibberellic acid (GA_3) from fruit using HPLC/UV-vis

마경나 하정민[1] 명승운[1]

경기대 자연과학부 화학과 [1]경기대 화학과

Gibberellic acid (GA_3) belongs to an important plant growth hormone involved in the control of different physiological proceses such as fruit external ripening and fruit development, and others. Analysis of gibbrellic acid from fruit using HPLC/UV-vis has always been extremely difficult, since gibberellic acid has little ultraviolet(UV) absorbance. Therefore, a simple and accurate analytical method for determination of gibberellic acid in fruit was developed. The method involves liquid-liquid extraction and derivatization using phenacyl bromide for effective and high sensitive HPLC/UV-vis analysis. For optimized liquid-liquid extraction condition, extraction times, extraction solvent and pH during sample preparation process were investigated. And also, experiment factors which are reaction time, reaction temperature and amount of derivatizing reagent and base, for the effective derivatization, were optimized. This method can be analysis of gibberellic acid from fruit by HPLC/UV-vis.

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Identification of Degradation Product of Lincomycin and Iopromide by Electron Beam in Aqueous Sample

함현선 이민지 조현우[1] 명승운

경기대 화학과 [1]경기대 자연과학화학과

Attention to the occurrence of pharmaceuticals in the environment has led to a need for the analysis and identification of its metabolites and degradation products, as well as parent pharmaceutical. But identification of degradation products of pharmaceuticals is a challenging task because they are present in very low concentrations. Identification of the degradation products of lincomycin (antibiotic pharmaceuticals) and iopromide (iodinated X-ray contrast media) under electrical beam was performed by chromatographic separation and mass spectrometric technique LC/ESI(+)-MS/MS. Electron beam (UELV-10-10S, klysotrn, 10 MeV, 1 mA and 10 kW) experiments for the spiked aqueous sample, which in fortified with lincomycin and iopromide, were performed at the different doses. Several degradation products of lincomycin and iopromide were identified by interpretation of mass spectra by mass spectrometry. According to the electron beam does, the degradation efficiencies were investigated. The concentration of remaining parent pharmaceutical with increasing electron beam does is reduced.

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The Analysis of Cholesterol Oxidation Products (COPs) in Milk Powder by HPLC/UV-Vis

이진주 박소연 명승운

경기대 화학과

Cholesterol present in milk products can undergo oxidation processes during heating and storage, and as a result of these processes yield various cholesterol oxidation products (COPs). COPs have been shown to have a variety of potentially atherogenic, cytotoxic, mutagenic and possibly carcinogenic affects. Also COPs cause cell membrane damage and inhibition of cholesterol biosynthesis. Because of negative effect on human, analysis of COPs in food is important. For the determination of COPs in milk powder, first of all, lipids was extracted from milk powder and transesterification was used for converting esterified oxysterols and triglycerides into fatty acid methyl esters. After esterfication, purification by solid-phase extraction (SPE) employing a aminopropyl cartridge was performed. Extracted COPs were derivatized with benzoyl chloride in order to increase the UV absorbance of compounds through derivatization attaching a chromophore to the functional groups of cholesterols. The derivatized COPs were analyzed on a C18 column (2.1×100 mm, 3.5 μm) using a mobile phase of water and acetonitrile simultaneously. The established method can be used to determine low mg/kg levels of COPs in milk powder.

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Application of judgment with ATR FTIR in differentiation of forgery document

남윤식 이강봉

KIST 특성분석센터

Red stamping inks has traditionally been an impression of one's name in personal or official documents written in China, Japan and Korea. Red stamping inks on questioned documents were studied to investigate the feasibility of micro-Attenuated Total Reflectance (ATR) FTIR spectroscopy as a tool in the forensic study. Red stamping in personal contract involved with mining development rights was claimed to be forged and to be given fake testimony. Analysis of red seals used in contract documents was carried out by micro-attenuated total reflectance (ATR) FTIR spectroscopy. The micro-ATR FTIR spectra for red seal inks stamped in contract document could differentiate between red seal inks, and they revealed that they were originated from different manufacturers. The results show that an accuser's claim on devolvement of mining development rights seems not to be authentic on the basis of micro-ATR FTIR spectra, and it was validated in a real case that this micro-ATR FTIR technique can be a valuable non-destructive tool for the objective analysis of questioned documents involving red seal ink.

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Simultaneous determination of bupropion, escitalopram, S-desmethyl citalopram fumarate, lamotrigine and quetiapine in human plasma by LC-MS/MS

박세민 정성우[1] 이지은 서온누리 송이 옥세윤 신성철

경상대 화학과 [1]경상대 원예학과

Liquid chromatography-electrospray ionization tandem mass spectrometry (LC-MS/MS) method is a powerful tool for analysis of drugs and their metabolites in different type plasma. LC-MS/MS method was developed and validated for the quantification of bupropion, escitalopram, S-desmethyl citalopram fumarate, lamotrigine and quetiapine in human plasma. Plasma samples were extracted by liquid-liquid extraction and protein was precipitated using 2% methanol. The analytes were separated on a SunFire 100 mm x 2.0 mm, 3.5 μm C_{18} column (waters) using a gradient mobile phase at a flow rate of 0.2 mL/min. The analytes were detected by a MRM (multiple reaction monitoring) mode. The analytical caliveration curve range was 0.03-500 ng/mL in human plasma. The validated method was successfully used in a clinical application.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Interaction of silica nanoparticles with serum proteins

전영은 김성종[1] 송남웅[2] 한상윤

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Interaction of injected nanoparticles (NPs) with serum proteins in the vein is known to be very important as it influences the behavior of NPs in a biological environment. More specifically, what a living organism may actually see is the dynamical corona of associated biomolecules rather than the simple nanoparticle itself, which defines the biological identity of the NPs. In this regard, we investigated adsorption of serum proteins on the surfaces of size and shape controlled silica (SiO2) NPs of 20 nm and 50 nm in diameter. The physicochemical properties of NPs were fully characterized using various methods including SEM and DLS. For the analysis of proteins interacting with NPs, gel electrophoresis (SDS-PAGE) and liquid chromatography - mass spectrometry (LC-MS/MS) analyses were utilized. In this poster, we present the interaction of representative serum proteins including human serum albumin with well-defined silica NPs in terms of adsorption profiles and kinetics, which reveals different behaviors for NP sizes.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of particle size and packing thickness on raman spectral features

이진아 정희일

한양대 화학과

Raman spectroscopy has been extensively utilized for quantitative analysis of solid power samples. When laser is illuminated on a powder samples for Raman spectral collection, along with Raman scattering, other kinds of scattering such as Mie scattering could occur simultaneously. The degree of other scattering events could vary depending on the particle size and also possibly influence on the resulting Raman spectral feature. In other words, the quantitative sample representation of acquired Raman spectra could vary depending on the particles size although composition of samples remains unchanged.In our study, the variation of accuracy for the determination of ambroxol concentration, when different sizes of sample particle are used for Raman measurement, has been investigated. For this purpose, 4 different sizes (over 150, 150-100, 100-50, under-50 ㎛) of both ambroxol and lactose samples were initially prepared, and binary mixture samples (ambroxol concentration from 9.0 to 15.0 wt%) were prepared using the same particle size. With the prepared sample, both back-scattering and transmission Raman spectra were collected by varying the packing thickness from 1 to 7 mm with an increment of 1 mm. The spectral features acquired by simultaneously varying the particle size of samples as well as the packing thickness were compared each other. Then, using each dataset, partial least squares (PLS) was performed to determine the concentration of ambroxol and the resulting accuracies were evaluated in relation with the particle size and packing thickness.

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Analysis of NSAIDs in environmental sample using three-phase hollow fiber-liquid phase microextraction (HF-LPME) and HPLC

차용병 명승운

경기대 화학과

The development of faster, simpler, inexpensive and more environmentally friendly sample-preparation technique is an important issue in chemical analysis. Liquid phase microextraction only needs to a little amount of organic solvent and simple preparation technique. Extraction efficiency in HF-LPME system depends upon a variety of factors which include extraction time, stirring rate, ionic strength of sample solution and acceptor phase. Influence of these parameters on the extraction efficiency by three phase HF-LPME was investigated. In a three-phase mode, the analytes are extracted from the aqueous sample, through the organic solvent, and further into the aqueous acceptor solution present inside the lumen of the hollow fiber. Seven NSAIDs were extracted from 4mL of aqueous solution with pH=3 (donor phase) into dihexyl ether immobilized in the wall pores of a porous hollow fiber and then extracted into the acceptor phase with pH=13 located in the lumen of hollow fiber. After the extraction, the acceptor phase was directly injected into the HPLC system for quantification. The developed method showed good precision and accuracy for the analysis of NSAIDs from aqueous sample.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effective determination of three tetracycline antibiotics using HF-LPME and HPLC-UV

오웅교 명승운

경기대 화학과

LPME (Liquid-phase microextraction) may be utilized as a green chemistry approach to reduce the consumption of hazardous organic solvents in the chemical laboratory. A simple and efficient preconcentration method was developed using three phase liquid phase microextraction prior to HPLC?UV for simultaneous extraction and determination of trace amounts of tetracycline antibiotics including tetracycline (TCN), oxytetracycline (OTCN) and chlortetracycline (CTCN) from aqueous sample. Optimized conditions with respect to several experimental parameters including the effects of the extraction solvent, extraction time, agitation speed, salting-out effect for the determination of tetracycline antibiotics from sample were established.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the determination of vanadium and arsenic species in various samples by ion chromatography coupled with inductively coupled plasma atomic emission spectrometry

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목포대 화학과 [1]목포대 자연대 화학과 [2]전남한방산업진흥원 시험분석팀

The elemental chemical speciation has been an important method of analysis because its toxic and biological effects cannot be determined only by the information of the total element, but they depend on the particular chemical forms of an element. These species differ mainly in terms of their oxidation state and whether they are present in inorganic or organic forms. Of the chemical species of vanadium (from -1 to +5), vanadium(Ⅳ) and vanadium(Ⅴ) mainly exist in the environment, and the vanadium(Ⅴ) is more toxic than the vanadium (Ⅳ). Inorganic arsenic arsenite (As^{3+}) and arsenate (As^{5+}) are more toxic than organic arsenic with arsenite (As^{3+}) being most toxic. Arsenobetaine (AsB) and arsenocholine (AsC) have been reported to be nontoxic. The chemical species can be converted into other species in the progress of sample preparation. In this study, the basic research of matrix and pH effects on elemental species were performed. In particular, the matrix interferences on the chemical species of arsenic and vanadium were investigated in various samples by IC-ICP-AES.

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Quantitative Analysis of Uric acid by fluorescence Quenching method based on CdTe nanoparticles with enzymatic uricase/peroxidase system

서민호 **B.T.Huy** 이용일

창원대 화학과

A simple synthetic procedure for CdTe nanoparticles was developed directly in aqueous phase. The CdTe nanoparticles are highly fluorescent and can be tuned the particle size by changing reaction time and pH values. The interaction between CdTe nanoparticles and hydrogen peroxide was investigated using different stabilizers including GSH, MPA, TGA. The results showed that the fluorescence quenching demonstrated excellent sensitivity to H2O2. The convenient optical detection methodology of uric acid was developed based on the fluorescence quenching of CdTe nanoparticles by H2O2 which was produced from the enzymatic reaction of uricase. The detection conditions, reaction time, the concentration of uricase were optimized. The results showed that CdTe nanoparticles could be used as a fluorescence probe for detecting uric acid. This optical analysis method could provide a new feasible, simple, and generic way to analyze numerous H2O2-dependent enzymes due to many enzymatic reactions can produce hydrogen peroxide.

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Analysis of sucralose in food samples by capillary electrophoresis with LED-induced in-column molecularly imprinted polymer/ solid phase extraction

안지용 AVVARU PRAVEEN KUMAR 임재민 이용일

창원대 화학과

Recently, we developed a novel in-column and open-tube molecularly imprinted solid phase extraction (MISPE) concentrator for capillary electrophoresis (CE) by using a miniaturized light emitting diode induced polymerization (LEDIP) system. The strategy was based on directly coating a short layer of MIP material (about 3 mm long) at the inlet end of the inner wall of separation capillary under the irradiation of LED, thus accompanying the advantages of simplicity, zero dead volume, and ease of automization. And then compared with the conventional method using hydrodynamic injection by MISPE fiber, the MISPE concentrator provides increase in sensitivity with a low loss of separation efficiency.In this work, LED-induced in-column MISPE was used for extraction of sucralose from food samples. Sucralose is an typical artificial sweetener. The majority of ingested sucralose is not broken down by the body and therefore it is non-caloric. And sucralose is approximately 600 times as sweet as sucrose. The in-column MISPE-CE system was applied for extraction and analysis of sucralose content in various food samples with good accuracy and precision. The developed miniaturized LEDIP system is also suitable for on-line renewing or fabricating MISPE concentrator conveniently. The in-column MISPE is show the high affinity and selectivity, and the high recoveries for MISPE-CE analysis.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric Detection and Quantification of Heparin with the Self-assembled Polydiacetylene Liposomes

조용석 안교한

포항공과대 화학과

Heparin, known as the most negatively charged biological molecule, is used as an anticoagulant during clinical procedures such as cardiovascular surgery or therapy.1 Also heparin plays an important role in the regulation of physiological processes such as inflammation, lipid transport and blood coagulation.2We have devised a new strategy for colorimetric detection and quantification of heparin in biological media, such as FBS, based on polydiacetylene liposomes. The electrostatic interaction between the negatively-charged heparin and the positively-charged polydiacetylene liposomes leads to color change from blue to red in aqueous solution. A sigmoid acid-base titration curve was obtained for the binding between the positively-charged liposome and the negatively-charged heparin, from which a linear calibration curve is extracted. Addition of anionic biopolymers such as chondroitin 4-sulfate or hyaluronic acid to the same liposome system only led to small color changes probably because of the lower charge density in these analytes. The sensing protocol was successfully applied to the determination of heparin in HEPES buffer and FBS samples in the linear relationship for concentration ranges of 0.30-5.35 U/mL and 0.67-4.33 U/mL respectively. Thus, the developed sensing system has potential for determination of the therpeutic dosing level of heparin (2-8 U/mL) during cardiovascular surgery and also for postoperative and long-term care (0.2-1.2 U/mL).3Reference1. Gemene, K. L.; Meyerhoff, M. E. Anal. Chem. 2010, 82, 1612.2. Whitelock, J. M.; Iozzo, R. V. Chem. Rev. 2005, 105, 2745.3. Zhan, R.; Fang, Z.; Liu, B. Anal. Chem. 2010, 82, 1326.

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HPLC-ICP MS에서 Br간섭을 제거한 Se의 정확한 분석법 개발 및 CE-ICP MS와의 비교

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한국교원대 화학교육과 [1]한국교원대 화학교육

셀레늄은 주로 음식을 통해 체내로 흡수되므로 생활수준의 향상으로 인해 건강에 관한 관심이 높아짐에 따라 식품 및 의약 분야에서 셀레늄에 대한 빠르고 정확한 분석이 요구되고 있다. 이번 연구에서는 팔중극자 반응셀(Octapole reaction cell, ORC)이 장착된 유도결합플라즈마 질량분석기(Inductively coupled plasma mass spectrometry, ICPMS)에 고성능 액체 크로마토그래피(high performance liquid chromatography, HPLC)를 연결하여 여러 식품 시료 중 셀레늄 화학종을 분석하였다. 먼저 Reversed-phase, Anion exchange chromatography 를 이용해 셀레늄 화학종을 분리하였고, Anion excahnge solid-phase-extraction(AE-SPE)를 사용해 Br 간섭을 제거한 뒤 post-column isotope dilution 을 이용하여 정량 분석을 하였다. 고래 근육의 분석 결과 주된 화학종은 SeMet 이었으며, ^{78}Se spike 를 이용해 분석한 SeMet 의 양은 9.40 (± 0.60) ppb 이었다. 마찬가지로, ICP MS 와 CE(capillary electrophoresis)를 연결하여 식품 시료 중의 Se 화학종을 분리 및 정량하고, CE-ICP MS 와 HPLC-ICP MS 의 결과를 비교해 보고자 한다.

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SEC-HPLC-ICP MS를 이용한 Se-rich yeast의 Se-containing metabolite 분리

김경미 박용남[1] 김은주[1]

한국교원대 화학교육 [1]한국교원대 화학교육과

셀레늄은 인체필수영양원소로 포유동물의 셀렌 결핍증은 암 발병률과 사망률의 증가,근육 신경 감소 및 면역 질환을 일으키는 질병과 연관되어 있다. Se-rich yeast 를 이용하여 섭취할 경우 셀레늄이 단백질에 싸여진 상태로 섭취되므로 셀레늄의 손실이 적고 장기간 복용(800μg/day)에도 독성이 없어 유용하다. 또한 음식에 있는 셀레늄에 비해 matrix 의 영향이 적고 soft conditions(37 C; pH 7.5)으로 종 분화 위험이 적어 셀레늄연구에 주로 이용된다. Se-rich yeast 는 특정한 셀렌단백질을 가지고 있지 않으므로 본 연구에서는 Se-containing metabolite 을 SEC-HPLC-ICP MS 로 분리하였다.Se-rich yeast 는 Alltech(S. Korea)의 Selplex (1903±36 mgkg?1 셀레늄을 포함하는 Saccharomyces cerevisiae)을 이용하여 SEC (Size Exclusion Chromatography, Superdex 75 PC 3.2/30)를 10mM ammonium acetate buffer (pH 9.5), 0.1mL min?1 에서 Metabolite fraction(M1, M2, M3)를 분리하였다. 다원자 동중간섭방해를 제거하기 위해 ORC (Octapole Reaction Cell)의 reaction gas 로 H2 gas 를 사용하였으며, ICPMS 와 HPLC 를 연결했을 때 탄소흡착에 의한 sampler cone, torch injector 막힘 등의 문제를 해결하기 위해 make up gas 로 Ar 과 O2 를 혼합하여(Ar 80%, O2 20%) 사용하여 탄소를 산화시켰다.

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발표분야: 분석화학

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Structural identification of fluorosurfactant using mass spectrometry

임영희 조혜성[1]

LG화학기술연구원 CRD연구소 분석센타 [1]LG화학기술연구원 CRD연구소

Fluorocarbon-based surfactants are synthetic organofluorine compounds that have multiple fluorine atoms. They are more effective at lowering the surface tension of water than comparable hydrocarbon surfactants. For polymer they are used as lubricant, antifogging and reducing plasticizer migration. To determine structure, fluorosurfactants were analyzed by mass spectrometry. MALDI-TOF MS and pyrolysis-GC-MS was used for analysis of fluorosurfactants.

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Forensic comparison of soil samples.

장유림 김기욱[1] 허상철[1] 민지숙[1]

이화여대 화학나노과학과 [1]국립과학수사연구원 화학분석과

Soil samples were collected around the National Forensic Service in Seoul (three plots) and in Gangwon-do (eight plots), as a preliminary examination to obtain local information and to review the homogeneity of soils from the forensic viewpoint. The sample of each spots were obtained within the soil surface and 30 cm depth from the small-scale($1m^2$) of the five sites (a, b, c, d, e). Among the samples of 53-500 ㎛ fraction, Color test was conducted using a spectrophotometer and main composition elements were tested through the X-ray fluorescence spectrometer (XRF). In addition carbon contents and carbon stable isotope ratio were measured by the element analyzer-isotope ratio mass spectrometer (EA-IRMS) for fractions less than 53 ㎛. The canonical discriminant analysis showed that 88.2% of the color was distinguished. The major compositions by the XRF had excellent distinction, and the canonical discriminant analysis showed that 96.4% was correctly distinguished.The EA-IRMS showed that $d^{13}C$ (‰) was enriched in the deep soil compared to the surface and the C amount (%) was higher in the surface. These results are easy to distinguish of depth rather than regional differences.The canonical discriminant analysis testing all 3 features of the soil correctly distinguished 100% of the soil. For the same area, however, depending on the depth was observed the difference of results. Therefore, we should be careful that the samples are not mixed with soils from different depths while taking samples on the spot, as well as good results can be obtained by taking samples for forensic comparison from various points in the same area.

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Fluoride Anion Complexation by Mono and Ditopic Receptors and Appplications in ISEs

김관겸 이은빈 김동완 김재상

경상대 화학과

A uranyl(salphen) and bis- uranyl(salphen) based fluoride selective potentiometric sensor of novel structures were tested as anion-selective ionophores in the plasticized PVC membrane. Optimized membrane electrodes displayed linear range from 1×10^{-4} to 1×10^{-2} mol L^{-1} with a detection limit of 2.6×10^{-5} mol L^{-1} and a Nernstian response of -58.7±0.5mV $decade^{-1}$ was observed at a glycine-phosphoric acid buffer (pH 3.0). The following selectivity sequence has been recorded for both ionophores: $F^- > NO_3^- >$ Benzoate $> NO_2^- >$ Oxalate $> Cl^- > CO_3^{2-} > CN^- >$ Acetate $> HPO_4^{2-} > HCO_3^- > H_2PO_4^-$. The complexed were characterized by NMR, UV-Vis, X-ray analysis.

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Enantioseparation of Basic Chiral Drug Ccompounds Using Roxithromycin as a Novel Chiral Selector by Capillary Electrophoresis

AVVARU PRAVEEN KUMAR 이용일[1]

창원대 [1]창원대 화학과

A great number of chiral selectors have been employed in capillary electrophoresis (CE) and among them macrocyclic antibiotics exhibited excellent enantioselective properties towards a wide number of racemic compounds. From macrocyclic antibiotics, the use of roxithromycin (RXM) as a chiral selector for separation of enantiomers has not been reported previously. RXM possesses advantages such as high solubility and low viscosity in the lower alcohols and very weak UV absorption. This work reports the use of RXM as a novel chiral selector for the enantiomeric separations of seven chiral drugs in CE. The enantioseparations are carried out using polar organic mixtures of acetonitrile (ACN), methanol (MeOH), acetic acid and triethylamine as run buffer. The influences of the chiral selector concentration, ACN/MeOH ratio, and applied voltage on chiral separation are investigated. Further, work on enantiomeric identification by coupling CE with mass spectrometry (MSS) under progress. Keywords: Capillary Electrophoresis, Enantioseparation, Chiral drugs, Roxithromycin as a Novel chiral selector.

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Development of SERS DNA sensor based on DNA displacement

김샛별 정회일

한양대 화학과

Development of DNA sensor is one of the major researches in analytical chemistry. Due to the importance of DNA detection, rapid, sensitive and cost-effective DNA sensor received a great attention. We present a simple electrochemical synthesis of 3 dimentional (3D) Au nanodendirte network porous structure and its application in SERS sensor. Due to the ultra high surface area and many hot spots from 3D nanodendrite structure, the SERS signal was much more increasing compare to normal gold substrate. And using displacement reaction of DNA helped to increase the specificity and sensitivity of DNA sensor.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-688**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural Elucidation of Acetaminotadalafil Found in a Dietary Supplement

김지원

식품의약품안전청 첨단분석팀

A new tadalafil analogue, acetaminotadalafil, was detected by HPLC in the bulk powders of illegal dietary supplement products. The product was isolated by semipreparative HPLC. The chemical structure of the new compound was elucidated by HPLC, ESI-(Q)TOF-MS, NMR, IR and circular dichroism spectroscopy and identified as an acetylated compound of aminotadalafil. The structure of the previously unknown compound was confirmed as (6R,12aR)-2-acetamino-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-pyrazino[1?,2?:1,6]pyrido[3,4-b]indole-1,4-dione and named as acetaminotadalafil.

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발표코드: **ANAL.P-689**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Survey of Macrolide Antibiotics in Foods, Korea

송재상 강명희[1] 박순희

서울지방식약청 유해물질분석과 [1]서울지방식품의약품안전청 유해물질분석과

가축 사육 중 질병 치료와 성장 촉진을 위해 일정량의 동물용의약품 사용을 허용하고 있다. 그러나 축산 농가 등에서의 동물용의약품 사용 빈도와 사용 농도가 매년 증가하고 있는 추세이며, 오남용에 따른 최종 식품 중 잔류문제가 발생하고 있는 실정이다. 본 연구에서는 전국 주요 대도시(서울, 부산, 인천, 대구, 대전, 광주, 울산)에서 유통 중인 축산물 5 종(소, 돼지, 닭, 계란, 우유) 300 건을 확률비례추출법으로 수거하여 마크로라이드계 4 종(키타사마이신, 아프라마이신, 카나마이신, 올레안도마이신)의 잔류량을 조사하였다. 함량조사는 식품공전 시험법에 따라 전처리하여 HPLC-MS/MS(THermo Fisher TSQ Quantum)으로 확인하였다. Method Validation 은 MRL 수준에서 3 반복 이상 회수율(%)시험을 실시하였고, 모든 항목에서 70~120% 범위 내의 결과를 확인하였다. 조사 결과 가장 빈번하게 검출되는 의약품은 올레안도마이신이였으며, 닭고기, 돼지고기에서 각 2 건으로 총 4 건이 검출되었다. 검출된 동물용의약품들은 잔류허용기준 이하로 검출되었으며, 이상의 모니터링 결과 동물용의약품의 잔류 위해성은 안전한 것으로 나타났다.

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장소: 부산BEXCO

발표코드: **ANAL.P-690**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of Methylmercury in Common Dolphin living in the Southern East Sea of Korea

박현미 오민석[1] 정민지[1] 이선화[1] 문명희[1] 김미혜[2] 최윤석[3] 손석연 박경수

KIST 특성분석센터 [1]연세대 화학과 [2]식품의약품안전청 오염물질과 [3]국립수산과학원 갯벌연구소

Delphinus delphis, which living in the southern East Sea of Korea was investigated for the study of methylmercury distribution in the big aquatic mammals. Methylmercury(MeHg) in 4 kinds of common dolphins(male, female, young and old) was determined with GC/ECD. Methylmercury was extracted with hydrochloric acid and toluene, and cleaned up with L-cystein solution.Limit of detection(LOD) and Limit of quantitation(LOQ) were 5.8μg/kg, and 17.7μg/kg, respectively. Calibration linearity was estimated by R^2 which was 0.99 and Relative Standard Deviation(RSD%) was 1.5%. These results could show us the understanding of bioaccumulation of methylmercury in the aquatic mammals from the food cycle of fish and the toxicological knowledge from this methylmercury concentration distribution. Keywords: common dolphin, methylmercury, concentration distribution

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발표코드: **ANAL.P-691**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

β-cyclodextrin capped CdTe quantum dots as a fluorescence sensor for chiral molecules

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창원대 화학과

A simple, accurate, and rapid analytical method for chiral compounds has been developed using β-cyclodextrin capped CdTe quantum dots (QDs) based on their fluorescence quenching property. The new fluorescence analysis pathway utilizes cyclodextrins or some other ligands to modify the surface of CdTe QDs which are easily prepared via a simple sonochemical procedure using β-cyclodextrine as surface coating agent. As a result of the remarkable changes of the fluorescence intensity depending on different chirals, it is possible for CdTe QDs to detect chirals selectively. The optimum experimental condition has been established and analytical performance including linearity, detection limits, and precision, has been evaluated.

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발표코드: **ANAL.P-692**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Modification of N-linked oligosaccharides by endoglycosidase with glucose as an acceptor

정수희 이용일 임재민

창원대 화학과

Endo-beta-N-acetylglucosaminidase (Endo-M) is a glycoside hydrolase on N,N'-diacetylchitobiose moiety in oligosaccharides bound to the asparaginyl reside of various glycoproteins through N-glycosidic linkage. Endo-M has also ability to transfer suitable acceptors to reducing end of oligosaccharides called transglycosylation. Transglycosylation can be useful tool for the remodeling of carbohydrate chain and thus various oligosaccharides could be modified by the enzyme reaction with acceptors.Endo-M has been utilized as a function of transglycosylation with the glucose acceptors for the modification of N-linked glycans. In this study, we have optimized the enzymatic conditions (concentration, reaction time, and temperature) of Endo-M for transglycosylation with the glucose and characterized the permethylated N-linked oligosaccharides from sialylglycoprotein (SGP) by mass spectrometry.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cellulose tris(3,5-dimethylphenylcarbamate) bonded Fe_3O_4@ZrO_2

김종화 AVVARU PRAVEEN KUMAR 이용일

창원대 화학과

Chiral discrimination of enantiomers is a very challenging task and of critical importance in many areas of analytical chemistry and biotechnology, particularly in drug design and synthesis. In particular, solution-based sensor systems capable of chiral recognition would be of tremendous pharmaceutical value. Here we report, at first, the chiral discrimination of D- and L- aminoic acids using a designed CDMPC @Fe_3O_4@ZrO_2nanopraticles that acts as a chiral selector by virtue of its different interaction to binding of the chiral species. The nanoparticles composed of magnetic cores with chiral ligands on their surface to possess simultaneously magnetic property and chiral recognition ability. Cellulose tris(3,5-dimethylphenylcarbamate) (CDMPC) has been proved to be a most effective chiral selector. The Fe_3O_4@ZrO_2core-shell nanoparticles have not been reported for chiral separation yet. So, in the present work, core-shell nanoparticles consisting of Fe_3O_4 nanoparticle cores and zirconia shells (Fe_3O_4@ZrO_2) were used for immobilizing CDMPC to separate racemic compounds. The successful immobilization of CDMPC onto the surface of zirconia-coated nanoparticles(CDMPC @Fe_3O_4@ZrO_2) was confirmed by infrared spectra and circular dichroism spectra. Finally, direct separation of diverse enantiomers involving the application of magnetic nanomaterials will be presented. Keywords: Magnetic nanoparticles, Fe_3O_4@ZrO_2core-shell nanoparticles, CDMPC selector, Chiral separation.

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발표코드: **ANAL.P-694**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of Home-built Solid-state NMR Probe with Receiver Coil for Special Object

최성섭 정지호 박유근 김용애

한국외국어대 화학과

The solid-state NMR has been used for various insoluble materials and biological sample, up to now. Analysis of membrane protein using solid-state NMR on lipid bilayer or bicelle samples, membrane-like environment, is valuable especially for a predominantly helical secondary structure. But, most of biological lipid samples have 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. Therefore, several probe designs have been developed in our lab to improve the probe efficiency.We also employed solid-state NMR methodologies originally developed for the study of membrane proteins in lipid bilayers for the in-situ analysis of liquid crystalline materials in LCD panels. Since liquid crystals samples in LCD panels, could not be analyzed by conventional MAS technique and instruments.Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore(NB) 1H-15N solid-state NMR probe with strip-shield coil to prevent heating by high RF power. 1H-15N 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 19F-13C double resonance solid-state NMR probe with a flat-square coil and the first application of this probe for the in-situ analysis of LCD panel samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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발표분야: 분석화학

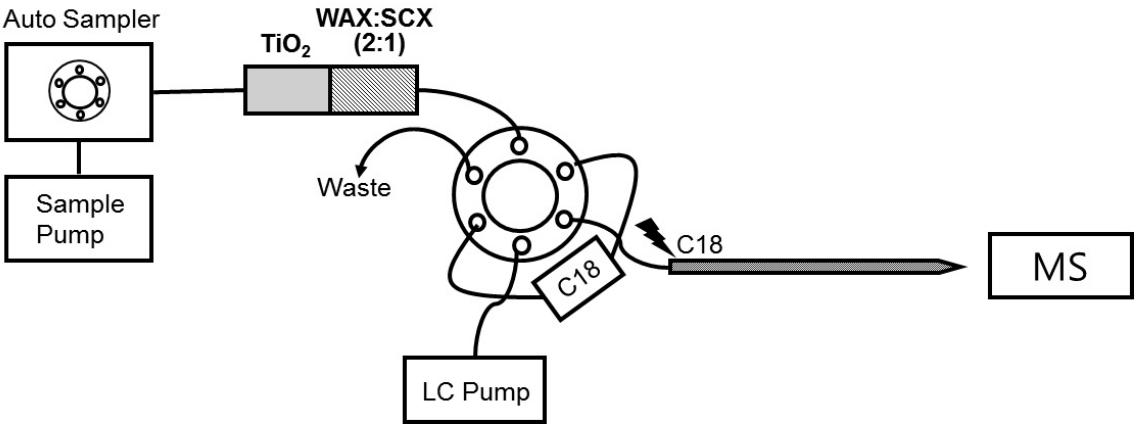
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Multidimensional System for Phosphopeptide Analysis using TiO2 enrichment and Ion-exchange Chromatography with Mass Spectrometry

조건 김진영 김영환 오한빈[1] 유종신[2]

한국기초과학지원연구원 질량분석연구부 [1]서강대 화학과 [2]한국기초과학지원연구원 연구장비 개발부

Although offline enrichment of phosphorylated peptides is widely used, enrichment for phosphopeptides using TiO2 is often performed manually, which is labor-intensive and can lead to irreproducible results. To address the problems associated with offline enrichment and to improve the effectiveness of phosphopeptide detection, we developed an automated online enrichment system for phosphopeptide analysis. A standard protein mixture comprising BSA, fetuin, crystalline, α-casein and β-casein, and ovalbumin was assessed using our new system. Our multidimensional system has four main parts: a sample pump, a 20-mm TiO2-based column, a weak anion-exchange, and a strong cation-exchange (2:1 WAX:SCX) separation column with LC/MS. Phosphorylated peptides were successfully detected using the TiO2-based online system with little interference from nonphosphorylated peptides. Our results confirmed that our online enrichment system is a simple and efficient method for detecting phosphorylated peptides.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-696**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

투명 은전극 제작 및 특성 평가

안경일 양성익[1]

경희대 화학과 [1]경희대 응용화학과

Recently, there have been significant interests in potential applications of flexible devices due to their potential applications in many areas including touch screens, flexible displays, printable electronics, OLED, OTFT, photovoltaics. Extensive efforts have been devoted in developing new material including alternative metal oxides, thin metal films, graphene, carbon nanotube to enhance their transparency and conductivity. We report on the single-pot fabrication of transparent Ag nanoparticle-based electrode on glass in solution. Our self-assembly based method allows the controlled deposition of Ag nanoparticles on substrate. The sheet resistance and transmittance can be controlled through the choice of reducing agent, capping materials, and reaction times.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

도료 내 VOC의 함유량과 방출량간의 상관관계

이나희 최민준[1]

중앙대 화학과 [1]숭실대 화학과

도료 내 VOC 함유기준에 관한 규제가 수도권에서 전국구로 내년 5 월 확대시행 된다. 휘발성유기화합물이라고 정의되는 VOC 물질들은 VOCs, TVOC 등 다양한 정의로 표현되고 있고, 도료 내 VOC 의 함유량과 방출량간의 상관관계에 대한 데이터는 아직 미비하다. 이에 다양한 종류의 도료를 이용해 함유량과 방출량의 기본방법인 ISO 11890-1/2, ISO 16000s 를 시행하여 둘의 상관관계 및 더 나아가 도료경화 시 방출량을 측정하는 Headspace 방법으로 값을 비교하고자 하였다. 방출량 시험은 경과시간 이후 분석을 하기에 함유량 값과의 절대적인 차이는 있을 것으로 보이지만, 전반적인 상관관계는 보일 것으로 생각한다. 또한 도료의 분야 별 상관관계도 비교해 볼 수 있다.

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장소: 부산BEXCO

발표코드: **ANAL.P-698**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Simultaneous Determination of Sibutramine and other weight loss substances in Weight loss functional foods

김지원

식품의약품안전청 첨단분석팀

A simple, specific, accurate and precise ion spray liquid chromatography/tandem mass spectrometry method was developed and validated for simultaneous determination of sibutramine and 28 other weight loss substances in weight loss functional foods. Chromatography was carried out on a UPLC BEH-C18 (Waters, 2.1mmx100mm,1.8 ㎛) Column with 0.1% Formic acid in DW:ACN (95:5) and 0.1% Formic acid in DW:ACN (5:95) at a flow rate of 0.25mL/min to gradient elution. The correlation coefficient of all the calibration curves were higher than 0.99. Coefficient of variation of intra- and inter-day variation was less than 13.7%. The recoveries ranged from 95.4% to 108%. Based on this results our developed methods to monitor illegal drug adulterations in dietary supplements using LC/MS/MS are simple, fast, reliable and applicable to drug adulteration screening.

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발표분야: 분석화학

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Validated corticoid signatures in human urine with liquid chromatography-tandem mass spectrometry

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SmartSCO, Clinical Diagnosis Division [1]연세대 화학과 [2]KIST 미래융합기술연구본부

Endogenous corticoids are produced in the adrenal cortex that mediates stress response. Since corticosteroid metabolism may be altered with disease states, the accurate and precise measurement of endogenous corticoids in biological specimens is necessary to understand their biochemical roles. An efficient quantitative profiling of 35 endogenous corticoids in human urine has been validated by liquid chromatography-tandem mass spectrometry (LC-MS/MS). After enzymatic hydrolysis with β-glucuronidase, samples were purified using a solid-phase extraction cartridge and then separated through a sub-2 μm particle C18 column (2.1 mm × 50 mm, 1.9 μm). The base-line chromatographic separation was accomplished with all corticoids including stereo-isomers, such as α-/β-cortol, α-/β-cortolone, and allo-tetrahydrocortisol/tetrahydrocortisol. The limit of quantification ranged from 0.2 to 10 ng/mL concentrations. Linearity as correlation coefficient was higher than 0.99 with the exception of α-cortolone, tetrahydrodeoxycorticosterone (THDOC), tetrahydrodeoxycortisol, and 5β-dihydrocortisone ($r^2 > 0.95$). The overall precision (% CV) of the assay were ranged within 0.29 - 89.8% (except for β-cortol, 5β-dihydrocortisol and THDOC). A validated method can be applied into inflammation mediated clinical events to evaluate metabolic changes of corticoids.

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장소: 부산BEXCO

발표코드: **ANAL.P-700**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Host-Guest Chemistry in the Gas Phase: Structures, Stabilities, and Dynamics of α,ω-alkyldiammonium Complexes of Cucurbituril

이신정 김준곤

포항공과대 화학과

Previously, our group reported the specific complex formation between the positive charged primary amine group of lysine side chain in peptides and cucurbit[6]uril (*Anal. Chem.*, 2011, 83, 7916). In this study, non-covalent interactions between cucurbiturils (CB[6] and CB[7]) and a series of α,ω-alkyldiammonium ions ($NH_3^+(CH_2)_nNH_3^+$, n = 4, 6, 8, 10, and 12) are probed using electrospray ionization ion mobility mass spectrometry (IMS). IMS measured collision cross section value and computational structural analysis provide structural insight of complexation details of alkyldiammonium with cucurbit[6]uril and cucurbit[7]uril via host-guest interactions. Of another interest is how the gas phase stability of complex ions can be changed depending on the cavity size of cucurbituril and the acyl chain length of diammonium ion. With the aid of low energy collision induced dissociation (MS^n) analysis, the relative stability of the complex ion is investigated. Combined IMS and MS^n provide further insight of dynamics of host-guest interactions between cucurbituril and α,ω-alkyldiammonium ion in the gas phase.

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장소: 부산BEXCO

발표코드: **ANAL.P-701**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimization of a Pressurised Liquid Extraction Method for Fluorescent Whitening Agents in Paper Samples

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고려대 화학과 [1]대구대 화학교육과

The method for the extraction of fluorescent whitening agents (FWAs) in paper materials has been developed. The procedure involves the extraction of the FWAs from coated printing paper by pressurized liquid extraction and the analysis of the extracts by ion-pair reversed-phase high-performance liquid chromatography with fluorescence detection. A central composite design was used to investigate the dependence of the recoveries of the FWAs on the temperature, percentage acetone:water ratio and the extraction time. Experimental data were then processed by using the multiple regression analysis in order to calculate a mathematical model representing the relationship between factors and responses and to determine the best experimental conditions for PLE method. These conditions corresponded to a temperature of 130 C, an extraction time 12 min and an 33:67 acetone:water ratio.

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장소: 부산BEXCO

발표코드: **ANAL.P-702**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Analysis of synthetic oligonucleotides arrays using Microscopic MALDI Imaging Mass Spectrometry

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Imaging mass spectrometry has become an advanced methodology for its capability of simultaneous detection of all desorbed analytes over a sample surface. Imaging mass spectrometer (IMS) coupled with matrix-assisted laser desorption/ionization (MALDI) and time of flight (TOF) makes possible macromolecules analysis with high sensitivity., An ion-optical microscopic lens system was designed and constructed to project the spatial origin of the desorbed ions from the sample surface onto the position sensitive detector(IONPIX, AMOLF, The Netherlands), for a microscopic MALDI IMS. A spatial resolution is determined by ionizing beam size, the quality of ion optics, magnification of microscope system, and the detector resolution. The spatial resolution down below 10 um can be achieved for a large field of view of 500 x 500 um^2 in preliminary experiments. The deposition of more spots in a field of view, means that more samples can be analyzed at a time. It results in reducing the time for analysis. This methodological approach is able to produce high throughput data with acquisition times reduced by more than three orders of magnitude compared with microprobe imaging technique. Its application to the high-throughput DNA analysis is also demonstrated.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-703**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Physical Property Analysis of Phospholipid Surfactant Layers Based on the Microfluidic Device: the Effect of Ozonolysis on the Model Surfactant Layers

최태수 김준곤

포항공과대 화학과

In the biological system, one of the representative air-liquid interfaces is the pulmonary surfactant (PS) system which comprises mixtures of phospholipids and proteins. The PS system participates in the breath cycle by controlling the surface tension and the fluidity of the interface in alveolar sacs. The present study provides the application of the microfluidic bubble generator for interfacial chemical reactions and resulted functional alteration studies related to PS system. Previously, we have found that only unsaturated phospholipids in the surfactant layer, which comprises saturated and unsaturated phospholipids, undergoes oxidation reaction by ozone. Then, the oxidized unsaturated phospholipid products dissolve into the bulk phase, leaving only saturated phospholipid at the air-liquid interface (*J. Phys. Chem. B*, 2010, 114, 9496). In the present study, we describe the alteration of physical properties such as oscillatory behavior, of the interfacial layer, which comprises saturated dipalmitoylphosphatidylcholine (DPPC) and unsaturated 1-palmitoyl-2-oleoylphosphatidylglycerol (POPG), under oxidative stress by ozone. Size and formation time changes of micro-bubbles by interfacial reaction by ozone are also described. For example, the model surfactant layer with ozone exhibits ~28% higher elasticity and takes five times longer period for the formation of bubble compared with when air is applied for bubble generation. The study reports on the application of micro-bubble generator for the investigation of air-liquid interfacial chemistry and physics which is distinct from conventional encapsulating applications of micro-bubbles.

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장소: 부산BEXCO

발표코드: **ANAL.P-704**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of uncharged or feebly charged small molecules by field-effect transistor biosensors

아칠성

한국전자통신연구원 차세대디스플레이연구단 전자종이연구팀

A new technique for the detection of uncharged or feebly charged small molecules (

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ANAL.P-705**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Immobilization of β-CD on glass surface and its application as a catalyst for oxidation of alcohols to ketones

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The trend of surface-modified materials e.g. glass, silicon, quartz and organic polymers is increasing rapidly in modern science and technology. Applications of such modified surfaces in synthetic or catalytic process have many advantages over traditional chemical methods e.g. easy separation from reaction mixture and low amount of reagents needed [1]. Among these materials, glass is more interesting because it is optically transparent, easily available at low cost and easy surface modification techniques are known for this material [2,3]. β-CD was covalently immobilized on glass surface and this functional glass surface was used to catalyze oxidation of alcohols to ketones. All reactions show high yield.

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장소: 부산BEXCO

발표코드: **ANAL.P-706**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of composite MIP films using silica microsphere and application to SPR gas sensing

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국민대 생명나노화학과

The volumetric shrinkage and deformation of molecularly imprinted polymers(MIPs) have been severe problems for gas sensing applications by causing reduction of the porous recognition sites. To resolve this problem, composite MIP films using functionalized silica particles were coated on the gold substrate via photopolymerization. The silica colloidal microspheres were synthesized using the Stober method. The surface of silica colloidal microspheres were modified to the thiol or acrylate functional groups using (3-mercaptopropyl)trimethoxysilane or 3-(trimethoxysilyl)propyl methacrylate. The thiol-acrylate reaction was used to form the covalent bonds between silica particles and MIP networks. The concentration and size of silica colloidal microspheres were controlled to reduce the shrinkage of polymer films and to obtain optimum condition for sensor applications. The stabilities of silica composite MIP films were turned out to be highly improved compared with the general MIPs through pillar effect. The sensitivity and selectivity of sensor films were tested for VOCs using surface plasmon resonance(SPR) technique.

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장소: 부산BEXCO

발표코드: **ANAL.P-707**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Iron-binding properties of low-molecular-weight succinoglycans isolated from *Sinorhizobium meliloti*

조은애 Muhammad Nazir Tahir[1] 김경태[2] 정선호[2]

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Iron is an essential element for all bacteria, and is also considered as a crucial factor in the bacterial virulence. In the present study, we have investigated the iron-binding properties of low-molecular-weight succinoglycans isolated from *Sinorhizobium meliloti*. The low-molecular-weight succinoglycans which are monomers (M1-M3), dimers (D1-D4), and trimers (T1-T6) of the succinoglycan repeating unit were purified with various chromatographic techniques. Surprisingly, T6, M3, and D3 bind Fe^{2+} even stronger than the well known Fe^{2+}-chelator ferrozine at pH 7. Also, the ferrous ion binding mode was confirmed with nuclear magnetic resonance (NMR) spectroscopy and electrospray ionization (ESI) mass spectrometry. These results demonstrate that T6 showing the highest chelating ability can effectively modulate iron biochemistry in *S. meliloti*.

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장소: 부산BEXCO

발표코드: **ANAL.P-708**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of methylated cyclosophoraose and its inclusion complexation with sulfadiazine

김환희 최재민[1] 조은애[1] 정선호[2]

건국대 생명공학 [1]건국대 생명공학과 [2]건국대 특성화학부 생명공학과

Methylated cyclosophoraose was synthesized with a family of neutral cyclosophoraoses isolated from *Rhizobium leguminosarum* biovar *viciae* VF-39. Its structure was characterized by nuclear magnetic resonance (NMR), Fourier transform infrared (FTIR) spectroscopy, and matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometry. Based on the enhanced hydrophobicity by methylation of cyclosophoraose, we investigated the inclusion property with water-insoluble antibacterial drug, sulfadiazine through phase solubility study in water and buffer solution (pH value of 2). The complex formation was also confirmed with NMR and FTIR spectroscopy. The results indicate the successful complexation between methylated cyclosophoraose and sulfadiazine.

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장소: 부산BEXCO

발표코드: **ANAL.P-709**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of the Complexation of Fisetin with Synthetic Cyclosophoroase dimer

정다함 Muhammad Nazir Tahir[1] PIAO JINGLAN[2] 정선호[3]

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Fisetin (3,7,3',4'-Tetrahydroxyflavone) is a pooly soluble flavonoid and therapeutic drug for various free radical mediated disease. The solubility of Fisetin can be enhanced by complexation with beta-cyclodextrin. Here, we synthesized novel cationic cyclosophoraose dimer, and investigated its inclusion property with fisetin. The cationic cyclosophoraose dimer was synthesized with cyclosophoraose isolated from *Rhizobium leguminoserum*, epichlorohydrin and choline chloride through a one-step polymerization procedure. The structure was also confirmed by nuclear magnetic resonance (NMR) spectroscopic and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometric analysis. In this work, the interaction between the synthesized cationic cyclosophoraose dimer and fisetin was studied through steady-state fluorescence, ultraviolet-visible (UV), Fourier transform infrared (FT-IR) spectroscopic and differential scanning calorimetric (DSC) analysis. The solubilization efficacy of cyclosophoraose dimer was higher than that of the parent cyclosophoraose and beta-cyclodextrin.

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장소: 부산BEXCO

발표코드: **ANAL.P-710**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of microbore hollow fiber enzyme reactor (mHFER)-based 18O-labeling method for the quantitative proteomics: its application to profiling the biomarkers in liver cancer sera

이선영 오동근 김소영 강덕진[1] 문명희[2]

한국표준과학연구원(KRISS) 바이오임상표준센터 [1]한국표준과학연구원 삶의질측정표준본부 [2]연세대 화학과

This study presents a simple proteolytic 18O-labeling method, which has been alternatively used for the quantification of targeted protein(s) in mass spectrometry (MS)-based proteomics, by means of which the formations of isotopically labeled peptides of targeted protein is easily carried out by a microbore hollow fiber enzyme reactor (mHFER). The conventional isotope labeling method in quantitative proteomics has several drawbacks such as a considerable time (at least 24 hours) required for proper isotope labeling equilibrium and back-exchange caused by residual enzyme activity. In order to overcome these drawbacks, the mHFER served as a promising tool for proteolytic 18O-labeling method was newly introduced and examined the efficiency in trypsin-catalyzed stable isotope 16O/18O-labeling of the C-terminal carboxyl groups of peptides by using a cytochrome C at two different conditions of heavy (18O) and light (16O) water. Both of resulting 16O/18O-labeled peptide solutions produced by mHFER were differently mixed in the ratio of 10:0 and 5:5, and followed by which those mixtures analyzed using nanoLC-ESI-MS-MS. From shotgun proteomic analysis, the ratios of 10:0 and 5:5 of 16O/18O-labeled peptide mixture were experimentally estimated as 0.81 + 0.13 and 1.13 + 0.51, respectively. In addition, it is promising that the developed mHFER-based 18O-labeling strategy can be effectively exchanged two light oxygens (16O) of the C-terminal carboxyl groups into two heavy ones (18O) in 30 min with high reproducibility. As a result, the developed proteolytic 18O-labeling method coupled with mHFER is an alternative tool for the identification and quantification of targeted protein(s) and also offers an accessibility of discovering a biomarker in relation to human diseases.

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장소: 부산BEXCO

발표코드: **BIO.P-711**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification of novel regulatory peptides against Sox2 in human embryonic stem cells

이상춘 박해철 Gedi Vinayakumar BAIG IRSHAD AHMED 윤문영

한양대 화학과

Sox2 is a transcription factor which is necessary for human embryonic stem (hES) cells differentiation. Earlier research proved that human cancer is frequently associated with overexpression of the cancer stem cell marker, Sox2. Therefore, the Sox2 has been a fascinating biomarker in prevention and vaccinization for various cancer tumors. In the present study, the Sox2 gene was amplified from the Human lung small cell carcinoma leaves by polymerase chain reaction and cloned into a pET28a expression vector. The expression plasmid carrying Sox2 gene was transformed into competent E. coli Rosetta2 (DE3) cells, induced by 0.5 mM IPTG at 18℃ for overnight and purified to homogeneity. The purified recombinant Sox2 provides a basis to screen novel peptides which binds with higher affinity and higher specificity to Sox2. Future studies of the candidate peptides ability to detect Sox2 and regulate several protein expression such as Nanog in hES were in progress and we believe these studies would significantly contribute in cancer tumor prevention and vaccinizations.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-712**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Screening of peptide binding on alpha and beta tubulin fromPhytophthora capsici by phage display

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한양대 화학과 [1]한양대 자연과학대학

Phytophthora blight of pepper is a completely destructive plant disease caused by the oomycete pathogen Phytophthora capsici. Phytophthora disease is responsible for major losses in pepper production and the pathogen can survive in soil in the absence of the host plant for many years.Cellular microtubules are known to play an essential role in nuclear division as components of the mitotic spindle and dimeric tubulin is their primary component. A key property of tubulin is its ability to assemble into microtubules via interaction between polymerized α- and β-tubulin monomers (heterodimer), and to undergo disassembly at appropriate times in the cell cycle.In present study, we screened alpha and beta tubulin binding peptides by M13 phage display method.

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장소: 부산BEXCO

발표코드: **BIO.P-713**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

PAMAM Derivatives using bipartite NLS Motifs of Mouse Fibroblast Growth Factor

이제일 최준식[1]

충남대 분석과학기술대학원 [1]충남대 생화학과

Polyamidoamine(PAMAM) dendrimer is one of the useful nanomaterials as gene delivery carriers and has comparatively excellent biocompatibility and biodegradability. However, It has relatively lower transfection efficiency than polyethyleneimine(PEI). In order to solve the transgene expression efficiency problem, we introduced a Nuclear Localization Signal(NLS) Peptide to PAMAM dendrimer. We introduce Mouse Fibroblast Growth Factor 3(FGF3) protein containing bipartite NLS motif, which has rich arginine residues. The entire NLS peptide of FGF3 protein is RLRRDAGGRGGVYEHKGGAORRRK. We select RRRK peptide, which is one of bipartite NLS. We performed synthesis of PAMAM-RRRK signal peptide and several experiments. PAMAM-RRRK indicated similar transfection efficiency corresponding to PEI in HEK 293 cell line and it also retained comparatively lower cytotoxicity than PEI. These results suggest that introduction of NLS peptide to dendrimer shows the possibility of an effective gene carrier for transfection.

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장소: 부산BEXCO

발표코드: **BIO.P-714**

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

장소혜

서강대 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, non-biocompatible 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.

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발표코드: **BIO.P-715**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

C-Terminal Acyl Shifts for a Stable Peptide-Drug Design

엄기동 이윤식[1]

서울대 기초과학연구원 [1]서울대 화학생물공학부

The objective of our approach is to prepare peptide-thioesters via the intramolecular O-S and N-S acyl shifts at peptide C-terminals, which can easily be converted to a stable peptide structure with a circular backbone resistant to endogenous enzymes. To evaluate acyl shift at the three different C-terminal linker structures (1, 2 for O-S acyl shift and 3 for N-S acyl shift in Figure) we added them on 2-chlorotrityl chloride resin, and then attached the same peptide sequence (TIGGIR) by using Fmoc chemistry. The synthetic yields gave 80-85% for 1 and 2 but 20-30% for 3 because the low yield of tertiary amide bond formation resulted in a strong steric hindrance of the dialkylamine coupling. An optimal condition converting 1 and 2 to peptide-thiocresol-thioester through O-S acyl shift and S-S external thiol exchange was established, even though differences in the linkers resulted in rates of O-S acyl shift and side reactions driven from the linkers, with a high conversion yield in the range of 60-83% for 2-4 h under various conditions depending on acidity and amount of the external thiol. Surprisingly the expected peptide-thioester product was obtained negligibly when 3 was exposed to the above condition; however, the peptide-MES- thioester was obtained with ~90% yield during a long time reaction when the above acidity and the external thiol were changed to a pH 4 cocktail buffer solution and sodium 2-mercaptoethanesulfonate (MESNa). Our technical approach for C-terminal acyl shift provides as a convenient tool to design stable peptide drugs against human diseases.

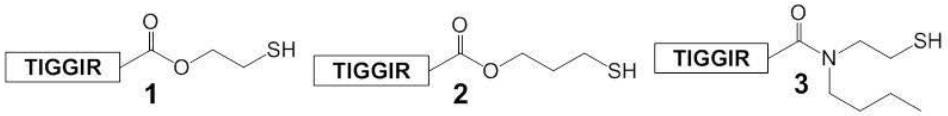

Figure. Three different C-terminal structures for C-terminal acyl shift. **1**: 5-membered O-S acyl shift, **2**: 6-membered O-S acyl shift, **3**: 5-membered N-S acyl shift

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-716**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal ion affinity purification of proteins by genetically incorporating metalchelatingamino acids

박나영

서강대 화학과

Affinity tags are efficient tools for protein purification. They allow simple one-step purification of proteinsto high purity. However, in some cases the tags cause structural and functional changes in a protein,and need to be removed. Therefore, affinity tags that are readily introduced into proteins with minimalperturbation and have specific affinity for purification are desired. Herein, two metal-chelating aminoacids derived from 2,20-bipyridine and 8-hydroxyquinoline were genetically incorporated into glutathioneS-transferase (GST) and the mutant proteins were purified by using the metal ion affinity of theunnatural amino acids. The purification of the GST mutants containing 2-amino-3-(8-hydroxyquinolin-3-yl)propanoic acid (HQA) showed that the proteins could be efficiently enriched in NieNTA by the metalion affinity of the unnatural amino acid and purified to excellent purity. This method should be veryuseful for general protein affinity purification, especially for proteins whose structure or function isaffected by affinity tags fused to N- or C-terminals.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **BIO.P-717**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of lipid compositions in Regulation of Photosynthesis

이길용 채원식[1] 안태규

성균관대 에너지과학과 [1]한국기초과학지원연구원 강릉센터

The photosynthesis in plants is designed to perform two opposing tasks. Firstly, it is composed to harvest sunlight efficiently. Secondly, it contains the phenomenon of dissipating excessive absorbed light energy as heat to avoid photo damage. These two functions act on thylakoid membranes which are composed of Monogalactosyldiacyglycerol(MGDG), digalactosyldiacylglycerol(DGDG),sulfoquinovosyldiacylglycerol(SQDF) and phosphatidylglycerol(PG). Numerious studies using such lipids have revealed that deficiency of these lipids primarily affects the structure and function of photosystem II. The specific function in the view of molecular level is still not understood. We reconstitute plant membrane protein inserting Light harvesting complex II (LHCII) into Giant Unilamellar Vesicle. By using this sample we observed that direct influence of plant's regulation in photosynthesis caused by protein complex structural change and protein-lipids interaction by fluorescence spectroscopy.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-718**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Colcemid inhibits the proliferation of vascular smooth muscle cells through the suppression of extracellular signal regulated kinase 1/2 (ERK1/2)

유지연 민용기

한국화학연구원 신물질연구본부

Colcemid is a microtubule-depolymerizing drug like vinblastine. We examined the effects of colcemid on the viability and proliferation in rat aortic smooth muscle cells. We also determined the mechanism by which the compound induces cell cycle arrest of the cells. Each group of colcemid (0.05, 0.1, 0.3 μM) treatment inhibited proliferation of the cells in a dose-dependent manner. colcemid did not decrease the levels of platelet-derived growth factor (PDGF) receptor and several protein kinases which had stimulated by exposing the cells to 25 ng/ml PDGF-BB. In contrast, the compound inhibited the extracellular signal regulated kinase 1/2 phospohrylation and arrested the cell cycle progression in the G0/G1 phase, which was related to the down-regulation of cell cycle regulatory factors such as cyclin D1/E, cyclin-dependent kinase (CDK)2/4. Further, colcemid induced cell cycle arrest in the G1 phase through up-regulation of p27kip1, but not of p21cip1. In order to examine the involvement of p27 and ERK-mediated signaling in colcemid-mediated growth inhibition of aortic smooth muscle cells, we determined the level of ERK phosphorylation by immunoprecipitates with anti-p27 antibody. Immunoprecipitation assay showed the decrease of p27-bound ERK1/2 only in the presence of colcemid. Also, colcemid shows the dramatic decrease of ERK expression in the cells transfected with its specific siRNA. The blockage of ERK by siRNA transfection significantly inhibited the colcemid-mediated decreases in the cell proliferation. These findings verify that colcemid mediates cell cycle arrest in the G0/G1 phase of PDGF-BB-treated cells through the inhibition of ERK1/2 phosphorylation. Our current findings suggest that colcemid contains anti-proliferative potential on aortic smooth muscle cells.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-719**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Doxorubicin exhibits a polo-like kinase 1 inhibitor in human colon cancer cells

김혜주 민용기

한국화학연구원 신물질연구본부

Polo-like kinase 1 (Plk1) has an important regulator of cell cycle progression in the pathology of many cancers, particularly mitosis. Also, Plk1 has a potential role in tumorigenesis. Drug repositioning is the application of known drugs and compounds to new indications. Accordingly, we investigated whether doxorubicin plays a Plk1 inhibitor in human colon cancer cells. We show that doxorubicin strongly inhibited cell proliferation Also, cell treated with doxorubicin accumulate in the G2/M phase of the cell cycle by FACs analysis. Several studies have identified mechanistic links that p53 and PLK1 negatively regulate each other that Plk1 inhibited the pro-apoptotic function of p53. We found that doxorubicin induced cell death by apoptosis occurs via p53-mediated prevention of caspase-independent mitotic death. Therefore, Plk1 inhibition leads to cell death in human colon cancer cells. We suggest that Plk1 inhibition have potential approach for cancer therapy.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-720**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

B-3575 enhances osteoblast differentiation through WNT and BMP2 signaling pathway via p300 and RUNX2 interaction in pre-myoblast C2C12 cells

배수정 김혜주 민용기

한국화학연구원 신물질연구본부

We demonstrated that novel compound B-3575 has an effect on bone formation in the pre-myoblasts C2C12 under the presence of bone morphogenetic protein (BMP)-2 in C2C12. BMPs are the most potent regulators of osteoblast differentiation among the local factors. We investigated the involvement of diverse BMP pathways on the induction of alkaline phosphatase (ALP) by B-3575. This compounds strongly enhanced osteoblastogenic differentiation ALP induction and smad 1/5/8 phosphorylation in this cell lines. RUNX2, the key transcription factor of osteoblast differentiation, was increased by B-3575 on osteogenic condition. We confirmed B-3575 blocked ALP induction and osteocalcin gene expression with noggin that highly selective inhibitor of both BMP signaling. In addition, we provide a molecular description for the cooperative effects of BMP and WNT canonical pathway on the expression of the early osteogenic marker RUNX2, Dlx3, Dlx5, Msx2 by B-3575 in the present of BMP2. We have uncovered that B-3575 have osteogenic properties, which are mediated by the interaction RUNX2 and p300. we suggest that B-3575 is beneficial therapeutics candidate for control bone formation.

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장소: 부산BEXCO

발표코드: **BIO.P-721**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inhibition screening of TCF/LEF activation by Luciferase assay in HCT116

박미경 김혜주 민용기

한국화학연구원 신물질연구본부

The Wnt/b-catenin pathway plays important roles in morphogenesis, normal physiological functions, and tumor formation. The Wnt signaling pathway controls beta-catenin, which enters the nucleus, where it interacts with members of the Tcf/Lef family and converts the Tcf proteins into potent transcriptional activators by recruiting co-activator proteins ensuring efficient activation of Wnt target genes including c-MYC, survivin and cyclin D1. We investigated whether 2320 chemicals of anti-cancer drug play a b-catenin inhibitor in colon cancer cells. First, we used the TCF reporter system in HEK 293 cells. HEK293 cells were transfected with a Tcf reporter gene (TOP-luciferase), which responds to the aberrant Wnt signalling activity by driving high levels of luciferase activity. We selected the best chemical `U-844` among 2320 chemical by reporter system. We found `U-844` inhibited c-myc, survivin and cyclin D1 expression level in HCT116 colon cancer. In conclusion, 'U844' inhibitions of Wnt target gene expression are important predictors of compound specificity.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-722**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Caffeoyl Dipeptide and Its Effect on PDGF-induced Vascular Smooth Muscle Cells Proliferation

양진경 곽선영 이윤식

서울대 화학생물공학부

The condition of oxidative stress is defined as elevated levels of free radicals or other reactive oxygen species (ROS), which can elicit either direct or indirect damage to the body. Caffeic acid (CA) is a well-known phenolic antioxidant, which exhibits a wide range of pharmacological activities and reduces oxidative stress. We prepared caffeoyl dipeptides to enhance the antioxidant activity and the stability of caffeic acid. Caffeoyl proline-histidine (CA-Pro-His) showed the excellent antioxidant activity among a small library of caffeoyl dipeptides containing histidine and/or proline. 1H-NMR study revealed that CA-Pro-His existed as s-cis conformation. From this, we assumed that proline provided a structural benefit, and thus, imidazole group of histidine could stabilize semi-quinone radicals of CA after hydrogen atom abstraction. Also, CA-Pro-His showed good ROS scavenging activity and anti-proliferation activity in cell systems without cytotoxicity.

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

Non-radiometric OGT Assay Method in a Microplate Format

김은주

대구대 과학교육학부/화학교육과

Dynamic O-linked-?-N-acetylglucosamine (O-GlcNAc) modification on the hydroxyl group of serine or threonine residues in nucleocytoplasmic proteins operates in a highly regulated manner in response to various cellular stimuli resembling phosphorylation. Different from phosphorylation, cycling of O-GlcNA is regulated by only two enzymes called as O-GlcNAc transferase (OGT) and O-GlcNAcase (OGA). OGT transfers GlcNAc from ?-linked UDP-GlcNAc to the hydroxyls of serine and threonine residues to form the ?-linked O-glycosyl proteins. A reverse enzyme, OGA returns glycosylated proteins to their unmodified state by catalyzing the removal of O-GlcNAc. Aided by the high-throughput enzymatic assays available for OGA, the design of potent and selective inhibitors for OGA has flourished in recent years. However, the lack of a rapid and simple method for continuously monitoring OGT activity has impeded the efficient discovery of potent OGT inhibitors. In this study we demonstrate a novel non-radiometric assay strategy for monitoring OGT activity in a microplate format using azide-labeled UDP-GlcNAc derivative (UDP-GlcNAz) as the sugar substrate. This method utilizes a microplate having a Ni ion captured on its surface and O-GlcNAc modified proteins with a poly-histidine tag as the protein substrates for OGT. This method developed here does not require the purification of the OGT enzyme allowing the rapid screening of chemical libraries for potent and selective OGT inhibitors.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-724**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Amino acid - conjugated polyamidoamine (PAMAM) induces efficiency of gene delivery

박정현 유광식 최준식

충남대 생화학과

Gene transfer using non-viral gene delivery carriers is studying widely. Non-viral gene delivery carrier shows low cytotoxicity. However non-viral gene delivery carrier has low transfection efficiency. We introduced Polyamidoamine (PAMAM) dendrimer that is widely used as a non-viral and polycationic vector for gene delivery. Amino acid - conjugated PAMAM dendrimer shows benefical results that is enhancement of transfection efficiency and a decrease in toxicity. We synthesized PAMAM dendrimer (generation 4, G4)-Histidine(H)-Lysine(K) / Ornithine(O) and compared this study with previous results (PAMAM G4-Histidine-Arginine). Lysine and Ornithine are cationic amino acid that contribute to condensation of DNA and contact with cell surface. Histidine has Imidazole group that induce “proton sponge” effect. We experimented the Gel retardation assay and Pico-green Assay for verification of PAMAM-DNA complex. Furthermore Toxicity was confirmed by MTT assay. Luciferase assay and Protein quantification were performed for confirmation of Transfection efficiency.

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장소: 부산BEXCO

발표코드: **BIO.P-725**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

OGT Inhibition Study Using Chemoselective Reaction in Combination with ELASA-based Enzymatic Assay

김은주

대구대 과학교육학부/화학교육과

OGT is the only enzyme that transfers single beta-N-acetylglucosamine (GlcNAc) from UDP-GlcNAc to the hydroxyls of serine and threonine residues of a large number of protein substrates. In concert with its counter enzyme, O-GlcNAcase, cellular O-GlcNAc levels are highly regulated. Dysregulation of O-GlcNAc cycling has been related to various diseases, including diabetes, cancer and neurodegenerative disorders. Selective and potent manipulation of O-GlcNAc in cells can be achieved by manipulation of these two enzymes' activities. As an attempt to discover enzyme-specific inhibitors of OGT we developed a rapid and simple method for continuously monitoring OGT activity using Ni-NTA coated 96-well plate. Using this method, we examined several known OGT inhibitors as well as a fluorescent UDP-GlcNAc derivative which has a fluorescein molecule through the amide linkage at C2 position for OGT inhibition. The fluorescent UDP-GlcNAc derivative was found to be as moderate inhibitor as UDP and the half maximal inhibitory concentration (IC50) of compounds examined in this study gave the similar values to the previously reported IC50 values.

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장소: 부산BEXCO

발표코드: **BIO.P-726**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enzymatically cleavable emphiphilic oligo-peptide micelles as a drug delivery system

송수정 최준식[1]

충남대 분석과학기술대학원 [1]충남대 생화학과

In this study, we report novel peptide micelles that composed of enzymatically cleavable peptides and can be applied as drug delivery system. GFLG (Gly-Phe-Leu-Gly) repeating sequence was conjugated with cationic amino acids (histidine and arginine). GFLG sequence is known to be cleaved by enzyme Cathepsin-B and may promote endosomal escape after intracellular internalization. Histidine and arginine modification helps to enhance the proton buffering capacity and transfection efficiency, respectively. Furthermore, synthesized GLFG3-His(n)-Arg peptides has two distinctive counter parts. GFLF3 unit serves as a hydrophobic tail and His(n)-Arg unit serves as a hydrophilic head group, respectively. Hence, they have a capability of forming a micellar structure in aqueous environment. Additionally, DOPE, a fusogenic helper lipid, was applied to more stable micellar formation. The hydrodynamic diameters of micelles were measured using dynamic light scattering method. To assess the possibility of application for drug delivery system, cytotoxicity was tested in cultured HeLa cells. Moreover, drug loading capability of synthesized micelles was measured using carboxyfluorescein (CF).

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발표코드: **BIO.P-727**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gene delivery carrier with PEI modified Polydiacetylene liposome

이영화 최준식

충남대 생화학과

The carrier based on Liposome has been investigated as gene or drug delivery system. In this study, we introduce a polyethylenimine(PEI) modified 10,12-pentacosadiynoic acid(PCDA) liposome. PEI has good transfection efficiency but it is known as a toxic material. We used to polymerization PCDA for gene delivery. PCDA and PEI were conjugated by 1-ethyl-3-[3-(dimethylamino) propyl] carbodiimide hydrochloride (EDC)/N-hydroxysuccinimide(NHS) coupling reagent. The synthesized polymer was determined by NMR spectroscopy and Fourier Transform Infrared Spectrometer (FT-IR). Agarose gel retardation and pico-green assay were performed to know the complex of the synthesized cationic polymer and plasmid DNA. The diameter of the polymer was analyzed by dynamic light scattering (DLS). Cytotoxicity of liposome was confirmed by MTT assay. We identify transfection efficiency of the PCDA-PEI liposome as luciferase assay.

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장소: 부산BEXCO

발표코드: **BIO.P-728**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of cationic liposomes with basic amino acids for gene delivery applications in vitro

배선주 최혜 최준식

충남대 생화학과

PDA(polydiacetylene) is made by photopolymerization of self-assembled diacetylene monomers. If diacetylene monomers are arranged systematically and close enough with distance of atoms , 1,4-addition polymerization will occur by the irradiation of 254nm ultraviolet rays and then PDA will have alternated ene-yne polymer chains at the main structure. Aqueous solutions of diffused PDA is tinged with blue which shows λmax 640nm . Visible color change from blue to red occurs in response to a variety of environmental perturbations, such as temperature, pH, and ligand-receptor interactions. Because cell membrane is composed of anionic lipids and glycoproteins, the net charge of cell membrane is anionic. Therefore, repulsive force is presented between cell membrane and DNA. So, many studies have been reported about using cationic polymer for non-viral vectors.In this study, we synthesized cationic peptides at the surface of PCDA liposome using SPPS (solid phase peptide synthesis) method and prepared liposome solutions at various molar ratios. When several mamalian cells were treated with the liposomes, high transfection efficiency and low toxicity was observed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-729**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel chroman derivative induced apoptosis in human cervical carcinoma HeLa cells

황지영 이명진 XuYi 신동수[1] 김동규[2]

인제대 화학과 [1]창원대 화학과 [2]인제대 의생명화학과

In this study, 1-((3R,4S)-4-(2-Ethoxy- 4-methyl-1H-pyrrol-1-yl)-3-hydroxy-2,2-dimethylchroman-6-yl)-3-phenylurea (S16), a novel 4,6-disubstituted 2,2-dimethylchroman was synthesized and its anticancer activity was investigated on the in vitro growth of human cervical carcinoma HeLa cells. In this study, we showed that S16 inhibited HeLa cell proliferation and viability in dose-dependent and time-dependent manner and the IC_{50} value was about 85 μM by using WST-8 assay. [^{3}H]thymidine incorporation and flow cytometry analysis significantly inhibited DNA synthesis and arrested HeLa cells at the G0/G1phase. Furthermore, the results from Annexin V-FITC/PI dual staining indicated that S16 induced early apoptosis in HeLa cells after exposure to S16 for 48hr. S16 treatment increased reactive oxygen species (ROS) and decreased mitochondrial membrane potential (ΔΨm). These results suggested that S16 induced apoptosis on HeLa cells.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-730**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functional expression and characterization of *carassius auratus* cytochrome P450 1A1 in *Shewanella oneidensis*

곽동건 강신원 박장수

부산대 화학과

Cytochrome P450 1A (CYP1A) is important in the biotransformation of xenobiotics, including polycyclic aromatic hydrocarbons, polychlorinated biphenyls, dioxins. Previous studies have reported a shewanella expression system for overproduction of c-type multiheme proteins. Here, we used shewanella to the functional expression of goldfish cytochrome P450 1A1. Since the periplasmic expression system is attractive, especially for protease-sensitive proteins, an expression vector containing a signal peptide was constructed for expressions in the periplasmic space of Shewanella oneidensis. The recombinant CYP1A1 protein containing a 6 × (His)-tag was expressed and was purified. Heme staining on SDS-gel electrophoresis proved binding of the heme to the protein. This work was supported for two years by Pusan National University Grant.

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장소: 부산BEXCO

발표코드: **BIO.P-731**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Cloning and characterization of full length of HSF1/2 isolate goldfish using RACE method

김지혜 박장수

부산대 화학과

In order to further establish goldfish as a vertebrate model for studying the mechanism of the heat shock response, it is necessary to sequence full length of HSF1 and HSF2. Heat shock factors (HSFs) are the main transcriptional regulators of the stress-induced expression of hsp genes. Organisms HSF1 was originally identified as the transcriptional regulator of the heat shock response, whereas HSF2 has not been implicated a role in the stress response. Organisms respond to circumstances threatening the cellular protein homeostasis by activation of heat-shock transcription factors (HSFs), which play important roles in stress resistance, development, and longevity. An efficient cDNA amplification procedure is described for determining of the 5’ and 3’ ends of mRNAs and cloning full-length cDNAs. The full-length genomic sequence of Heat shock transcription factor (HSF) recovered from liver tissue sample of a goldfish which was isolated with total RNA from liver of goldfish determined using RT-PCR and RACE (Rapid Amplification of cDNA Ends) methods.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-732**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functional Expression of a Cystine-rich Knot Peptide (ASPA) in Escherichia coli periplasm

이상언 강신원 박장수

부산대 화학과

Asteropsin A (ASPA), containing six-cysteine residues in 37 amino acids, was firstly isolated from the marine sponge Asteropus sp., which could enhance Ca2+ influx in murine cerebrocortical neuron cells following the addition of the Na+ channel activator veratridine. To further verify the characterization and mechanism of ASPA, its functional expression is urgent. Here, we showed that ASPA could be functionally expressed in the periplasmic area of E.coli by jointing a mini-tag (YoaJ) in the N-terminal of ASPA. The DNA sequences of ASPA and YoaJ were cloned into pQE30 vector by PCR technology, together with a six-histindine tag and a TEV recognition site. Recombinant YoaJ/ASPA was expressed in E.coli strain M15[pREP4], and purified by Ni2+-column. After digestion by TEV protease, functional ASPA was obtained by HPLC purification.*This work was supported for two years by Pusan National University Grant.

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발표코드: **BIO.P-733**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Gene Transfection efficiency of PAMAM Generation 4 conjugated enzyme-cleavable GFLG peptides.

손상재 이슬기[1] 최준식[1]

충남대 [1]충남대 생화학과

In the gene and drug delivery system, PAMAM dendrimer has been used as an ideal nanoparticle. So, we synthesized novel gene delivery carrier based on PAMAM G4. The oligopeptide polymer, GFLG sequence was selectively cleaved in the lysosome. Therefore, we adopted GFLG sequence to enhance the transfection efficiency. Also, we selected Arginine and Histidine to increase proton sponge effect and tranfection efficiency. Synthesized PAMAM G4 derivatives were evaluated their characterizations by various analysis ways. At first, complexes weight ratio of combined PAMAM G4 derivatives with pDNA were determined using agarose gel electrophoresis at 100V. Second, to identify the ability in vitro, we performed luciferase activity and MTT assay on the HeLa cells. As a result, the yield of synthesized PAMAM G4 derivatives was calculated by 1H-NMR, and we can be conformed that they were combined with amino-acid over 90%. PAMAM G4 derivatives with pDNA were completely retarded at 8:1(polymer:pDNA). Their size was determined between 100nm and 200nm. In results of transfecetion efficiency and cytotoxicity, PAMAM G4-GLFG-R revealed commonly transfection efficiency and somewhat higher cytotoxicity at the polymer concentration of 2mg/ml. On the other hand, PAMAM G4-GLFG-H-R indicated the highest transfection efficiency and lower cytotoxicity. In summary, we synthesized novel gene delivery carrier containing the enzyme-cleavable linker. So, GFLG sequence was adopted because the sequence can be broken by Cathepsin-B. Finally, we found the GFLG sequence to more enhance their transfection efficiency. Moreover, the carrier containing the Histidine showed remarkable transfection efficiency.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **BIO.P-734**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorophore-free Nanoprobes for Optical Imaging Based on the Self-assembly of Biofriendly Polyelectrolytes

신다혜

충남대 분석과학기술대학원

Here, we describe the fabrication of multispectral nanoparticles crosslinked with glutaraldehyde, which could provide multicolor optical imaging modality. The self-fluorescent Poly(γ-Glutamic Acid) (γ-PGA)/PLL(PEG) and γ-PGA/Chitosan nanocomposites were synthesized by electrostatic assembly and crosslinking between γ-PGA and two different cationic polymers, poly-L-lysine and Chitosan. The unique optical properties caused by crosslinking were analyzed by fluorescence spectra and UV/Vis spectra. Also, we could confirm that the fluorescence intensity can be regulated by adjusting the reaction time of crosslinking and the volume of crosslinker. The fluorescence images involving multispectral properties of nanocomposites are obtained by using appropriate optical filters. To demonstrate the fact for the possibility of biological application, intracellular delivery capacity was evaluated by flow cytometry at various concentrations. We have shown a possibility that the nanocomposites are expected to be a promising multimodal agent for the labeling, detection, monitoring and a variety of biomedical applications.

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발표코드: **BIO.P-735**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembled γ-PGA/Cholesterol Nanogel as Anticancer Drug Delivery Carriers

홍지현 임용택[1]

충남대 분석과학기술대학원 [1]충남대 분석과학기술대학원 분석과학기술학과

In this research, Poly(γ-Glutamic Acid) (γ-PGA)/Cholesterol nanogels were synthesized and their properties were evaluated. The γ-PGA/Cholesterol nanogels exhibited amphiphilic nature due to the hydrophilic γ-PGA backbone and the hydrophobic cholesterol side chain. The hydrophobic core was used for the encapsulation of doxorubicin (DOX), a model anticancer drug. The average size of γ-PGA/Cholesterol nanogel was 20-30 nm in aqueous phase. After encapsulating DOX into γ-PGA/Cholesterol nanogels, the particle size increased up to 400-500 nm. The zeta potential of the γ-PGA/Cholesterol nanogel was negative due to the ionized carboxylic group of γ-PGA located in the shell of nanogel. γ-PGA/Cholesterol nanogels showed controlled release of DOX in vitro condition and efficient uptake into cancer cell. The γ-PGA/Cholesterol nanogels are expected to be widely used as drug delivery carriers after loading with other therapeutic drugs, such as proteins and siRNA for cancer therapy.

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Mechanical properties of Artificial Mitochondrial Membranes

이두호 신관우[1]

서강대 화학과 [1]서강대 화학과 및 바이오융합과정

A cellular membrane is a physical boundary that differentiates cellular components from the outside. The adsorption and transport of molecules across the cellular membrane are intimately related to many important biological phenomena such as transport of ions or signal transduction. At a same time, the membrane maintains a basic cellular shape, and structure, and understanding its physical and mechanical properties are very important. Recently we developed an apparatus equipped with a microscopy and single cell manipulators, which is enabling us to monitor a deformation of individual artificial cellular structures, by aspiring the lipid vesicle with controlled pressure. By comparing the exerted pressure with the extent of surface area extension, we can calculate the modulus of lipid vesicles. In this study, we assembled a mitochondria-like lipid vesicles, composited with major lipid compositions (phophatidylcholine and cardiolipin). Since cardiolipin (CL) is a kind of lipid, but found only at mitochondria, we could determine the effects of CL in terms of physical properties, and shapes. It is well known that the mitochondria inner membranes have a unique shape ~ wavy and folded. In this study, we will present, how the content of CL in lipid vesicles influences the structural characteristics. Finally, we can discuss how the molecular structure of CL is responsible for the natural shape and physical structures of the mitochondria inner membranes.

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Reconstitution of proteorhodopsin into vesicles: monitoring proton-pump activity with pH sensing dyes

김희연 신관우[1]

서강대 화학과 [1]서강대 화학과 및 바이오융합과정

Proteorhodopsin(PR), the light-driven proton pump, is an retinal protein family type Ⅰ found in the marine bacterium. This is seven transmembrane α-helices proteins which carry retinal as a chromophore. The proton transports from inside to outside of membranes after illumination at pH above the pKa of the proton acceptor. There are so many methods for the reconstitution of membrane proteins into vesicles to make practical applications of properties of proton pumping by rhodopsin. Representative strategies for the functional reassembly of membrane proteins into vesicles are organic solvent-mediated reconstitutions, mechanical means and detergent-mediated reconstitutions. In this study, proteorhodopsin was reconstituted into artificial vesicles by the detergent-mediated method. Rhodopsin into artificial vesicles can support light-induced pH gradients like rhodopsin in real cells because this still maintains the activity. pH changes by proton pumping were measured with ratiometric analysis of pH sensing dyes. Fluorescence dyes like a pyranine dye and FITC also can be encapsulated into vesicles. The intensity of the dyes sensitively indicates the pH inside of vesicles. For accurate measurement of the pH of samples, fluorescence dyes were selected according to types of rhodopsin. As a result, we can detect pH changes with a fluorescence spectrophotometer and a confocal microscope.

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microcompartmentation of artificial cells

정성희 신관우[1]

서강대 화학 [1]서강대 화학과 및 바이오융합과정

A major difference between eukayotes and prokaryotes is the presence of physical compartments (membrane bound) within the cell. In a real cell, there are many physical compartments. There are major two reasons that the actual cell can make up compartmentalization. First, each part of the compartmentalized cells constitutes not pure water but gel-like solution. It makes cells withstand external force and maintain their original form. Second, various compartmentalization within a one cell makes it possible to perform many functions in a cell where specific processes may occur or are restricted too. In my experiment, I made Giant unilamellar vesicle(GUV)s using agarose gel, that is artificial cell based on the fact that cells made up of gel-like solution to provide a similar environment to cytoplasm. It has high internal rigidity compared to usual vesicles swollen by only water.Furthermore, GUVs were made by mixing two or more polymers that have different chemical properties and then by changing external environment like temperature or pH, I could observe change of the interior structure that artificial cells constitute microcompartment, or the boundary of the cells disappears. Finally, I would like to make GUVs containing beads that can lean to one side in an artificial cell by changing chemical or physical properties of inner structure. Movement of these beads can play a role to mimic nucleus of cell division in a real cell.

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Analytical characterization of aza-indole alkaloids in the biosynthesis of Catharanthus roseus

이향렬

한국교통대 생명공학과

Aza-indoles are important pharmacophores that have similar size and biological properties of indole. Here we have synthesized 4- and 7-azaindole tryptamines and showed that they are successfully incorporated in the biosynthesis of monoterepene indole alkaloids (MIAs) to form novel azaindole alkaloids by enzymatic reactions of strictosidine synthase(STR) and strictosidine glucosidase(SDG) monitored by UPLC/MS. By using HPLC equipped with a HPLC photo diode array(PDA) detector, each of the UV spectra of azaindole alkaloids was obtained and characterized. When hydrophilicity of azaindole alkaloids was compared, 4-azaindole alkaloids were more hydrophilic than 7-azaindole alkaloids.

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Encapsulation of Quercetin into PLGA Nanoparticles by Pluronic F127 and Poly(vinyl alcohol)

조상희 임용택[1]

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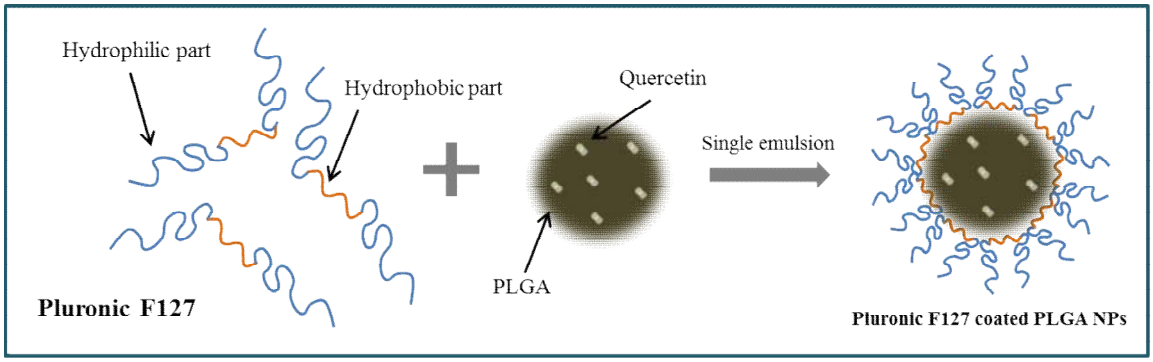
The antioxidant molecules, quercetin, 3,3',4',5'-7-pentahydroxy flavones, have been encapsulated into poly(D,L-lactide-co-glycolide) (PLGA) nanoparticles (QC-PLGA NPs) for the improvement of their poor aqueous solubility and stability, by O/W emulsion solvent evaporation method . Two surface modifying agents, Pluronic (F127) and PVA molecules, were used for the coating of PLGA NPs during the fabrication procedure. In this research, F127 coating strategy was adopted for the increase of mucus penetration property of QC-PLGA NPs by polyethylene glycol part in F127. The sizes and zeta potentials of QC-PLGA NPs coated with F127 and PVA were 138 ± 22.6 nm and 108.2 ± 19.2 nm, -22.24 mV and -23.43 mV respectively. Antioxidant assay indicated that QC-PLGA NPs were able to maintain the antioxidant property similar to that of free Quercetin at equivalent concentration and MTS assay showed that QC-PLGA NPs is non-toxic.



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Molecular Basis of Docking Interaction between ERK2 and its Substrate ELK-1

임동원 허용석

건국대 화학과

Mitogen-activated protein kinases (MAPKs) play central roles in many physiological processes including cell growth, differentiation, oncogenic transformation, apoptosis, and immune response by mediating extracellular stresses to cellular signals. The efficiency and specificity of these MAPK signal pathways are modulated by docking interactions between individual MAPK and the kinase interaction motif in its upstream kinases, scaffolding proteins, substrates, and phosphatases. Here, the crystal structure of extracellular signal-regulated protein kinase 2 (Erk2) in complexed with the peptide derived from its substrate Elk-1 was determined at a resolution of 2.2 angstrom. In the complex structure, the peptide docks to the docking groove of Erk2, which is away from the ATP pocket or substrate recognition site and the peptide binding induces the conformational rearrangements of the activation loop, which is buried in the inactive form of Erk2, being exposed to the surface of the protein. This structure implicates the structural basis of the regulation of MAPK signaling by specific docking interactions

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Structural Insight for the Recognition of 3-phosphoinositides by MTMR8.

유기영 허용석

건국대 화학과

Phosphatidylinositides play important roles in cellular recognition and membrane trafficking. Myotubularin families have been emerged as key regulators of phosphatidylinositol 3-phosphate and phosphatidylinositol 3,5-bisphosphate, which regulate traffic within the endosomal-lysosomal pathway. These myotubularins belong to a unique subgroup of phosphatase that dephosphorylate inositol phospholipid, rather than phosphoprotein, as physiological substrates. Mutations in MTMRs, myotubularin-related proteins, lead to diseases such as type 4B Charcot-Marie-Tooth. Here, the crystal structure of human MTMR8, a homologuolus myotubulatin, is determined at the resolution of 2.95 angstrom. MTMR8 shows the first structure of a dimeric interface of the catalytic domain and the specificity of MTMR8 toward phosphoinisitide substrates. This structure will provide the molecular mechanism of the MTMR regulation by dimerization and the specific recognition of substrates.

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Enhanced gene expression by complexation of EBNA-1 gene and PAMAM-Arg polymer

최혜 배선주 송수정[1] 최준식

충남대 생화학과 [1]충남대 분석과학기술대학원

An Epstein-Barr virus (EBV)-based plasmid contains the EBV nuclear antigen 1 (EBNA1) gene and EBV replication origin (oriP) sequence. Since EBNA1 (the only EBV-encoded protein) is combined with oriP, it is replicated simultaneously with chromosomal DNA in human, primate, and canine cells and is faithfully segregated at a stable copy number upon cell division. Consequently, it can be used to stably express gene inserts over a prolonged time in target cells. We have previously shown that the polyamidoamine (PAMAM) dendrimer can be surface-modified with l-arginine. Arginine is present at a high frequency in the trans-activator of transcription (Tat) sequences of human immunodeficiency virus (HIV). It presents high membrane permeability and permits effective transfer of DNA into the nucleus. In this study, we constructed two kinds of recombinant DNA by inserting the luciferase gene and enhanced green fluorescence protein (eGFP) gene as reporter genes into the pCEP4 plasmid vector. We measured dynamic light scattering (DLS) and zeta potential after preparing PAMAM-based cationic polymer/EBV-based plasmid complexes. We performed transfection of HEK 293 cell lines with the polyplexes, and monitored luciferase activity and green fluorescence protein (GFP) expression. Our results show that PAMAM-based cationic polymer/EBV plasmid complexes provide enhanced and sustained gene expression.

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Gene delivery effects of PAMAM dendrimer modified with signal peptide from simian virus 40T

이제일 정진우 최준식[1]

충남대 분석과학기술학과 [1]충남대 생화학과

Nuclear Localization Signal(NLS) Peptide is specific signal facilicating translocation into the nuclear and it enables inflow of optimum particle of 26nm whereas particles below 9nm can pass Nuclear Pore Complex(NPC) under absence of NLS peptide. Polyamidoamine(PAMAM) dendrimer is widely using cationic polymer in the gene delivery system research. It has low cytotoxicity and relatively good transfection efficiency but it indicates less transfection capacity in comparison with viral vector or Polyethyleneimine(PEI). Therefore, we introduced one of the NLS peptides in order to improve transgene expression capacity. The utilized NLS is KKKR peptide sequence of simian virus 40 T-antigen and it has rich primary amine group. In light of these information, The NLS peptide KKKR anticipated* that it has possibility of proton buffering effect occurrence. Therefore, we process this study.

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Selective Dephosphorylation by Scp1 and PP2A in Phosphorylated Residues of Smad2

김영준

건국대 응용생화학과

Phosphorylation and dephosphorylation of proteins have relevance to enzymatic activity or stable regulation of protein. It has been known as vital mechanism, and phosphorylated residues exist about 30 percent in the intracellular protein. Protein phosphatases have a important role in cellular events as a regulator. Scp1 specifically dephosphorylates phosphorylated Ser(5) (phospho.Ser5) of the heptad-repeats (YSPTSPS) of the C-terminal domain(CTD) of RNAP II. PP2A has been known a ubiquitous and conserved Serine/Threonine phosphatase with wide substrate specificity and multiple cellular functions, and among the targets of PP2A are proteins of oncogenic signaling cascades, such as Raf, MEK, and AKT. Smad2 is a signal transducer and transcriptional modulator that mediate multiple signaling pathways. With already phosphorylation certificated residues of SMAD2 proteins, relative activities of SCP1 and PP2A against them have been compared by malachite green assay. Through this comparison, we investigated the difference of substrate specificity between SCP1 to PP2A .

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Mechanism of action of Copper ion on the activity of protein tyrosine phosphatase 1B

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중앙대 화학과 [1]서강대 화학과 [2]서강대 바이오융합기술

Copper is an essential cofactor for a number of proteins and enzymes that are critical to human life. Its beneficial role, however, is counterbalanced by its potential contribution to cellular toxicity at high levels. Among the several biological targets of the cytotoxicity of copper, inhibition of protein tyrosine phosphatases(PTPs) and their related cell signaling cascades has been demonstrated. Regarding the copper ion inhibition of PTPs, previous studies indicated that the active site cysteine residue in PTPs may be inactivated by ROS. However, it has been reported that the Cu2+ inhibition of human vaccinia H1-related phosphatase(VHR) is more potent than H2O2 in the cell free system, suggesting that comprehending the oxidative mechanism for the Cu2+ inhibition of VHR does not seem to be straight forward and the high potency of Cu2+ inhibition observed for PTPs has remained unexplained. Therefore, we investigated the effect of Cu+ on the inhibition of PTP1B, suggesting that the regulation of PTP1B could be caused by oxidizing the active site cysteine and by coordinating some residues on enzyme.

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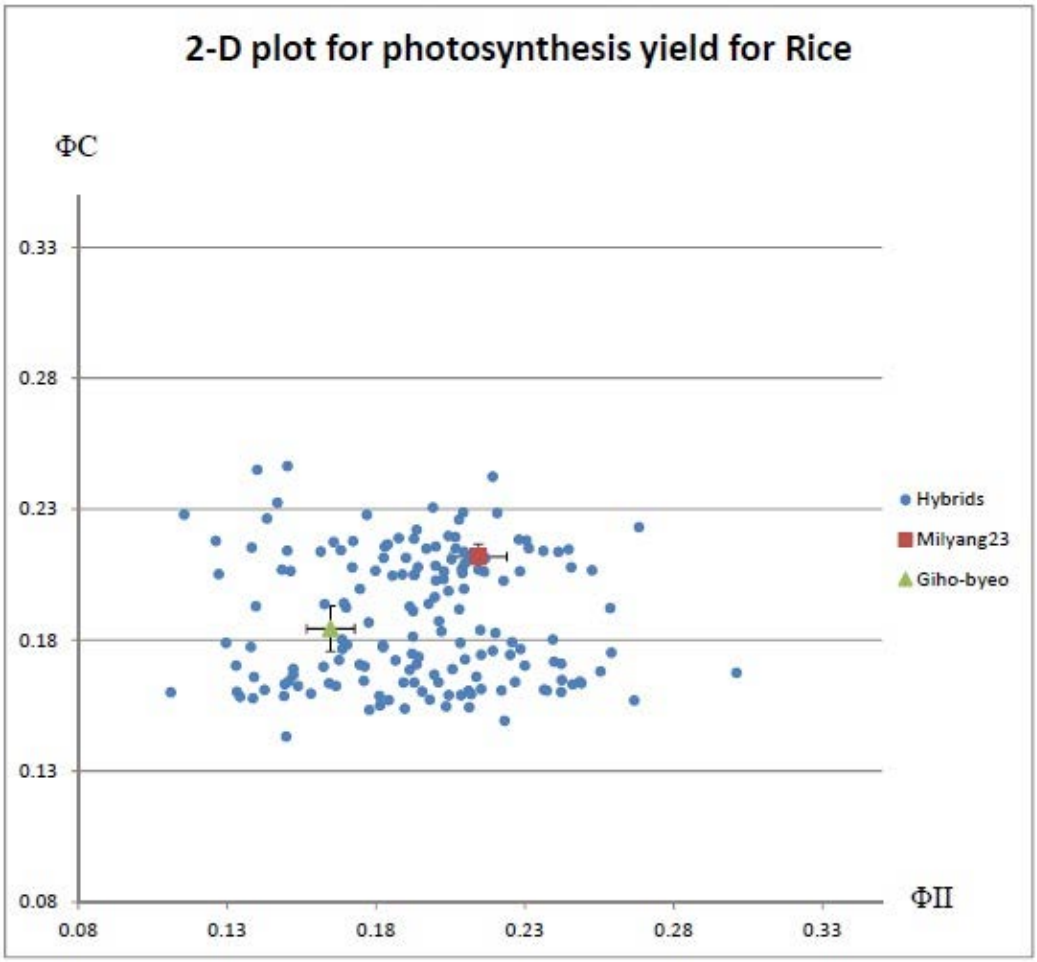
2D plot for photosynthetic yield of Korean rice varieties

NGUYEN MINH THANG

성균관대 에너지과학과

Photosynthetic organisms emerged right after the first living thing appeared on earth and have driven life by capturing energy from sunlight until now. High absorption ability of photosynthesis pigments (most importantly: chlorophyll a), can be the double?edged sword and lead to the damage of photosynthetic system by producing ROS (Reactive oxygen species), therefore, photosynthesis always keeps the balance between light capturing and utilizing. In this research, we develop a method for fast, non-destructive investigation of the balance between gain and risk in plant to reveal the best among photosynthesis plants. The method bases on the behaviors of plants which are treated with sun-mimicking light, by tracing chlorophyll a fluorescence using Pulse Amplitude Modulated (PAM) Fluorometry. Two parameters represent potential gain (ΦII ? photosystem II quantum yield, amount of light energy drive sugar formation) and risk (ΦC - photophysical decaying quantum yield, lead to ROS) of energy capture will be used for conducting the map so-called 2D plot that shows the good and the bad photosynthetic plants. The 2-D map is plotted from data obtained in Summer 2011 and 2012 at experimental field in Kunwi, Korea, for 2 rice varieties Milyang23 (Oryza sativa indica) and Giho-byeo (Oryza sativa japonica) and their 162 hybrid lines. All 164 samples have its own position in the map which showed the variation of genetic recombinant between lines, the group of good recombinants can be identified. The research also provide useful reference for create high productivity plant in term of light energy capture.



THE KOREAN CHEMICAL SOCIETY

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Streptavidin-based multivalent peptide inhibitors

권혁성 박지웅[1] 안대로[1]

고려대 생명공학과 [1]KIST 테라그노시스연구단

HIF1α is a transcription factor found in mammalian cells growing at low oxygen concentrations. Under hypoxia, HIF1α interacts with p300 and translocates to the nucleus where it transcribes the target genes, including vascular endothelial growth factor (VEGF) mRNA and genes for other cytoprotective proteins. Thus, a control agent for the HIF1α activity can be useful in therapeutic applications for diseases such as cancer and stroke. In this work, we have designed and prepared streptavidin-based multivalent peptide inhibitors to control HIF1α activity. We have also evaluated potency of the multivalent peptide inhibitors at the cellular level as well as in vitro

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Study on hierarchical structure of collagen and actin protein

박수진 신관우[1]

서강대 바이오융합과 [1]서강대 화학과 및 바이오융합과정

Protein fibers are most abundant materials which consist of inside and outside cells such as collagen and cytoskeleton. Stringy in nature, collagen connects and supports other bodily tissues, like skin, bone and tendons. Cytoskeleton (actin, neurofilament and etc.) is important part of a cell structure. It spans the cytoplasm to supply back up, shape, elasticity and protection to the contents of the cell. The aim of this study is to control the structure of protein fibers. We chose collagen and actin to build up fibril network in vitro. We changed pH, ion-concentrations and other parameters to find the optimized conditions. With these results, we can model a real cell containing protein fibers network in the future.

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Characterization of IF-inserted hybrid proteins and their effects on the fibril formation of α-synuclein

신은숙 최지은[1] 이경희

세종대 화학과 [1]세종대 화학

In order to regulate the fibril formation of specific target proteins such as α-synuclein (AS) and IAPP, we have studied the function of molecular chaperones engineered to exhibit more powerful activities. For this aim, we have inserted the IF domain from SlyD of E.coli into FKBP12 and F36V using recombinant technology in the previous study. The FKBP hybrid proteins (FKBP, FKBPIF, F36V and F36VIF) were overexpressed by IPTG induction and purified using Ni2+-affinity chromatography. To in vitro confirm the improved functions of IF-inserted hybrid proteins, we have conducted the CS aggregation assays and the PPIase (peptidyl-proyl cis-trans isomerase) assays. We have also performed the ThT fluorescence assay to monitor the fibril formation of α-AS and several related mutants in the presence or in the absence of inhibitors. We will discuss the role of IF-inserted hybrid chaperone proteins on regulating the fibril formation based on these results.

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DNA-coated micelles and their application in immunoassays

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과학기술연합대학원대 Nanomaterial&Science [1]KIST 테라그노시스연구단

Immunological techniques, and in particular, immunoassay, have proved to be one of the most important tool, which can be applied to investigate the disease biomarkers and pathogenic biological agents which often present at low levels in clinical samples. In order to improve the sensitivity and multiplex detection, a wide variety of assay designs and formats have been developed over the years. In this study, we described the DNA-coated, nano-sized micelles in which the DNA strands play a role as signal generators in an immunoassay. This micelle-based immunoassay was evaluated for quantification of a liver cancer biomarker and the sensitivity of the method was compared with those of the conventional methods.

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Amphipathic a-helical peptides with phenyl alanine promotes alternative splicing in mRNA of survival of motor neuron; possible therapeutics for spinal muscular atrophy

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서울대 화학교육과 [1]광주과학기술원(GIST) 생명과학부

Spinal muscular atrophy (SMA) is a neurodegenerative disease that is the leading genetic cause of infant mortality. SMA patients usually lacks the SMN1 (survival of motor neuron 1) gene, leading to selective motor neuron degeneration. SMN2 gene is present in all SMA patients and nearly identical to SMN1 but has one nucleotide mutation that causes exon 7 skipping, resulting in a truncated, unstable SMA protein. Thus, small molecules that can induce alternative splicing and preventing exon 7 skipping could be therapeutic drugs. Cell based screening with luciferase reporter and in-house peptide library was carried out to select peptides that could promote alternative splicing and include exon 7. Amphipathic a-helical peptides with phenyl alanine were identified as a stimulant of exon 7 splicing and increases SMN protein levels in vitro. Unlike previously identified molecules that stimulate SMN production via SMN2 promoter activation, the selected peptides directly bind to stem-loop hairpin structures near exon 7 and induce inclusion of exon 7. Synthetic peptides offer an alternative to oligonucleotide-based therapeutics that are being developed for a number of disease-associated splicing defects.

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Selective Polyamine Derivatives for using as Chemotherapeutic Agents

이유리 이명희 유재훈

서울대 화학교육과

Polyamines such as spermine and spermidine, abundant in cells, play pivotal roles for many biological events. Their concentrations, thus, should be finely controlled in cells. N^1,N^{11}-diethylnorspermine (DENSPM), a polyamine analog, is known to up-regulate polyamine catabolism by increasing expression of spermine/spermidine N^1-acetyltransferas (SSAT1). Then, a significant reduction of polyamine levels is observed in DENSPM-treated cells and tissues, resulting in more sensitized cells and tissues against many types of anti-cancer agents. Owing to this beneficial function, DENSPM is used as an additive of chemotherapeutic agents especially in drug-resistant cancers. The goal of our work is to identify polyamine analogs, which induce SSAT1 more than DENSPM in order to improve polyamines catabolism. We made a library of short peptides and combined them with spermine or spermidine derivatives. The combined peptidyl polyamines were screened against SSAT1 to select the best suiting substrate. Information from the screening was used for constructing polyamine analogs to down-regulate polyamines pools. A development of additive chemotherapeutic drugs for sensitizing drug-resistant cancers could possibly help for another type of anti-cancer drugs.

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NMR study of hydrogen exchange of various DNA recognized by DNA-binding motif for AtSPL14.

박진완 이준화

경상대 화학과

Proteins with a conserved Cys- and His-rich SQUAMOSA promoter binding protein (SBP)domain are transcription factors restricted to photosynthetic organisms that possess a novel two Zn-fingerstructure DNA-binding domain. Despite the fact that altered expression of some SBP-encoding genes hasprofound effects on organism growth and development, little is known about SBP domain protein targetgenes. Misexpression of the Arabidopsis thaliana AtSPL14 SBP domain gene confers resistance toprogrammed cell death and modifies plant architecture. A consensus DNA-binding motif for AtSPL14was identified by systematic evolution of ligands by exponential enrichment (SELEX) or random bindingsite selection (RBSS). DNA recognized by AtSPL14 contained the core binding motif (GTAC) found forother SBP domain proteins, but mutational analyses indicated that at least one additional flanking nucleotide is necessary for effective AtSPL14-DNA interaction. Comparison of several SBP domain amino acid sequences allows us to hypothesize which specific amino acids might participate in this sequence-specific DNA recognition. Here we have performed NMR hydrogen exchange experiments on the DNA recognized by AtSPL14.

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Hydrogen exchange study of winter flounder type I antifreeze protein.

최용근 이준화

경상대 화학과

Antifreeze proteins (AFPs) protect cold-blooded organisms by binding small ice crystals and inhibiting their growth. Structure of Type I AFP isoforms HPLC6 from winter flounder consists of a single α-helix that is 37 residues long, single α-helix that contains three 11 amino acid repeats (Thr-X_2-Asx-X_7), where X is generally Ala. Hydrogen exchange properties of the amide and side-chain protons were measured to probe differences in hydrogen bond strength between the winter flounder type I AFP (HPLC6 isoform) and its two mutants, A17L- and A20L-AFPs. S4 amide protons in all three AFPs are not exchange-protected by H-bonding interaction according to statistical analysis of protein and peptides. However, N16/N27 and R37-Hη protons in all three AFPs exhibit H-bond interaction. The hydrogen exchange rate constants (k_{ex}) of the amide and side-chain protons were determined by water magnetization transfer experiments and inversion recovery experiments at temperature in the range of 1~45℃. The R37-Hη proton of the wt-AFP is rapidly exchanged and shows negative peaks at short delay times, whereas the side-chain resonances (Hδ21 and Hδ22) of the N16/N27 residues, which are the most slowly exchanging protons, exhibit still positive up to 1s. In A17-AFP, where Ala residue at 17 position is changed to Leu, the peak intensities of the N16/N27 amide protons show larger dependence on the delay time after selective water inversion compared to the wt-AFP. Contrast to A17L-AFP, the A-to-L substitution at 20 position does not affect on the k_{ex} values of the N16/N27 amide protons.

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Antibody Transducer: Targeted Antibody Delivery into Live Cells

강효진 정상전[1]

한국생명공학연구원 바이오나노연구센터 [1]한국생명공학연구원 바이오나노연구단

Antibody transduction into live cells will be very effective tool for targeted live cell imaging and targeted delivery method. However, live cells did not uptake the antibodies naturally. Recently, several methods for internalization of antibodies into living cells have been developed such as electroporation, microinjection, and transfected gene mediated intracellular expression of antibodies. However, these methods have some disadvantages, electroporation and microinjection damage the cell membrane or decrease cell viability, and intracellular expression of antibodies is not stable. Therefore, other antibody delivery methods using cell-penetrating peptides (CPPs) have been developed. CPPs have been employed for the cellular delivery of proteins, DNA or nanoparticles as their complexes. There have been reported several CPPs such as penetratin, Arg8, HIV-1 TAT, MPS, etc. In this study, we have fused FcBP with CPPs to develop antibody transducer. FcBP (Fc binding peptide) consists of 13 amino acids and a novel soluble surface linker and which specifically binds to Fc domain of immunoglobulin G, and we have previously used to efficiently capture antibodies on various solid surfaces. In this work, FcBP with various CPPs were constructed and tested for transduction of fluorescence-labeled Abs. This represents the first peptide reagents, enabling targeted antibody delivery into live cells without any detergents or other physical methods.

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Predicting the complex structure between calcium bound CAPN1 and CAST4 domain from bovine

채한화

농촌진흥청 국립축산과학원/동물유전체과

The Ca+2 bound CAPN1/CAST system plays a central role in the proteolysis of key myofibrillar proteins which are related to meat tenderness but no crystal structures or molecular modeling data are available for the complex system. An important key to understanding CAPN1 inhibition by CAST is to determine at the molecular level how CAST interacts with CAPN1 to inhibit its protease activity. In this study, a 3D structure model of CAPN1 bound CAST4 complex from bovine was built by comparative modeling based on the only known template structure as CAPN2/CAST4 complex from rat. The complex model suggests certain residues of the bovine CAST4, notably TIPPKYQ sequence, and the structural elements of these residues which are important for CAPN1 inhibition. Especially, as CAST4 dock near the flexible active site of CAPN1, conformational changes at the interaction site after binding could be directly related to CAST4 inhibitory activity. These functional interfaces will serve as to guide the site-mutagenesis to research the bovine CAPN1 structure-function relationships for meat tenderness. Also this can aid the design of small molecule inhibitors to prevent uncontrolled and unspecific degradation by over-activated CAPN linked to human disease as well as Alzheimer's disease and cataract formation.

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Rapid total protein analysis of saliva assisted with microwave digestion

인용하 김동민[1] 서현정[2] 박창원[3] 김양선[4]

(주)아스타 연구소 [1]ASTA & HST R&D [2]건국대 생명공학과 [3]주식회사 아스타 R&D [4]ASTA(주) 연구소

Information from saliva accounts for the roles in altered health state as well as in therapeutic and toxicologic monitoring of pharmacokinetics. One of the promising techniques in proteomics, microwave-assisted enzymatic digestion has been come up with for protein identification. In this study, optimization of enzymatic digestion of total proteins involved in saliva was attempted in the use of microwave. Total proteins from saliva was digested into peptides by trypsin and these were profiled in the spectrum by matrix assisted laser desorption/ionization mass spectrometry. The results showed that it was able to complete reaction within few minutes. There were several factors influencing in the reaction such as protein denaturation, the power of microwave and the amount of enzyme. But the reaction time was not highly associated with the digestion yield. According to the results, microwave-assisted enzymatic digestion is thoroughly suggested in proteomic analysis of total protein.

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Protein digestion efficiency of Microwave-Assisted Enzymatic Reaction with Water Bubbling System.

김동민 서현정[1] 양준영 박창원[2] 김양선[3]

ASTA & HST R&D [1]건국대 생명공학과 [2]주식회사 아스타 R&D [3]ASTA(주) 연구소

In proteomics research, enzymatic protein digestion is very important. However, traditional enzymatic digestion system need to long reaction time normally. In recent years, microwave has applied to protein digestions and completed most of digestion reactions with in several minutes. However, the disadvantage of microwave assisted enzymatic reaction system is producing more miss-cleavage peptides compared to traditional enzymatic digestion system. In this study, a reaction chamber with water bubbling effect has been developed and tested BSA and glycoproteins were digested with several enzymes such as trypsin, chymotrypsin and PNGase F. The digestion efficiency of microwave system was evaluated by BSA tryptic and chymotryptic digestion. The obtained digests were identified by MALDI-TOF MS with the sequence coverages that were comparable to those obtained by using traditional in-solution digestion. In the BSA tryptic and chymotryptic digestion data, the sequence coverage was more than 80% , 50% and one miss-cleavage peptide of BSA has been measured in most of repeated experiments with water bubbling chamber. With the assistance of microwave, digestion time was substantially reduced to 10 minutes compared to 16 hours for traditional in-solution digestion and the high sequence coverage and higher numbers of the identified peptides indicated its excellent digestion performance.

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Practical application of oligonucleotide-linked immunosorbent assay (OLISA) to detection of Herpatitis C virus(HCV)

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KIST 테라그노시스 [1]연세대 화학과 [2]KIST 테라그노시스연구단

Previously, we have developed an immunoassay called oligonucleotide-linked immunosorbent assay (OLISA). OLISA is a very useful method for identifying multiple analytes in serum samples with improved detection sensitivity. Herein, as a practical application of this OLISA method, we attempt to detect antibodies of a hepatitis C viral antigen using OLISA for the diagnosis of Hepatitis C virus (HCV) infection.

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Inhibitory Effect of Active Compounds Isolated from *Impatiens balsamina*(Garden Balsam) for Melanogenesis

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한밭대 화학생명공학과 [1]한밭대 응용화학생명공학부 [2]한밭대 생명공학과

The ambient levels of harmful ultraviolet (UV) radiation emitted by the sun are increasing due to destruction of the ozone layer. Therefore, our skin is exposed to more UV radiation and often suffers from various harmful effects of UV. Melaninpigmentation in human skin is a major defense mechanism against UV light of the sun, but abnormal hyperpigmentation such as freckles, chloasma, lentigines and other forms of melanin hyperpigmentation could be serious aesthetic problems. Therefore, potent active agents for the improvement of hyperpigmentation are sought for their cosmetic use. Many chemicals such as hydroquinone, arbutin, kojic acid, and ascorbic acid are well known for their melanogenic inhibitory functions. In this paper, the efficacy of whitening was tstudied with a purifed naphthaquinone from Impatiens balsamina Linne, classified into Balsaminaceae. Methoxynaphtoquinone isolated from Garden Balsam as the active naphthaquinone. For the efficacy of whitening studies, melanin content assay, measurement of cell proliferation, radiometric tyrosinase assay, RNA preparation and reverse transcription-polymerase chain reaction (RT-PCR), western blotting experiments were carried out.

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The length of L2 loop is critical for caspase-7 active site conformation

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Caspase-7 serves as one of apoptotic executioners to cleave the majority of cellular substrates in apoptotic cells. The enzyme expressed as a proenzyme is activated by other caspases upon cell death signals. Crystal structures of caspase-7 revealed a large conformational difference of caspase-7 active site before and after activation, meaning that the activation accompanies a large conformational change of loops constituting the active site. In spite of extensive structural and biochemical analyses, however, a detailed molecular mechanism of the caspase activation remains to be solved. Here, we demonstrate that active sites conformation is close correlation between lengths of caspase-7 L2 loops into S2 subsite. We engineered caspase-7 mutagenesis series on L2 loops and crystallized procaspase-7 with its specific inhibitor, Ac-DEVD-CHO. The determined structure showed the first procaspase-7 bound to a specific caspase inhibitor, implying that the engineering itself gave caspase-7 a catalytic activity. Surprisingly, each heterodimeric structure showed different conformations corresponding to the precursor and matured caspase-7. Biochemical analysis with the mutants demonstrated that the length of L2 loop is pivotal for the enzyme activity.

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Induction of autophagy by spermine through p53 activation in HT1080 cells.

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동의대 화학과 [1]동의대 자연대학/화학과

Autophagy is a cellular catabolic pathway by which long-lived proteins and damaged organelles are targeted for degradation. In recent years, the accumulated evidence indicate that autophagy is associated with a number of pathological processes, including cancer, muscular disorder and neurodegeneration in addition to longevity. Polyamines such as putrescine, spermidine and spermine are low molecular weight cations present in mammalian cells. The efficacy of the spermine was investigated on autophagy through histone deacetylation and p53 activation in human fibrosarcoma cell line, HT1080. In this study, it was observed that spermine modulates the proteins associated with autophagy and apoptosis. The expression level of HDAC1 was increased in HT1080 cells. In contrast, the expression level of proteins such as acetyl-p53, p-p53 and caspase-9 inducing apoptosis was increased, On the other hands, while the level of Ac-histone H3, MDM2 and Bcl-2 expression was reduced in the presence of spermine compared to blank group, the level that of SIRT1 and p300 activation was not changed. These results suggest that the activation of p53 may play a key role in both autophagic degradation related with and regulation of lifespan.

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Buforin IIb as a peptide vector for the nonviral delivery of nucleic acids

김지수 하상수

경희대 화학과

RNA interference (RNAi) is a natural response of eukaryotic cells to double-stranded RNA (dsRNA) leading to silencing of homologous gene transcripts by ~21 nucleotide (nt) dsRNAs, termed short interfering RNAs (siRNAs). While siRNAs have been rapidly appreciated to silence genes, efficient and non-toxic vectors for primary cells and for systemic in vivo delivery remain lacking. Several siRNA-delivery vehicles, including cell-penetrating peptides (CPPs), have been developed but their utility is often restricted by entrapment following endocytosis. Hence, developing CPPs that promote endosomal escape is a prerequisite for successful siRNA implementation. We here present buforin IIb, a synthetic analog of buforin II that contains a proline hinge between the two α-helices and a model α-helical sequence at the C-terminus (3× RLLR), in order to facilitate endosomal release of siRNAs. Stable buforin IIb-conjugated siRNAs enter entire cell populations and rapidly promote endosomal escape, resulting in robust RNAi responses in MCF-7 cells, with buforin IIb-mediated delivery being independent of cell confluence. These results imply that the peptide, in addition to having utility for RNAi screens in vitro, displays great therapeutic potential.

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Methanol extracts of ginkgo fallen leaves induces apoptotic cell death in murine melanoma cell line

박혜정 오영희 이동환 김문무 류준하

동의대 화학과

The purpose of this study is to examine apoptotic effect of methanol extracts of Ginkgo fallen leaves (MEGFL) on B16F1 cells. *Ginkgo biloba* is a deciduous castle chaplain and their leaves include various kind of flavonoid like flavonol-O-glycosides. Previous studies reported that MEGFL has therapeutic properties against a number of diseases, such as cerebrovascular diseases, blood circulation disease and hypertension. During cell death process, a variety of death-associated proteins including p53, caspase-3 and -9, cytochrome C and bax are known to be produced in cytosol. In this study, MEGFL treatment at 10 μg/mL to B16F1 cells induced apoptotic cell death, which was characterized by DNA fragmentation. MEGFL significantly increased expression levels of caspase-3, cytochrome C and p53 in a dose-dependent manner. Our data indicate that MEGFL exhibit to induce apoptotic cell death by increasing the expression of cell death-associated proteins in melanoma cells.

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Ursolic acid induces apoptosis in human colon adenocarinoma cells called SW480.

남향 김문무 이동환 류준하 오영희

동의대 화학과

The objective of this study is to assess the effect of ursolic acid, a triterpene, on induction of apoptosis in human colon adenocarcinoma cells called SW480. Treatment of cells with nontoxic concentration of ursolic acid showed the presence of apoptotic bodies and induced DNA fragmentation in a dose dependent manner. The apoptotic proteins such as p53 and caspase-3 were found to be up-regulated while the anti-apoptotic protein such as bcl-2 was down-regulated in cells treated with ursolic acid. The expression level of p53 was found to be increased in cells treated with ursolic acid compared to blank group, but the expression level of p-p53, acetyl-p53, p-p21, bax, bcl-2, caspase-3 and caspase-9 were down regulated in ursolic acid treated cells compared to blank group. Above these results demonstrate that ursolic acid induce apoptosis via p53 modulation.

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Effect of ethanol extract of *Oenanthe javanica* on melanogenesis and antioxidant activity

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동의대 화학과

The aim of this study is to investigate the effect of ethanol extract of *Oenanthe javanica* (OJE) on melanogenesis in melanocyte (B16F1). *Oenanthe javanica* is well known as a plant effective for liver detoxification. To determine whether OJE effects melanin synthesis in cellular level, we cultured B16F1 melanoma cell in the presence of different concentrations of OJE. In the present study, we examined the antioxidant effects of OJE on DPPH radical scavenging activity, reducing power, lipid peroxidation and DNA oxidation. In this study it was observed that OJE exhibited the highest inhibitory effect on lipid peroxidation and hydroxyl radical among reactive oxygen species and blocked DNA oxidation induced by hydroxyl radical produced by fenton reaction. Furthermore , the inhibitory effect of OJE on production of melanin was determined by DOPA Assay and tyrosinase activity. OJE increased melanin synthesis above 10μg/ml. In addition, the OJE dose-dependently increased tyrosinase activity. These findings demonstrate that OJE with antioxidant activity can regulate the melanogenesis in melanoma cells

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Effects on Osteogenesis by Functionalized MWCNT on Titanium

김경하 안영창 조민호 윤일규 문명진 장원철[1]

단국대 화학과 [1]단국대 첨단과학대학

Carbon nanotubes (CNTs) have unique chemical durability, mechanical strength, electrical and structural properties. therefore, CNTs have received enormous attention in biomedical applications, as drug delivery systems, biosensors, and bone scaffolds material. Titanium is widely used in the field of orthopedic prosthesis or a dental-implants, due to their non-toxicity and inherent biocompatible property. We coated titanium, a common material for dental implants, with carboxylated multiwalled carbon nanotubes (MWCNTs). Furthermore, the aminated MWCNTs of negative charge surface made by hexamethlyenediamine covalent bond on carboxylated MWCNTs. The purpose of this study is to test whether functionalized MWCNT are able to support the adhesion, proliferation, and differentiation of MC3T3-E1 preosteoblast cells in vitro, and if so, how these processes are compared to those occurring under standard culture conditions (TiO_2). As a results, MC3T3-E1 preosteoblast cells cultured on the functionalized MWCNT coated titanium showed higher viability, proliferation, and differentiation compared to the oxidation titanium surface (TiO_2). Therefore, we suggest that the functionalized MWCNT coated titanium surface can be used to improve the osseointegration of titanium implants by enhancing bone formation.

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Investigation of SNP-SNP Interaction of Ku70/80 Associated with Breast Cancer

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단국대 화학과 [1]단국대 첨단과학대학

Double strand break (DSB) can result from variety factors such as UV light, ionizing radiation, genotoxic chemicals and reactive oxidative species (ROS). If not repaired or error of repair systems, double strand break can lead to genetic code change genome instability and transformation to carcinoma. Double strand break is repaired by two major repair pathway that homologous recombination (HR) and non-homologous end joining (NHEJ). In human, NHEJ is the predominant repair pathway. Ku70 and Ku80 are major repair gene in NHEJ, these two gene is formed a KU heterodimer. The major role of KU is the first protein to bind to ends of DSB region. In this study, we investigated of SNP-SNP interaction of Ku70/Ku80 associated with breast cancer susceptibility by PCR-Denaturing high performance liquid chromatography (DHPLC) assay. Our results show that SNP-SNP interaction of Ku70/80 is no effect of breast cancer risk. However, T allele of Ku80 is increase of breast cancer risk compared to G allele (OR = 1.902, 95% CI = 1.007-3.605, p value = 0.038).

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발표코드: **BIO.P-770**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-yield Expression and NMR Structural Studies of Antimicrobial Peptides, LPcin Analogs

정지호 김용애

한국외국어대 화학과

Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of proteose-peptone. LPcin is a good candidate as a peptide antibiotic because it has an antibacterial activity but no hemolytic activity. 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 in our lab. These three LPcin analogs show better antibioitic activities than LPcin and no toxicity at all.In order to understand the structural correlation between LPcin structure and antimicrobial activity under the membrane environments, we tried to express and purify as large as amounts of LPcin and three different LPcin analogs. We finally optimized and succeed to overexpress in the form of fusion protein in Escherichia coli and purified with biophysical techniques like Ni-affinity chromatography, dialysis, centrifuge, chemical cleavage, and reversed-phase semiprep HPLC. In order to identify the purified peptides, we performed Mass, CD and NMR spectrometry for their characteristic structure in membrane environments. In here, we will present the optimizing processes for high-yield expression and purification and solution NMR spectra and solid state NMR spectra for antimicrobial mechanisms.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The high-throughput screening of small CTD phosphatase 1

박지혜 신인재

연세대 화학과

Small CTD phosphatase 1 (Scp1), carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 1, is a phosphatase enzyme found in eukaryotes. Scp1, a newly discovered class of phosphatase, was reported to specifically dephosphorylate phosphorylated Ser5 (phosphor.Ser5) of the tandem heptad repeats of RNA polymerase II's carboxy-terminal domain. In recent years, the repressor element 1-silencing transcription factor/neuron-restrictive silencer factor (REST/NRSF) protein, among the best-characterized proteins in neuronal gene silencing, recruits Scp1 to the repressor element 1. Thus, inhibition of Scp1 might increase the expression of neuronal genes in non-neuronal cells. For this reason, small molecule inhibitors of Scp1 can possibly be a potent drug to treat neurodegenerative disease. In this project, we have tried to discover the inhibitors of Scp1 which allow neuronal gene expression and induces neuronal differentiation. At first, human Scp1 gene was cloned into an appropriate plamid vector, then subsequently expressed in E. coli and purified using Ni2+-NTA affinity beads. To identify the inhibitors for Scp's, we screened a number of libraries (~7000 compounds) using pNPP as the substrate. The screened compounds showed no inhibition of Scp1 activity. Other libraries are currently being assessed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Langmuir Monolayer Study of Mitochondrial Inner Membrane Lipids

Phan Dinh Minh 신관우[1]

서강대 화학과 [1]서강대 화학과 및 바이오융합과정

Mitochondrion is known as a power-house of mammalian cells, where ATP generation is carried out. The three major components composing of the mitochondrial inner membrane are phosphatidylcholine (PC, 40% in weight), phosphatidylethanolamine (PE, 40%) and cardiolipin (CL, 20%). The cardiolipin (CL) is a complex phospholipid only found in the energy-transducing membranes of bacteria and mitochondria. It is known as an essential component in maintaining structure and biological functionality of mitochondrial inner membrane. For better understanding, the mixing properties of CL and other abundant phospholipids in inner membrane of mitochondria, PC, have been investigated. In this work, we have studied ?-A isotherm to understand the compression diagram, and lead to knowledge of thermodynamic and mechanical properties of mixing monolayer as a function of CL content. And we find that at certain amount of cardiolipin, 20% molar fracture, the whole physical properties of mixing monolayer will be ruled as the same of cardiolipin. The fluorescent microscopy, then, is used to visualize the model of CL effects upon mixing monolayer's properties, as well as prove the role of CL in inducing the 3D folding structure on monolayer system, which is relevant to the interestingly folding structure of cristae in real organelle. Finally, the detail structures of monolayer, in term of electron density profiles, thickness and roughness, at gas phase as reference, pressure of 30mN/m as relevance to lipid packing in real cell, and collapsed phase are characterized at atomic scale by X-ray reflectivity.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of PET/MR/NIR trimodal imaging probe based on polyelectrolyte nanogels

박혜선 신다혜 노영욱 임용택[1]

충남대 분석과학기술대학원 [1]충남대 분석과학기술대학원 분석과학기술학과

Challenges in diagnostic imaging have led to an explosion of interest in combining modalities to more accurately interpret disease and abnormalities in vivo. By combining dual- and triple imaging modalities, many shortcomings that are present for single-modality imaging methods can be overcome. We have designed and synthesized positron emission tomography (PET)/magnetic resonance (MR)/near-infrared (NIR) trimodal imaging nanoprobe in a facile synthesis process based on the ionic gelation of biocompatible polyelectrolytes. Synthesized MnFe2O4 nanoparticles in organic solvents were encapsulated in the ionic nanocomplex in aqueous solutions by ligand exchange on the particle surface prior to gelation process.Amine functionalized ionic nanocomposite surfaces were used to modify for labeling imaging agents for PET and NIR imaging. The macrocyclic chelator, 2-(p-isothiocyanatobenzyl)-1,4,7-triazacyclononane-N,N',N"-triacetic acid ((p-SCN-Bn)-NOTA) and NIR fluorescent dyes, IRDye800? were sequentially conjugated on the particle surfaces. NOTA modified nanopartigles allowed chelation of gallium-68 for PET imaging. We quantitatively evaluated and controlled tri-functional properties of the particles. This facile method for the preparation of multimodality imaging probes based on polyelectrolyte composites and their surface modifications has a promising potential for application in many other biomedical and clinical research fields such as cell trafficking, and in vivo imaging fields.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Near-Infrared Emitting Polymer Nanogels for Efficient Sentinel Lymph Node Mapping

노영욱 박혜선 임용택[1]

충남대 분석과학기술대학원 [1]충남대 분석과학기술대학원 분석과학기술학과

Sentinel lymph node (SLN) mapping have been widely used to predict the metastatic spread of primary tumor to regional lymph nodes in clinical practice. In this research, a new near-infrared (NIR) emitting polymer nanogel (NIR-PNG) having a hydrodynamic diameter of about 30 nm, which is optimal for lymph node uptake was developed. The NIR emitting polymer nanoprobes were designed and synthesized by conjugating IRDye800 organic dye to biodegradable pullulan-cholesterol polymer nanogels. The NIR-PNG nanoprobes were found to be photostable compared with the IRDye800 free dye at room temperature. Upon intradermal injection of the NIR-PNG into the front paw of a mouse, the nanoprobes entered the lymphatic system and migrated to the axillary lymph node within 2 min. The NIR fluorescence signal intensity and retention time of NIR-PNG in the lymph node were superior to the corresponding properties of the IRDye800 free dye. A immunohistofluorescence study of the SLN resected under NIR imaging revealed that the NIR-PNG nanoprobes were predominantly co-localized with macrophages and dendritic cells. Intradermal injection of NIR-PNG nanoprobes (100 μg in 100 μl water) into the thigh of a pig, permitted real-time imaging of the lymphatic flow towards the SLN. The surgeon was quickly able to identify the position of the SLN within 1 min with the help of the NIR fluorescence images. Taken together, the experimental results demonstrating the enhanced photostability and retention time of the NIR-PNG provide a strong evidence for the potential utility of these polymer probes in cancer surgery such as SLN mapping

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Epithelial cancer cell imaging by aptamer-decorated polydiacetylene liposomes

정윤경

울산과학기술대 그린에너지연구부

A innovative tumor-targeted imaging probe that possesses the combined advantages of non-antigenic aptamer and robust fluorogenic PDA has been devised for targeting EpCAM protein overexpressed in cell membrane of epithelial cancer cell line. DNA aptamers displaying low nM Kd for EpCAM selected through our developed SELEX process were utilized as affinity agents for recognition of EpCAM, which is visualized by fluorogenic transitions of PDA.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution Structure of Microcystin-LR by NMR

원호식 권애진

한양대 응용화학과

Microcystins compose toxic and cyclic heptapeptides produced by diverse cyanobacteria. The formula for these compounds is cyclo[2,3-didehydro-N-methyl-Ala-D-Ala-L-X-erythro-3-methyl-β- D-Asp-L-Y-Adda-γ-D-Glu], where Adda is 3-amino-9-methoxy-2,6,8-trimethyl-10-phenyldeca-4E,6E-dienoic acid, and X and Y are two of several common L-amino acids. These microcystins are powerful inducers of tumours and inhibit the serine/threonine phosphatases(PP-1 and PP-2A) for growth. Microcystin-LR associates with high molecular, liver cytosolic components. In this study, we isolated microcystin-LR from cyanobacteria(blue-green algae) obtained from Dae-cheong Dam. Microcystin-LR was extracted from purification by HPLC method and identified by LC-MS/MS and DAD detector. 1H-NMR and 2D NMR(COSY, TOCSY, NOESY) experiments were accomplished in DMSO-d6 and signal assignment of microcystin-LR was made. The solution structure of this compound was investigated with use of 2D NMR and distance information. The distance information between proton pairs was obtained by NOE cross peak intensities of NOESY spectrum. On the basis of these distance data, distance geometry and molecular dynamic were carried out to determine the tertiary structure of microcystin-LR.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Phylogenetic analysis of protein kinase C isoforms

임선영 소재원

인하대 화학과

In order to study the evolutionary relationship of the PKC isoforms in various species ranging from yeast to human. Here, we searched, identified, and extracted the PKC sequences from at least 19 different species representing different phyla from yeast to human and aligned the PKC catalytic domain sequences of these proteins to create a phylogenetic tree. Our phylogenetic tree of the PKC isoforms of 19 different species clearly showed the grouping of the PKC isoforms into four branches, namely, aPKCs, cPKCs, and two distinct branches of nPKCs. The PKCdelta and PKCtheta formed the one branch and the PKCepsilon and PKCeta formed the other branch in the phylogenetic tree. Furthermore, we found that in the phylogenetic tree of the PKC catalytic domains, the archetypal yeast PKC isoforms are clustered in the aPKC branch, while in the phylogenetic tree of the PKC C1A domains, the yeast PKC isoforms are clustered in the cPKC branch. In addition, comparison of the domain architectures shows that the yeast PKC isoforms are similar to the nPKC isoforms except for the presence of two Hr1 repeats in yeast. These findings led us to predict that the three classes of the PKC isoforms have been evolved independent of each other rather than by divergence from a common ancestral pair. We next modeled the three-dimensional structures of the PKC catalytic domains from these species and aligned them to see the structural similarities between them. We were able to group the PKC isoforms into distinct clusters on the basis of the structural similarities of their catalytic domains. Furthermore, our studies on the evolutionary pattern of the PKC catalytic domain structures showed that the amino acid residues which lie in and around the active site cleft are evolutionarily well conserved.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Induction of apoptosis by 2,4,6,8-tetrakis(2-methoxyphenyl)-3,7-diazabicyclo[3.3.1] nonan-9-one derivative

이명진 황지영 XuYi 김동규[1]

인제대 화학과 [1]인제대 의생명화학과

In previous study, we examined that 2,4,6,8-tetrakis(2-methoxyphenyl)-3,7-diazabicyclo[3.3.1] nonan-9-one has anticancer effect on HeLa cells. So, novel 9 compounds were derived from 2,4,6,8-tetrakis(2-methoxyphenyl)-3,7-diazabicyclo[3.3.1] nonan-9-one and they were prepared to evaluate their cytotoxicity in HeLa cell line by using WST-8 assay. Among those compounds, compound 6 had most significant so we choose compound 6 for examining as anticancer drug. Its IC_{50} value was about 25μM. In addition, compound 6 inhibited clearly the proliferation of HeLa cell. Though its mother compound had less IC_{50}, compound 6 had radical scavenger function. We could compare their radical scavenger effect by using DPPH radical scavenger assay. Also, compound 6 led intracellular ROS to increase in time-dependent manner. Results from cell cycle arrest analysis showed that compound 6 induced G1 phase arrest of HeLa cell. We found that compound 6 induced apoptosis by Annexin V-FITC/PI double staining assay. Morphologic results showed compound 6 induced remarkable changes like cellular shrinkage and disruption. Moreover, compound 6 led intracellular $\Delta\Psi_m$(mitochondrial membrane potential) at HeLa cell to decrease. Gathering those data, we could regard compound 6 as good candidate for anticancer drug and antioxidant.

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발표분야: 생명화학

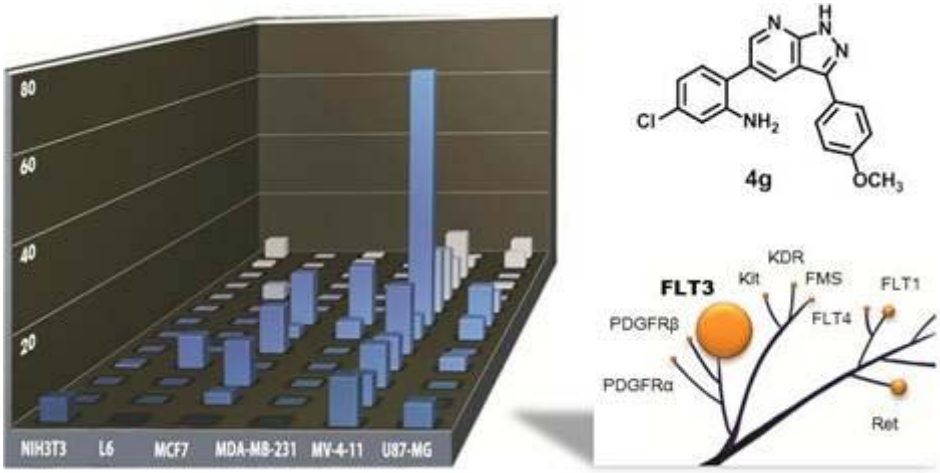
발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of highly selective FLT3 kinase inhibitor from phenotypic cell viability profiling

이상희 조아라 박승범

서울대 화학부

We discovered a novel molecular framework 4 containing heterobiaryl pyrazolopyridine moiety as a selective FLT3 kinase inhibitor from the phenotype-based viability profiling. Compound 4g showed the outstanding selectivity in cellular cytotoxicity against MV-4-11 leukemic cell via the induction of apoptosis. The hypothesis-driven deconvolution elucidated that compound 4g selectively blocked the phosphorylation of FLT3 and its downstream effector, such as ERK and STAT5, only in MV-4-11 cells. The inhibitory effect of 4g on in vitro enzyme function and FLT3 phosphorylation in cells proved FLT3 kinase as a direct molecular target of 4g. Finally, the kinase activity profiling of 4g verified its excellent selectivity toward FLT3 over 40 representative kinases including receptor tyrosine kinase (RTK) family.



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발표코드: **BIO.P-780**

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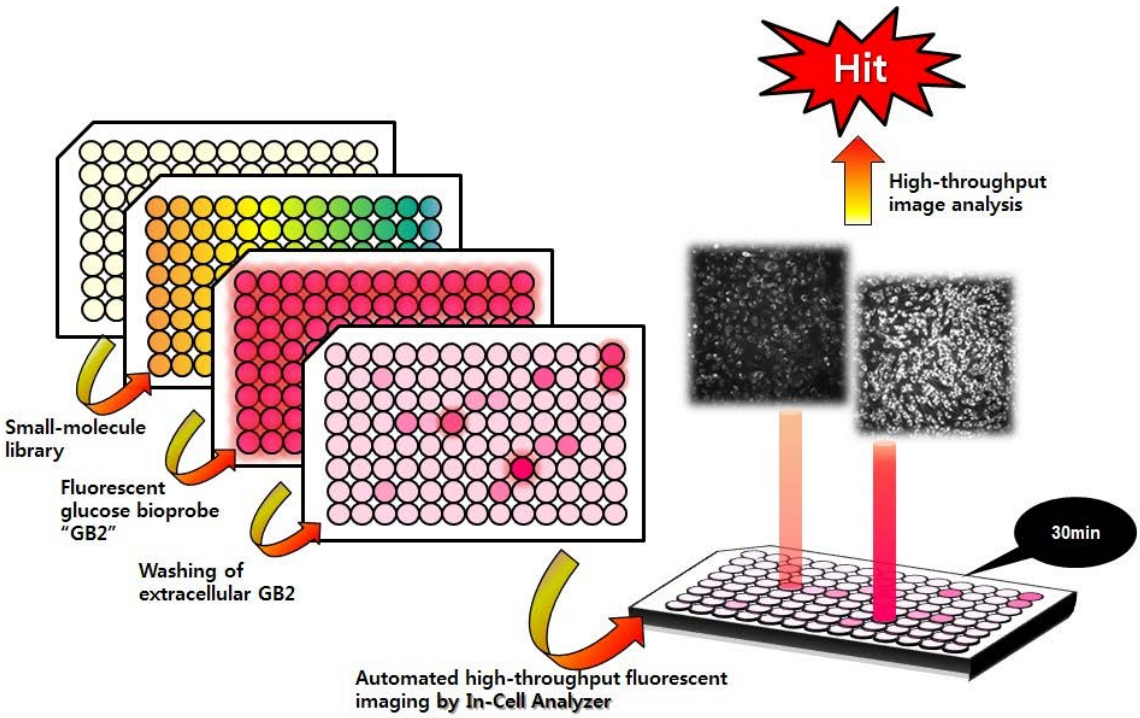
Development of Image-Based High-Throughput Screening for Monitoring Glucose Uptake in Live Cells

조아라 박종민

서울대 화학부

We previously developed novel fluorescent glucose analogue GB which is applicable to fluorescence-image based, real-time and quantitative monitoring of glucose uptake in living cells. Because of its instinsic physological chacter that it does not serve as substrate for hexokinase, however, we consistently observed substantial release of GB2 from the cells. To avoid this potential problem for its application to large-scale compounds screening, we introduced inhibitor of glucose transporter ‘phloretin’ in glucose uptake monitoring assay. From this improvement, we developed rapid and reliable high-throughput screening assay for glucose uptake in living cell. On the basis of the importance of glucose homeosis in human, image-based HTS system for monitoring glucose uptake in live cell would be a powerful tool in the discovery of therapeutic agents for related disease. Furthermore, image-based assay at cellular level allows dual tracing of other cellular aspects and glucose utilization, providing intensive screening system and potential to discover undiscovered relation between glucose utilization and novel cellular process.



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발표코드: **BIO.P-781**

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Poly(A)-targeting molecular beacons: Fluorescence resonance energy transfer-based in vitro quantitation and time-dependent imaging in live cells

김민영 하상수

경희대 화학과

Quantitation of poly(A)-RNA, time-dependent visualization of intracellular poly(A)$^+$-RNA localization in living mammalian cells, and time-resolved intracellular binding dynamics of molecular beacons at the single-molecule level using a fluorescence resonance energy transfer (FRET)-based molecular beacon are described. FRET-based molecular beacons were designed as poly(A)-targeting probes to be oligonucleotides that contained Cy5 and Cy3 fluorescent dyes at the strand ends and a poly(A)-targeting sequence inside the strand. Our ratiometric analysis using poly(A)-targeting probes allowed for highly specific and wide-ranging detection (from 1.25 nM to 0.5 μM) of poly(A)-RNA, as well as for determination of K_d values, and revealed a distribution of the probe itself and localization of the target RNA sequence in cells. Furthermore, time-dependent FRET-mediated fluorescence changes at the single-molecule level caused by the folding-induced gradual conformation changes in live cells were observed.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Studies on Temperature Effect in Photochemistry of o-Alkylphenacyl Benzoates

장미 권은주 박봉서

동국대 화학과

Our recent study revealed that photochemistry of o-alkylphenacyl benzoates showed strong dependency on irradiation temperature in the product selectivity. At low temperature, benzocyclobutenols (CB) were formed preferentially over indanones (IN) in photolysis of all the o-alkylphenacyl benzoates that we had studied. Difference of the reaction energy barrier to CB and IN was higher for mono-alkyl substituted phenacyl benzoates than for tri-alkyl substituted ones. We have carried out a quantum chemical calculation for the reaction using Gaussian-09 package and obtained an interesting clue on the origin of the product selectivity and the temperature effect. The product selectivity turned out to be entropy driven and the tri-alkyl substituted ketones go through the earlier transition state than the mono-alkyl substituted ones.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Methanolysis of a-Keto ester via 1,2-Shift of Methanol in Hemiacetal Intermediates

송송이 최여정 최지혜 박봉서

동국대 화학과

a-Keto ester is an important family of organic compounds in biochemistry[i]and synthetic organic chemistry. It has also been applied in many fields such as herbicides, fragrance delivery system, and photoinitiator of polymer synthesis. While the compounds are stable in non polar solvents, they readily form hydrates and hemiacetals of keto carbonyls in the presence of water and alcohols, respectively. In the course of our studies on photochemistry of phenacyl carboxylates, we had a chance to prepare and work with 2,4,6-trimethylphenacyl phenylglyoxylate, which we found it very unstable in methanol even at ambient temperature. The resulting products of the decomposition turned out to be a-hydroxy-2,4,6-trimethylacetophenone and methyl phenylglyoxylate, methanolysis products. The seemingly simple conversion, however, had a twist in reaction pathways according to our further investigation into the chemical change. The reaction occurred via a hemiacetal of the keto carbonyl apparently by 1,2-shift of the methoxy group. Such a reaction pathway for alcoholysis of a-keto ester has not been documented in literature to the best of our knowledge. We, therefore, prepared several a-keto esters and studied their reaction mechanism of the methanolysis. Kinetic analysis as well as substituent effects led us to identify the reaction pathway.

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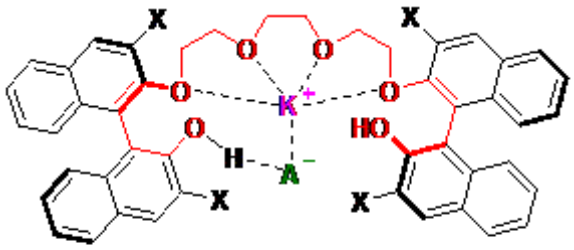
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Cooperative Organocatalysis using a High-Performance Chiral Anion Generator

오중석 박상연 권유경 안순아 송충의

성균관대 화학과

Cooperative catalysis, the simultaneous binding and activation of reacting partners resulting in both the pre-organization of the substrates and stabilization of the transition state structures, is a fundamental principle in enzymatic catalysis. For cooperative catalysis using small organic molecules, we recently developed a new structural motif for multifunctional catalysts that can be used to generate a chiral anion from an inorganic salt in “one phase”. Using this chial anion generator as an organocatalyst, excellent catalytic activity and enantioselectivity have been achieved for a range of organic reactions. The single crystal X-ray structure of the complex of the catalyst and a potassium salt (e.g. KF) provides interesting insight into the origin of the catalytic activity and stereoselectivity.



Chiral Bis-Hydroxy Polyether
Chiral Anion Generator

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Aminoarylvinyl Group-containing Anthracene Derivatives for Organic Light-Emitting Diodes

김혜정 이금희 김영관[1] 윤승수

성균관대 화학과 [1]홍익대 기초과학과

A series of fluorescent materials based on anthracene containing aminoaryl groups were synthesized via the Horner-Wadsworth-Emmons reaction for applications to efficient organic light-emitting diodes(WOLEDs). The OLEDs were fabricated with a device structure of ITO/NPB (40 nm)/Alq_3: orange-red dopant materials 1-3 (1%) (20 nm)/Alq_3 (40 nm)/LiF (2.0 nm)/Al. Among these, the device using compound 3 as a dopant material exhibited higher efficiencies than others with a luminous efficiency of 3.83 cd/A and a power efficiency of 1.43 lm/W at 20 mA/cm^2, respectively. The peak wavelength of the electroluminescence was 552 nm with $CIE_{x,y}$ coordinates of (0.542, 0.433) at 7V.

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장소: 부산BEXCO

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발표분야: 유기화학

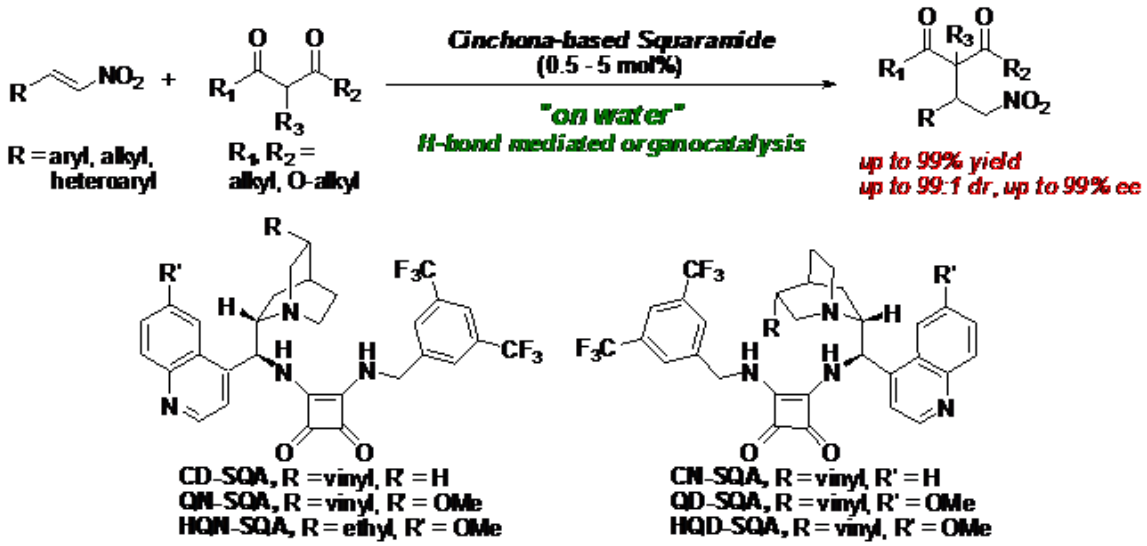
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrogen Bonding Mediated Enantioselective Organocatalysis on Water:Significant Rate Acceleration and Enhanced Stereoselectivity

배한용 송충의[1]

성균관대 자연과학부 화학과 [1]성균관대 화학과

Nature uses water as a solvent for biosynthetic reactions to sustain life. The “hydrophobic effect” is a key element in enzyme catalysis, in determining the structures of proteins and nucleic acids, and in the binding of antigens to antibodies. Due to movements toward green chemistry and an increased scientific effort to mimic nature, tremendous effort has recently been applied toward developing enantioselective organocatalytic reactions in an aqueous environment. Chiral secondary amines have been shown to be viable catalysts in an aqueous environment for several C-C and C-heteroatom bond-forming processes, which proceed via iminium or enanmine intermediates. However, introducing water as a solvent in the hydrogen-bonding-mediated asymmetric catalysis still remains a challenge, because water can interfere with the organocatalysis by its capacity for disrupting hydrogen bonds and other polar interactions. In this symposium, we will present the successful results of H-bonding-mediated enantioselective organocatalysis in an aqueous environment. Enantioselective Michael addition using a bifunctional cinchona-based squaramide organocatalyst was dramatically accelerated in brine compared to the reaction in organic solvents, due to the hydrophobic hydration effect. Remarkably, in most cases, diastereo- and/or enantioselectivity also were enhanced in brine. Catalyst loading at 0.5 mol% was sufficient to complete most reactions within 10 min, affording the Michael adduct in up to >99% yield and >99% ee.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-787**

발표분야: 유기화학

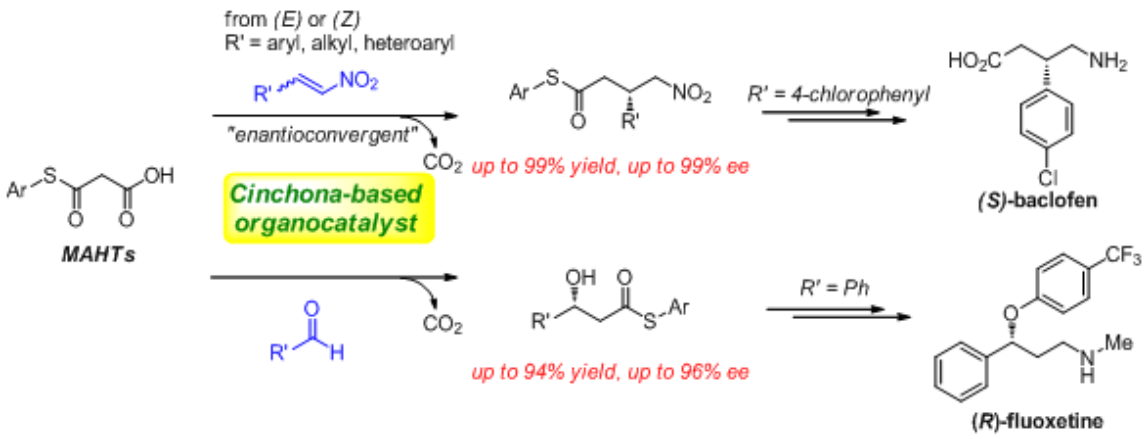
발표종류: 포스터, 발표일시: 수 16:00~19:00

Biomimetic Organocatalysis using Malonic Acid Half-Thioesters (MAHTs) as Enolate Precursors: Mimicry of Polyketide Synthases

배한용 심재훈[1] 송충의[1]

성균관대 자연과학부 화학과 [1]성균관대 화학과

Nature uses the enzymatic activation of malonic acid half thioesters (MAHTs) to generate ester enolates or their equivalents that smoothly undergo the chain elongation step by decarboxylative Claisen condensation. Inspired by these biocatalytic processes, a few groups have independently reported on a Metal-catalyzed aldol reaction and Michael addition reaction using MAHTs as direct thioester enolate donors. Meanwhile, other groups independently demonstrated that organocatalytic asymmetric transformations can also be accomplished with MAHTs via hydrogen bond catalysis using organocatalysts. Unfortunately, the catalytic activity and enantioselectivity achieved in their work were insufficient for synthetic use. In this symposium, we present that some cinchona-based organocatalysts serve as remarkably effective catalysts for biomimetic enantioselective organocatalysis using MAHTs as enolate precursors in asymmetric Michael addition reaction and asymmetric direct aldol reaction. In addition, the synthetic utilities of our protocols are demonstrated in the formal synthesis of (S)-baclofen and (R)-fluoxetin. Details of the mechanistic hypothesis and the basis for enantioselectivity will also be presented.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-788**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Red Fluorescent Donor-π-Acceptor Type Materials based on chromene moiety for Organic Light-Emitting Diodes

윤진영 이금희 김영관[1] 윤승수

성균관대 화학과 [1]홍익대 기초과학과

We have synthesized a novel red dopant for applications in organic light emitting diode (OLEDs) by introducing a triphenylamine and julolidine segment as an electron donor and chromene moiety as an electron acceptor in donor-π-acceptor type emitting core. Organic light-emitting diodes (OLEDs) with the structure ITO/NPB (50 nm)/Alq3 ; dopant (30 nm, 2 or 5 %)/BCP (10 nm)/Alq3 (40 nm)/Liq (2 nm)/Al has been fabricated to investigate their electroluminescent properties. A device using Red 1 as a dopant showed efficient red electroluminescent properties with a maximum luminous, a power efficiencies of 1.25 cd/A, 0.80 lm/W and the CIE coordinates of (0.59, 0.40) at 7V, respectively.

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장소: 부산BEXCO

발표코드: **ORGN.P-789**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Indium-mediated intermolecular heterocyclizations of 2-nitroanilines toward quinoxalines

이근수 이병민[1] 김병효

광운대 화학과 [1]한국화학연구원 신화학연구단

The first ionization potential of indium (5.8 eV) is lower than reducing metals such as zinc and close to that of alkali metals suggests that the metal ought to participate readily in single electron transfer processes. Quinoxalines are important nitrogen containing heterocycles possessing various biologically and chemically useful properties with applications in dyes, pharmaceuticals, organic semiconductors. In continuation of our efforts for searching for efficient synthetic methodology using indium, 2,3-dimethylquinoxalines were successfully synthesized from the 2-nitroanilines with 2,3-butadione using indium/indium(Ⅲ) chloride in good yields (80-96%). 2,3-Diphenylquinoxalines were synthesized also from 2-nitroanilines with benzil using indium/indium(Ⅲ) chloride or indium/acetic acid in reasonable yields (59-90%).

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장소: 부산BEXCO

발표코드: **ORGN.P-790**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Heteroleptic Ru(II) Complexes Ligated with DTDP Ligand and Anchoring Ligands for Efficient Dye-Sensitized Solar Cells

오현주 박세주 김병효

광운대 화학과

Dye-Sensitized Solar Cells (DSSCs) based on the principles of natural photosynthesis is a non-polluting clean technology to convert light into electrical energy. In the DSSCs, sensitizer is the key component to harvest the light energy. Up to present, a variety of dyes has been developed to improve the durability and the efficiency of energy conversion. Herein, new heteroleptic ruthenium(II) complexes [Ru(DTDP)L(NCS)2] was synthesized by using structurally rigid DTDP ligand (DTDP = 1,3-dihydro-1,1,3,3-tetramethyl-7,8-diazacyclopenta[1] phenanthren-2-one) and several counter anchoring ligands L (L = 4,4'-dicarboxy-2,2'-bipyridine, 4,4'-bis(E-carboxyvinyl)-2,2'-bipyridine, 4,7-dicarboxy-1,10-phenanthroline, 4,7-bis(E-carboxyvinyl)-1,10-phenanthroline). Our newly synthesized ruthenium(II) complexes show similar characteristic features of absorption with N719 over visible range of the light. Hence newly synthesized our ruthenium(II) complexes were examined as sensitizers. DSSCs based on these new dyes show reasonable efficiencies comparable with that of the N719 sensitized standard cell.

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장소: 부산BEXCO

발표코드: **ORGN.P-791**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of novel Ruthenium complexes and their application to DSSCs

김민기 김병효 김지혜[1]

광운대 화학과 [1]한미정밀화학(주) 화학과

The sun radiates more energy onto the Earth's surface than is consumed globally in one year. Solar cells are developed to utilize the power of solar energy. Among them, the dye sensitized solar cells (DSSCs) widely attract the attention by advantage of cost and manufacturing process. Ruthenium complexes have been well known as dye of DSSCs. The efficiency of solar cells is determined by metal-to-ligand charge-transfer (MLCT). In general, conjugated ligands are more absorptive sunlight than non-conjugated ligands. Thus we synthesized new heteroleptic ruthenium complexes that have 4,7-bis(E-carboxyvinyl)-1,10-phenanthroline and other N-containing heterocyclic ligands. Ru(4,7-bis(E-carboxyvinyl)-1,10-phenanthroline)2(NCS)2 shows broad and intense MLCT band absorption with high molar extinction coefficient.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-792**

발표분야: 유기화학

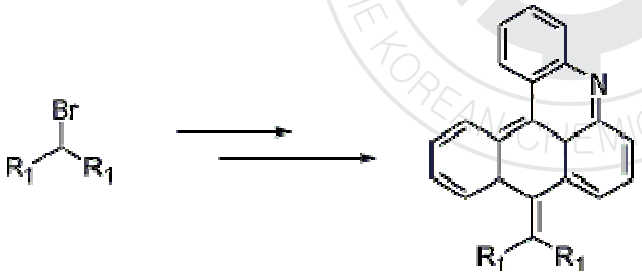
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photoluminescent Properties of New Ceramidine Derivatives

이소하 박병선[1] 태진성[1] 김인태[2]

KIST 화학키노믹스연구센터 [1]연세대 화학과 [2]광운대 화학과

A series of new ceramidine derivatives have been synthesized by 4-5 steps involving Wittig reaction of ceramidonine with various triphenylphosphonium bromides. Their UV and photoluminescence properties are also reported, and the compounds showed medium to strong photoluminescence between 502 and 522 nm at a concentration of 1x10-5 M CH2Cl2.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-793**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Various Dendrimers Containing Fluoreneas a Core Chromophores via Click Chemistry

최인화 한승철 이재욱

동아대 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 various emissive dendrimers having the core chromophore via the copper-catalyzed 1,3-dipolar cycloaddition reaction between alkyne and azide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-794**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Frechet Dendrimers Containing a Chromophore Core

곽승환 한승철 이재욱

동아대 화학과

The Glaser-type coupling is a classic reaction to prepare 1,3-diynes through homo-coupling reaction from terminal alkynes. Glaser-type coupling reactions have been applied in numerous research fields from total synthesis of polyyne natural products to the straightforward elaboration of highly conjugated new materials. Taking advantage of these facts, herein we will present the efficient strategy for the convergent synthesis of emissive Frechet-type dendrimers containing a chromophore from alkyne focal point functionalized Frechet-type dendrons via homo-coupling reaction of terminal alkyne. The dendrimers will be characterized by 1H and 13C-NMR spectroscopy, IR spectroscopy, mass spectra, GPC, UV, and PL.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-795**

발표분야: 유기화학

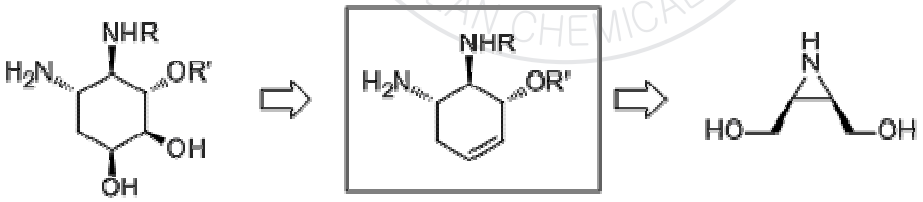
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereodivergent Syntheses of Diaminocyclitols

강한영 이가은

충북대 화학과

Aminocyclitols belong to a wide class of compounds that exhibit interesting biological properties. In particular, diaminocyclitols have been known to exhibit inhibitory properties for glucose metabolism and antibiotic activities. Synthesis of various diaminocyclitols has been reported in which two amino groups are located in the ring with diverse patterns of substitution. Our efforts for the synthesis of amino- and diaminocyclitols, based on the synthetic pathway previously developed for the synthesis of oseltamivir phosphate, will be presented. Some of advanced synthetic intermediates for the target diaminocylitols, one of which is shown below, have been prepared.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-796**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Unexpected formation of 1,3-diaminopropan-2-ol derivatives by migration of amino group through azetidinium intermediate

윤준 한민수 남기달[1] 한호규[2]

고려대 화학과 [1]KIST 생체분자기능연구센터 [2]KIST 생체과학연구부

Azetidinium ions are useful versatile intermediates for nitrogen containing heterocyclic syntheses. As a part of our continuing efforts to develop novel biologically active 1,3-diaminopropane derivatives, we designed novel compounds through structure analysis and molecular modification of currently marketed compounds. In the course of the syntheses of target compound, we found unexpectedly a formation of 1,3-diaminopropan-2-ol derivatives of which structure was determined by 1H, 13C NMR spectra and X-ray crystallographic analysis. Here, we will present a proposed reaction mechanism involving migration of amino group through azetidinium intermediate in the formation of 1,3-diaminopropan-2-ol derivatives. Several examples of the analogues will be presented also.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-797**

발표분야: 유기화학

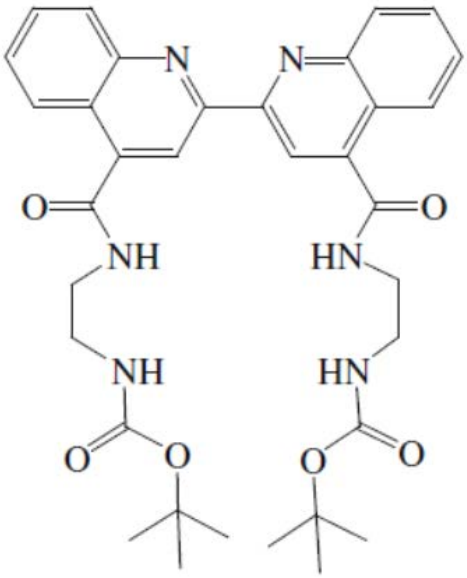
발표종류: 포스터, 발표일시: 수 16:00~19:00

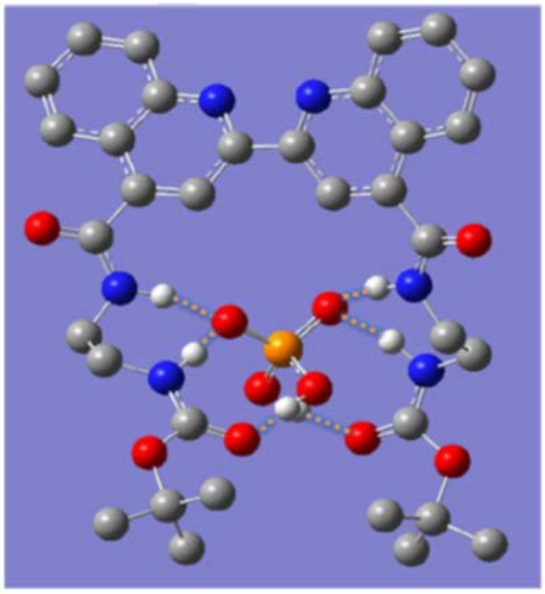
The new fluorescent receptor based on two amide hydrogens and two carbamate hydrogens anchored at 4,4'-position of biquinoline.

김영희 강종민

세종대 화학과

We have designed and synthesized a new fluorescent receptor 3 utilizing biquinoline as a molecular scaffold. The receptor 3 has two amide hydrogens and two carbamate hydrogens anchored at 4,4′-position of biquinoline. Fluorescence and 1H NMR titration showed that receptor 3 bound anions with different stoichiometry depending on the shape of anions and its association constants for anions reflected the basicities of anions. Receptor 3 bound chloride, acetate and benzoate in 1:2 stoichiometry and had a highest affinity for acetate. Tetrahedral shaped dihydrogen phosphate bound receptor 3 in 1:1 stoichiometry, although its affinity was low.





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THE KOREAN CHEMICAL SOCIETY

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장소: 부산BEXCO

발표코드: **ORGN.P-798**

발표분야: 유기화학

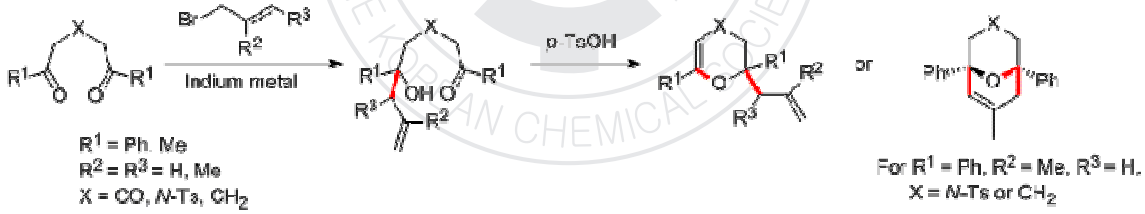
발표종류: 포스터, 발표일시: 수 16:00~19:00

Indium-mediated regioselective mono-allylation of 1,5-dicarbonyl compounds and dehydrative cyclization to 2,3-dihydro-*4*H-pyran-4-ones and 3,4-dihydro-2*H*-[1,4]oxazines

김성환 김세희 임진우 김재녕

전남대 화학과

An indium-mediated Barbier type mono-allylation of 1,5-dicarbonyl compounds and a subsequent acid-catalyzed dehydrative cyclization afforded 2,3-dihydro-4*H*-pyran-4-ones and 3,4-dihydro-2*H*-[1,4]oxazines in good to moderate yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-799**

발표분야: 유기화학

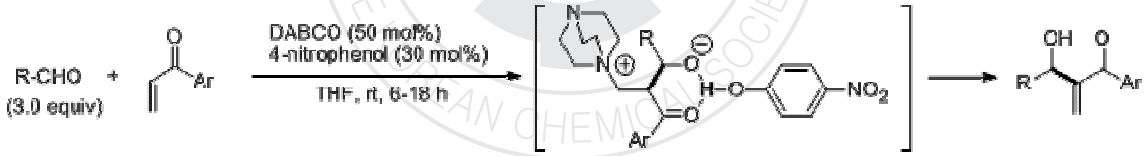
발표종류: 포스터, 발표일시: 수 16:00~19:00

A practical synthesis of Morita-Baylis-Hillman adducts of aryl vinyl ketones catalyzed by a proton donor

김성환 김세희 임철희 김재녕

전남대 화학과

An efficient and practical synthesis of Morita-Baylis-Hillman (MBH) adducts of aryl vinyl ketones was developed using DABCO and 4-nitrophenol as a proton donor. Addition of a proton donor and the use of excess amounts (3.0 equiv) of aldehydes were highly beneficial for the yields of MBH adducts of aryl vinyl ketones.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-800**

발표분야: 유기화학

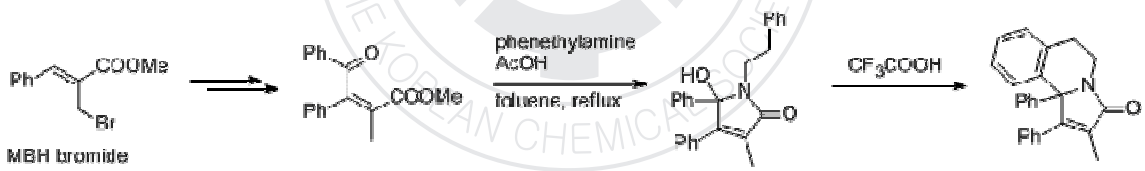
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis of 5-hydroxy-3-pyrrolin-2-ones from Morita-Baylis-Hillman adducts

임철희 김성환 임진우 김재녕

전남대 화학과

An efficient synthetic method of various 5-hydroxy-3-pyrrolin-2-one derivatives has been developed starting from the Morita-Baylis-Hillman (MBH) adducts. In addition, some synthetic applicability of the prepared 5-hydroxy-3-pyrrolin-2-ones was demonstrated including the synthesis of lactam-fused tetrahydroisoquinolines.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-801**

발표분야: 유기화학

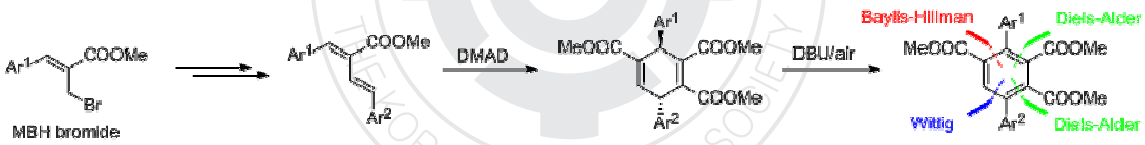
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis of poly-substituted terphenyl, quaterphenyl and quinquephenyl derivatives from Morita-Baylis-Hillman adducts

임철희 이현주 박가현 이준승 김재녕

전남대 화학과

Poly-substituted terphenyl derivatives were synthesized from the Morita-Baylis-Hillman (MBH) bromides via a sequential Wittig reaction with aryl aldehydes, Diels-Alder reaction with DMAD, and a final aerobic oxidation process.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-802**

발표분야: 유기화학

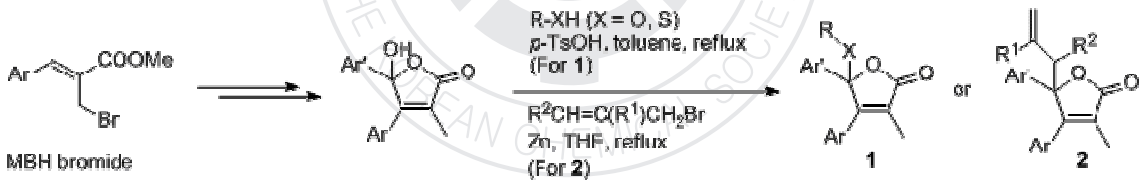
발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient synthesis of various γ-substituted butenolides from Morita-Baylis-Hillman adducts

임진우 김고훈 김세희 김재녕

전남대 화학과

An efficient synthesis of various γ-substituted butenolides was carried out from the corresponding γ-hydroxybutenolides, which were prepared from Morita-Baylis-Hillman (MBH) adducts via a consecutive bromination, indium-mediated Barbier type reaction, and K_2CO_3-mediated concomitant lactonization/aerobic oxidation.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-803**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-catalyzed tandem alkynylation, propargyl-allenyl isomerization, and 6π-electrocyclization of Morita-Baylis-Hillman adducts to naphthalenes

임진우 김고훈 김세희 김재녕

전남대 화학과

An expedient synthetic approach of naphthalenes was developed from the reaction of Morita-Baylis-Hillman (MBH) bromides and arylacetylenes. The synthesis was carried out via a tandem copper salt-catalyzed alkynylation, propargyl-allenyl isomerization, and 6π-electrocyclization protocol.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-804**

발표분야: 유기화학

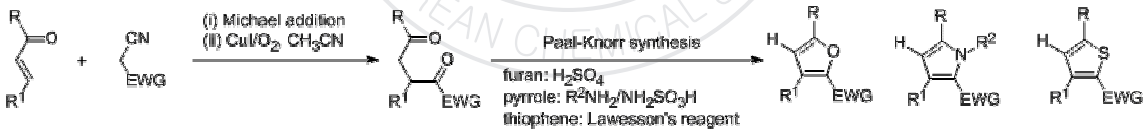
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile regio-controlled three-step synthesis of poly-substituted furans, pyrroles, and thiophenes: consecutive Michael addition of methyl cyanoacetate to α,β-enone, CuI-mediated aerobic oxidation, and acid-catalyzed Paal-Knorr synthesis

김세희 임진우 임철희 김재녕

전남대 화학과

An efficient synthesis of poly-substituted furans, pyrroles, and thiophenes was carried out in a regio-controlled manner via a three-step process; (i) conjugate addition of methyl cyanoacetate derivatives to α,β-enones, (ii) CuI-mediated aerobic oxidation, and (iii) Paal-Knorr type synthesis of five-membered heterocycles.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-805**

발표분야: 유기화학

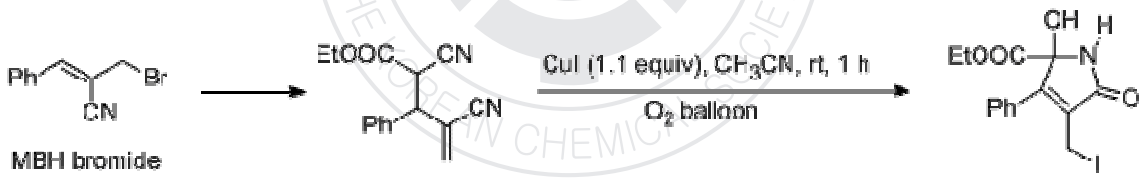
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot synthesis of 5-hydroxypyrrolin-2-one derivatives from modified Morita-Baylis-Hillman adducts via a consecutive CuI-mediated aerobic oxidation, allylic iodination, hydration of nitrile, and lactamization

김세희 김성환 이현주 김재녕

전남대 화학과

5-Hydroxypyrrolin-2-one derivatives were synthesized in moderate yields from modified Morita-Baylis-Hillman (MBH) adducts under the CuI-mediated aerobic oxidation conditions.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-806**

발표분야: 유기화학

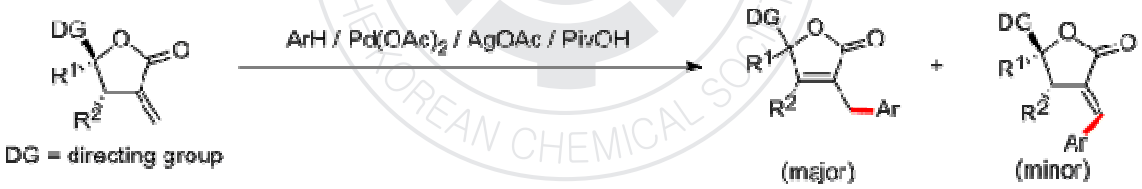
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed chelation-controlled oxidative arylation of α-methylene-γ-butyrolactones

김세희 김고훈 이현주 김재녕

전남대 화학과

Palladium-catalyzed chelation-assisted oxidative arylation of α-methylene-γ-butyrolactones with arenes selectively provided butenolides as major products along with low yield of arylidene lactones. The selective formation of butenolides is the result of a chelation between the palladium center and a directing group.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-807**

발표분야: 유기화학

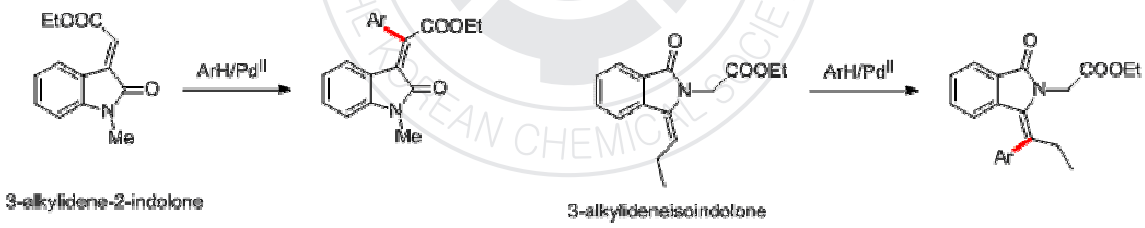
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed oxidative arylation of 3-alkylidene-2-indolone, 3-alkylideneisoindolone, and related compounds

이현주 김고훈 임진우 김재녕

전남대 화학과

A palladium-catalyzed oxidative arylation was examined with less reactive trisubstituted olefins such as 3-alkylidene-2-indolone, 3-alkylideneisoindolone, and alkylidenephthalides. Such trisubstituted olefins bearing a suitable directing group could form the corresponding tetrasubstituted olefins in moderate to good yields with highly electrophilic arylpalladium species



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-808**

발표분야: 유기화학

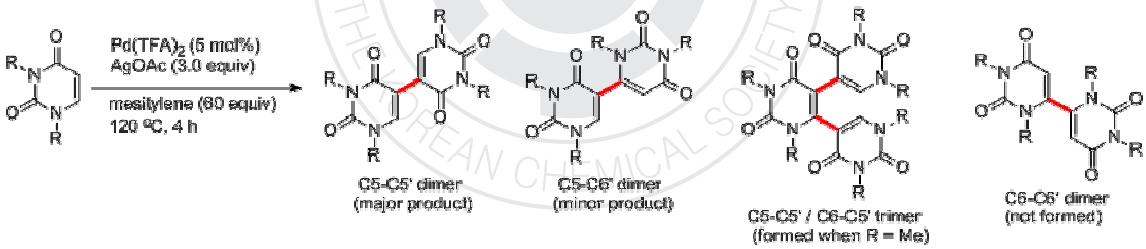
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium(II)-catalyzed oxidative homo-coupling of 1,3-dimethyluracil derivatives

김고훈 이현승 김성환 김재녕

전남대 화학과

A palladium-catalyzed oxidative homo-coupling of 1,3-dimethyluracil was examined. Two types of uracil dimer, C5-C5' linked dimer and C5-C6' linked dimer, were obtained in variable yields depending on the conditions along with a low yield of C5-C5' and C6-C5' linked uracil trimer.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-809**

발표분야: 유기화학

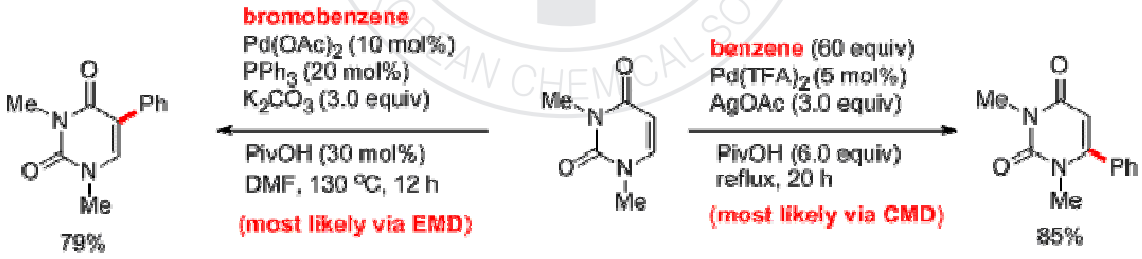
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed direct 5-arylation of 1,3-dimethyluracil with aryl bromides: an electrophilic metalation-deprotonation with electrophilic arylpalladium intermediate

김고훈 이현승 임철희 김재녕

전남대 화학과

An efficient method of palladium-catalyzed direct 5-arylation of 1,3-dimethyluracil was developed with various range of aryl bromides including electron-deficient aryl bromides. 5-Aryluracil derivatives were obtained in moderate to good yields regioselectively most likely via an electrophilic metalation-deprotonation process.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-810**

발표분야: 유기화학

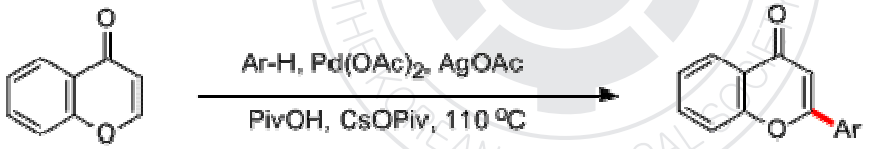
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed oxidative arylation of chromones via a double C-H activation: an expedient approach to flavones

김고훈 이현승 김세희 김재녕

전남대 화학과

A palladium-catalyzed oxidative arylation of chromones was examined. A regioselective 2-arylation of chromone was carried out via a double C-H activation process. The procedure provided an expedient approach for the preparation of flavone derivatives.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-811**

발표분야: 유기화학

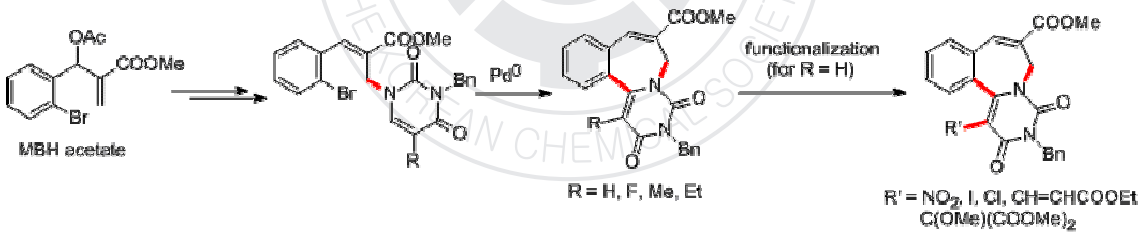
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed synthesis of benzo[*c*]pyrimido[1,6-*a*]azepine scaffold from Morita-Baylis-Hillman adducts: an intramolecular 6-arylation of uracil nucleus

이현승 김고훈 김세희 김재녕

전남대 화학과

Palladium-catalyzed intramolecular arylation at the C-6 position of uracil moiety was examined. Morita-Baylis-Hillman (MBH) adducts bearing an uracil moiety at the primary position served an efficient way to a benzo[*c*]pyrimido[1,6-*a*]azepine scaffold.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-812**

발표분야: 유기화학

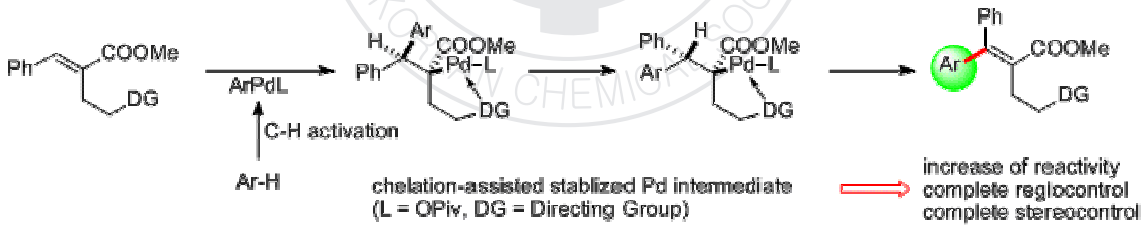
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed chelation-assisted stereo- and regioselective synthesis of fully-substituted methyl cinnamates by oxidative Heck arylation

이현승 김고훈 김성환 김재녕

전남대 화학과

Fully-substituted methyl cinnamate derivatives were synthesized via a palladium-catalyzed oxidative Heck arylation protocol in a completely stereo- and regioselective manner. The stereo- and regioselective outcome as well as the excellent yields of products were originated from the stabilization of the palladium intermediate.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-813**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nonsymetric Diarylanthracene OLED 물질의 합성과 평가

김소영 정용석[1] 권수한[1]

충북대 대학원 화학과 유기 및 생화학전공 [1]충북대 화학과

청색발광은 풀칼라를 위한 전자발광 소자로의 응용에 매우 중요하다. 청색발광물질로서의 가능성을 확인하기 위하여 antrhracene 에 메틸기가 치환된 phenyl group 및 naphthyl group 이 치환된 phenyl group 을 도입하여 비대칭형 신규화합물을 합성하였다. 또한 비대칭형 신규화합물에 trifluorometyl group 을 도입하였다. 합성한 청색발광물질재료로 발광소자를 만들어 광학적·전기적 특성평가를 하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-814**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hindered rotation in dibenzylamino-1,3,5-triazines

이은옥 김영준

충남대 화학과

The room temperature 1H NMR spectra of di-, and tri- substituted 1,3,5-triazines show two signals for the protons of benzyl position. At elevated temperatures, the two signals displayed only one signal and coalesced.As a result, the free energy of coalescence ($\Delta G_c^{\ddagger}$) for C-N bond rotation in the dibenzylamine-1,3,5-triazines was measured from not only coalescence temperature but also line shape analysis. Their activation energies were between 17kcal/mol and 19kcal/mol and will be provided useful information about the electronic effects.

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-815**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Silica supported ceric ammonium nitrate (CAN-SiO2): Efficient catalyst for the cascade synthesis of biologically active 3-aryl-3,4-dihydro-1,2,4 benzothiadiazine-1,1-dioxides

Dindulkar Someshwar 정연태

부경대 이미지시스템공학과

A silica-gel-supported ceric ammonium nitrate (CAN-SiO2) was found effective catalyst for cascade synthesis of diversified 3-aryl-3,4-dihydro-1,2,4-benzothiadiazine-1,1-dioxides using 2-aminobenzenesulfonamide and benzaldehydes at room temperature. The reaction allows rapid cyclization (10?70 min) with 5 mol % ceric ammonium nitrate impregnated on silica gel to give desired product in good to excellent yield without further column purification. The protocol uses inexpensive and environmentally friendly CAN-SiO2 as the catalyst, and no ligand or additive was required.

Scheme 1. Supported CAN catalyzed synthesis of 3-aryl-3,4-dihydro-1,2,4-benzothiadiazine-1,1-dioxides.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-816**

발표분야: 유기화학

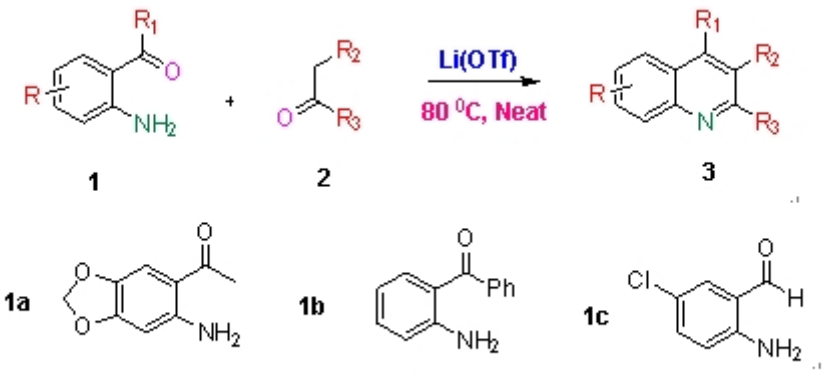
발표종류: 포스터, 발표일시: 수 16:00~19:00

Lithium Triflate Li(OTf): Highly Efficient and Reusable Catalytic System For The Synthesis Of Diversified Quinolines under Neat conditions

Atar Amol Balu 정연태

부경대 이미지시스템공학과

A series of diverse polyfunctionalized quinolines were easily prepared in excellent yields via a Friedlander reaction of o-aminoarylketone or o-aminoarylaldehyde with α- methylene ketones using lithium triflate as an expeditious catalyst under solvent free conditions. The protocol provides a practical and straight forward approach toward highly functionalized quinoline derivatives in excellent yields. The catalyst is easily recoverable and less sensitive to moisture make this protocol more advantageous



Scheme

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-817**

발표분야: 유기화학

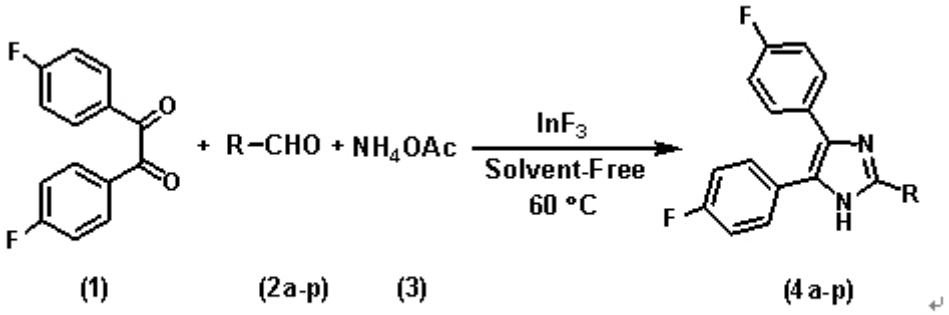
발표종류: 포스터, 발표일시: 수 16:00~19:00

Indium trifluoride: A highly efficient catalyst for the synthesis offluorine-containing 2,4,5-trisubstituted imidazoles under solvent-free conditions

Mudumala Veeranarayana Reddy 정연태

부경대 이미지시스템공학과

A new green protocol has been developed for the synthesis of fluorine containing 2,4,5-trisubstituted imidazoles via one-pot, three-component condensation reaction of 4,4-difluorobenzil with aldehydes and ammonium acetate using reusable indium (III) fluoride (InF3) as Lewis acid catalyst under solvent-free conditions. This protocol provides a novel and improved method for obtaining fluorine containing 2,4,5-trisubstituted imidazoles in terms of good yields with little catalyst loading.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-818**

발표분야: 유기화학

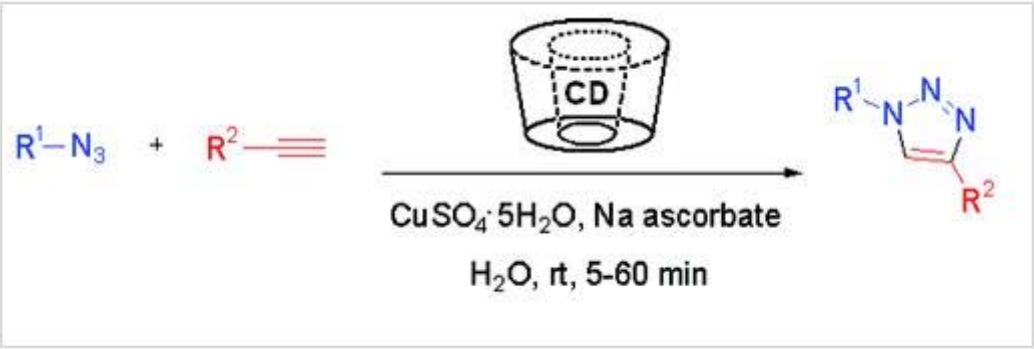
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Azide-Alkyne Cycloaddition Reaction in Water Using Cyclodextrin as a Phase Transfer Catalyst

신정아 임영권 이경희

국방과학연구소 4본부 2부

Cyclodextrins are cyclic oligosaccharides containing α-1,4-linked glycopyranose units, with a hydrophilic hydroxyl group on their outer surface and a hydrophobic cavity in the center. CDs are capable of forming inclusion complexes with many chemicals by taking it up into the cavity. These inclusion complexes have been shown to improve stability, solubility of poorly water soluble chemicals. 1,4-Disubstituted-1,2,3-triazoles were obtained in excellent yields from azides and terminal alkynes in H2O in the presence of catalytic amount of β-cyclodextrin as a phase transfer catalyst. Also, a one-pot CuAAC reaction was carried out successfully, affording 1,4-disubstituted-1,2,3-triazoles in good to high yields starting from an alkyl bromide, sodium azide, and terminal alkyne. The results of this reaction will be discussed in detail.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-819**

발표분야: 유기화학

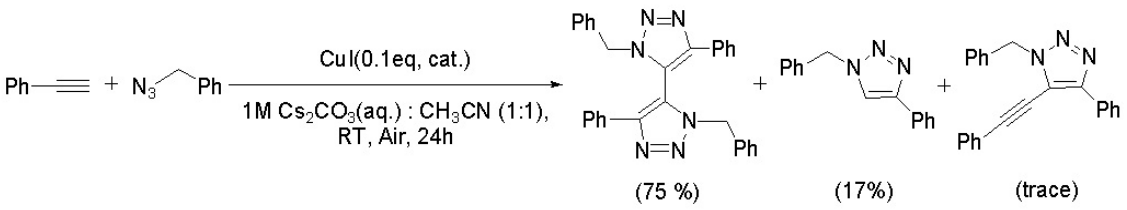
발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient bistriazole formation by copper(I)-catalyzed 1,3-dipolar cycloaddition

윤선영 김상현 전홍배

광운대 화학과

The 1,2,3-triazole formation by copper(I)-catalyzed 1,3-dipolar cycloaddition of organic azides with alkynes, a click reaction, is one of the most attractive field in organic synthesis. According to the paper published by Kevin Burgess in 2007, however, the use of carbonate base in the cycloaddition reaction afforded bistriazoles as major product for only alkynes with propargylic oxygen atom. In this study, we tried to synthesize the bistriazoles in good yields for all kinds of general alkynes with or without propargylic oxygen atom, and find the optimal reaction condition using phenylacetylene and benzyl azide for bistriazole formation. As a result, we found that the best reaction condition for the bistriazole formation is the use of phenylactylene (2 mmol) and 1M Cs_2CO_3:CH_3CN (1:1, 10 mL) per 1 mmol of benzyl azide with a catalytic amount of CuI. Furthermore, this reaction condition was applied to various organic alkynes and azides to provide the corresponding bistriazoles in good yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-820**

발표분야: 유기화학

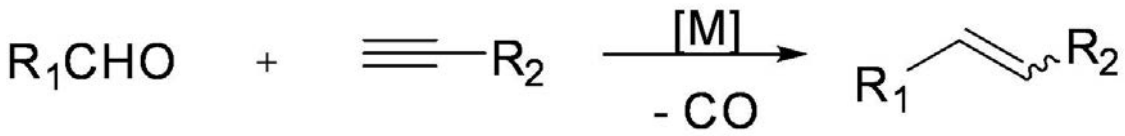
발표종류: 포스터, 발표일시: 수 16:00~19:00

The First $RuCl_3 \cdot (H_2O)_x$-Catalyzed Decarbonylative Olefination of Aromatic Aldehyde and Terminal Alkyne

김세진 송정아 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

We have developed extremely efficient decarbonylative olefination of aromatic aldehyde with terminal alkyne by using $RuCl_3 \cdot (H_2O)_x$ as a catalyst. This is the first example of ruthenium trichloride-catalyzed decaronylative 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)



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-821**

발표분야: 유기화학

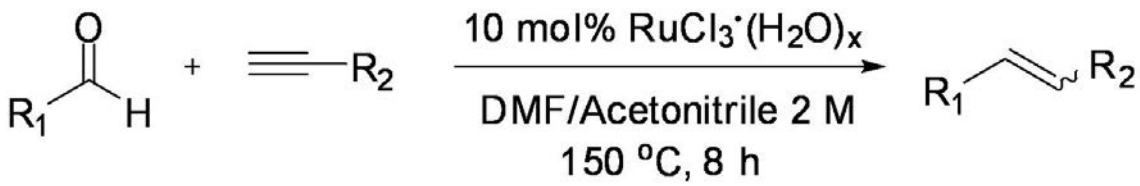
발표종류: 포스터, 발표일시: 수 16:00~19:00

General $RuCl_3 \cdot (H_2O)_x$-Catalyzed Decarbonylative Olefination of Aldehydes and Terminal Alkynes

김세진 송정아 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

We have evaluated the substrate scope of general catalytic system for the decarbonylative olefination reaction of aldehydes and terminal alkynes. The E/Z mixture of olefin products are obtained at high yields. The result of our study will be discussed at the presentation in details. This work is supported by the NRF (WCU project R33-10169)



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-822**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Metathesis-Based Strategy for the Identification of Cyclic Peptoids

김아림 **Robert H. Grubbs[1]** 권용억

이화여대 화학.나노과학과 [1]The Arnold and Mabel Beckman Laboratory of Chemical Synthesis, Division of Chemistry and Chemical Engineering, California Institute of Technology

Various chemical tools which have high binding affinity and high specificity against proteins must be developed in chemical biology and drug discovery. Peptides are attractive candidates for those purposes but they have serious limitation such as poor cell permeability, protease-sensitivity, etc. Thus, there have been increasing needs for the development of new peptidomimetics with improved pharmacokinetic characteristics. Among them, peptoids, N-alkylated glycine oligomers where side chains are directly attached to nitrogen atom rather than ?-carbon of peptide, possess many advantages over peptides. In addition, many biologically interesting natural products have been found in cyclic forms. Cyclic molecules generally exhibit an enhanced cell permeability and improved resistance to enzymatic degradation. They might also be presumed to possess high binding affinities against their target proteins. Therefore we have been interested in the development of cyclic compounds library as chemical tools. Recently, we reported the efficient synthesis of cyclic peptoids using solid-phase ring-closing metathesis (RCM). In addition to our previous efforts, we have developed a sequencing strategy of cyclic peptoids for screening studies. In this presentation, the metathesis-based strategy that cyclic peptoids can be easily sequenced by MS/MS analysis will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-823**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid-Phase Synthesis of Linear and Cyclic Glycopeptoids

장우정 권용억

이화여대 화학.나노과학과

Glycosylation, one of the most abundant post translational modifications in all living cells, plays very important roles in cell-cell recognition, protein folding, stabilization, cell growth, cell differentiation, neuronal development, immunological response, bacterial and viral infections, etc. It produces huge structural diversity in proteins which is necessary for the functionalization of nascent proteins. Abberant glycosylation can lead to numerous genetic disorders. Thus, well-defined glycoconjugates or glycopeptidomimetics can be served as biological probes and lead compounds for glycobiology and drug development. While peptides are an attractive class of molecules to synthesize glycopeptides, they possess undesirable drawbacks including sensitivity to proteases, limited cell permeability and poor bioavailability. Thus, there have been increasing needs for new peptidomimetics with improved pharmacokinetic characteristics. Among them, peptoids, N-alkylated glycine oligomers where side chains are directly attached to nitrogen atom rather than α-carbon of peptide, possess many advantages over peptides. As glycopeptide mimetics, we envisioned to develop glycopeptoids in both linear and cyclic forms. Glycopeptoids were prepared on solid-phase by using many commercially available primary amines and synthetically prepared sugar amines. Especially, diastereomeric sugar monomers were differentiated by using different amine linkers, resulting in successful sequencing of glycopeptoids by tandem mass spectrometry (MS/MS). Cyclic glycopeptoids were also synthesized on solid-phase in very high yields. In this presentation, the successful synthetic approaches to linear and cyclic glycopeptoids on solid-phase will be discussed.

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발표코드: **ORGN.P-824**

발표분야: 유기화학

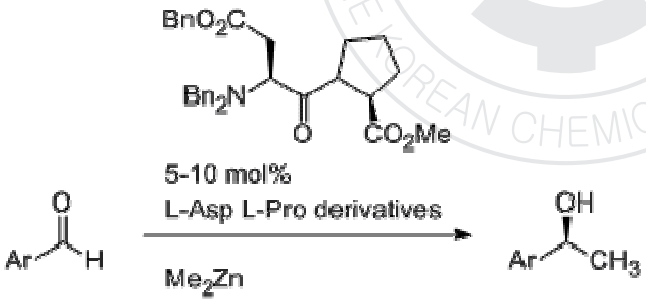
발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of Dipeptide-Derived Catalysts for the Enantioselective Addition of Dimethylzinc to Aldehydes

강석용 박용선

건국대 화학과

A new class of modular chiral catalysts derived from various amino acid-L-Pro dipeptides was prepared, and the catalysts were tested for their ability to catalyze the enantioselective addition of dimethylzinc to aromatic aldehydes. Dipeptides derived from L-Asp-L-Pro were identified as effective catalysts for the addition at room temperature with up to 97:3 er and 95% yield.



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-825**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Trend of Fluorescent Probe for Redox Active Biological Analytes

이동남 홍종인

서울대 화학부

Photo-oxidation mechanism based probe 1-Zn(II) for redox-active targets was designed and synthesized. It showed high selectivity for flavins over other biological oxidants and its sensing behavior was measured by various photo-physical methods. A positively charged Zn(II)-DPA moiety in 1-Zn(II) facilitated the recognition of biologically active flavins by modulating an electrostatic effect of a dianionic 5´-phosphate site of FMN and FAD toward isoalloxazine ring. 1-Zn(II) showed a possibility for quantitative analysis of flavins in micro-molar concentration range and in vitro human cell tests which can be utilized to monitor the flavin-linked medical studies. Detailed evidence for the photo-oxidation based sensing mechanism will be presented. We expect that redox mechanism based sensing system will be a new method for the detection of redox active biological targets.

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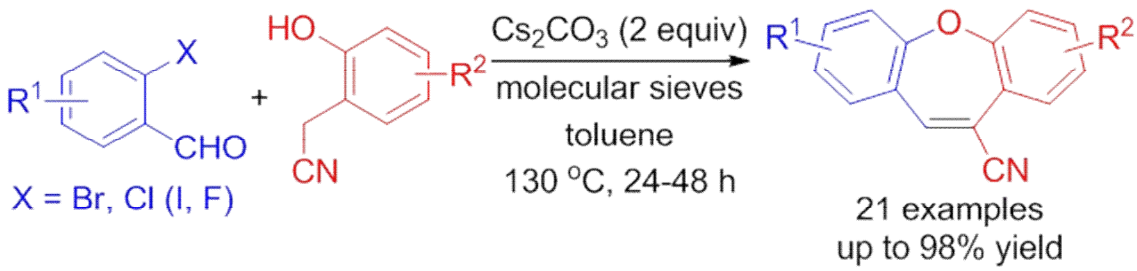
발표코드: **ORGN.P-826**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Transition-Metal-Free Synthesis of Dibenzo[*b,f*]oxepins from 2-Halobenzaldehydes and (2-Hydroxyphenyl)acetonitriles.

최영록 임혜선[1] 김범태[2] 임정연[2] 이봉향[2] 허정녕[2]

고려대 화학과 [1]충남대 신약전문대학원 [2]한국화학연구원 의약화학연구센터

Dibenzo[*b,f*]oxepin is an important motif in natural and medicinal compounds, which have been shown to exhibit antimycobacterial and anti-inflammatory activities, respectively. 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 sought to develop an efficient synthesis of dibenzo[*b,f*]oxepin via a one-pot Cu-catalyzed aryl ether formation/aldol condensation reaction. Serendipitously, we observed that the formation of dibenzo[*b,f*]oxepin occurred even in the absence of a copper catalyst. Herein a one-pot transition-metal-free, base-mediated synthesis of dibenzo[*b,f*]oxepins was developed. The reaction of 2-halobenzaldehydes with (2-hydroxyphenyl)acetonitriles proceeds via a sequential aldol condensation and intramolecular ether formation reaction in the presence of $Cs_2CO_3$and molecular sieves in toluene. To further extend the scope, the optimized protocol was employed to obtain various dibenzo[*b,f*]oxepins from a broad range of substituted 2-bromo- and 2-chloro-benzaldehydes and (2-hydroxyphenyl)acetonitriles.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-827**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and photophysical studies of novel near NIR 1,7/1,6-diaminoperylene-3,4,9,10-tetracarboxylic acid bisimides

RAMACHANDRAN 정연태

부경대 이미지시스템공학과

In this paper, we have synthesized novel near NIR 1,7/1,6-diaminoperylene-3,4,9,10-tetracarboxylic acid bisimides from the corresponding bromo derivatives. The near NIR compounds have been completely characterized by UV-Visible, fluorescence, NMR, electrochemcial and DFT calculations. This compound can be used as stable near NIR dyes

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-828**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution and solide combinatorial synthesis of terephthaloyl bis-amides for medidate

이상협 박혜정[1]

대구가톨릭대 생명화학과 [1]대구가톨릭대 화학과

Unsymmetrical terephthaloyl bis-amide are found in many biologically active compounds both synthetic and natral. In this presentation, using the aluminum amide reagents derived from a variety of amine species, including primary, secondary, aliphatic, and aromatic amines in solution-phase and optimization of solid-phase reaction conditions in various cases well be discussed.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-829**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Decoration of gold nanoparticles with receptor-fluorphore supramolecular ensemble for sensitive sensing of anionic species

이창희 김진주 Punidha Sokkalingam[1]

강원대 화학과 [1]India

Gold nanoparticle which is decorated with deep cavity calix[4]pyrrole was prepared and fully characterized. This nano-receptor exhibits elevated fluoride anion binding and sensing behavior as compared to its monomeric congener while maintaining selectivity towards fluoride anion. The covalent attachment of calix[4]pyrrole to the gold nanoparticle was accomplished by treating the dodecanethiol functionalized AuNPs with a calix[4]pyrroles bearing terminal thiol groups flanked by the flexible polyethylene glycol linker. TEM image shows that the average diameter of the particles is ~ 4 nm and remains almost in the uniform size even after hybridization with receptors. The content of receptors in the nano particle was determined by TGA analysis and estimated to be as nearly 38.3% by weight, which corresponds to 69 receptors per nanoparticle. The resulting hybrid receptor strongly binds with fluoride anion over an order of magnitude higher (at concentrations of three orders of magnitude lower) than the monomeric entity in dichloromethane. The receptor-nanoparticle conjugate showed significant aggregation upon addition of biphenolate anion due to anion-mediated anchoring of nanoparticles. Moreover the chromenolate complex of nanoparticles exhibits sensitive “turn-on” fluorescence upon addition of pico-molar concentration (~10-11) of fluoride anion. The elevated fluoride anion binding affinity was demonstrated through 1H NMR spectroscopy. The receptor-nanoparticle conjugates were able to extract fluoride anion from aqueous layer to organic medium, which was not possible by the analogous monomeric receptor.

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장소: 부산BEXCO

발표코드: **ORGN.P-830**

발표분야: 유기화학

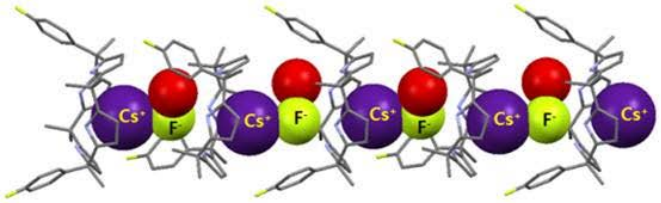
발표종류: 포스터, 발표일시: 수 16:00~19:00

Elusive Mono-Hydrated Fluoride Anion Finally Captured

이창희 김진경 punidha sokkalingam[1]

강원대 화학과 [1]IIT

A 'Picket calix[4]pyrrole' bearing well-defined binding domain allowed to capture the mono-hydrated fluoride anion that has been elusive for a long time. The structure of the receptor-bound, mono-hydrated fluoride was fully characterized by single crystal X-ray diffraction analysis as well as low temperature NMR spectroscopy. The mono-hydrated fluoride was only observed when CsF was treated with host in aqueous acetonitrile. Only fluoride anion-bound complex was seen when TBAF was treated under the identical condition. The further analysis revealed that the complex formed a three dimensional, salt mediated organic framework in solid state.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-831**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

1,3-Dipolar Cycloaddition Reactions of meso-Alkylidenyl Porphyrinoidswith Azomethine Ylides

이창희 박도우 이가원

강원대 화학과

1,3-Dipolar cycloaddition reaction of azomethine ylides has been drown attention to the chemical modification ofporphyrin skeleton. We applied this reaction to the meso-alkylidenyl porphyrinoids synthesized very recently by our group. The reaction of in- situ generated azomethine ylide (generated from the reaction of N-methyl glycine and formaldehyde) with diethyl malonylidene-(m-benzi)porphyrin or its expanded analogs afforded new adducts. The reaction took place regioselectively on the pyrrole adjacent to the meso-alkylidenyl double bond in the case of (m-benzi)porphyrin analogues. On the other hand, the same reaction of diethyl malonylidene-(mbenzi)pentaphyrin afforded different regioisomer which can be purified by oxidation. The reaction is very clean albeit slow product formation. All the products were fully characterized by spectroscopic means including MOLDI-TOF mass spectrometry. The reaction can generate wide variety of new porphyrinoids which can be potentially in various porphyrin-related applications.

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장소: 부산BEXCO

발표코드: **ORGN.P-832**

발표분야: 유기화학

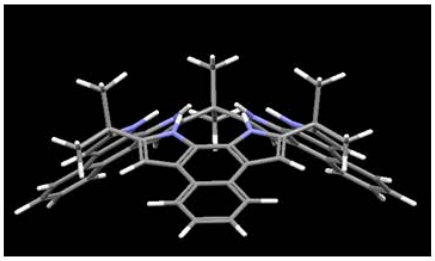
발표종류: 포스터, 발표일시: 수 16:00~19:00

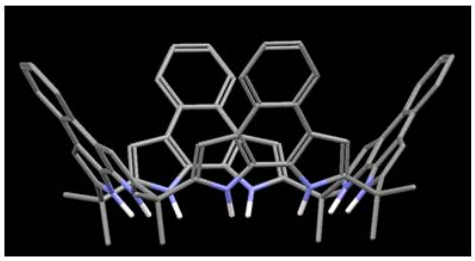
First Synthesis of Calix[n]naphthobipyrroles (n=3,4) and Their Anion Recognition Properties

이창희 김수진

강원대 화학과

Calix[n]naphthobipyrroles (n=3,4) were synthesized and characterized. The synthesis accomplished by building block approaches. The anion recogntion properties were carried out with proton NMR spectroscopy and ITC. The results indicated that the synthesized hosts can bind with multi-oxoanions other than halide anions in particular, the synthesized receptors showed higher affinity toward sulfate and phosphate anion. Spectral red shifts were also observed upon anion binding in UV-vis spectra.





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장소: 부산BEXCO

발표코드: **ORGN.P-833**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Supramolecular Dicationic Calix[4]pyrrole-Indicator Ensemble for Sensitive Detection of Pyrophosphate through IDA

이창희 sandeep kaur

강원대 화학과

IDA (Indicator Displacement Assay) is well known and getting popular method for simple conversion of synthetic receptor into optical sensor. The technique is that the reversibly binding indicator to the receptor is replaced by analytes followed by release of indicator which shows different optical signal from the receptor-indicator ensemble. Based on this principle, we here report a Dicationic calix[4]pyrrole?indicator ensemble that shows excellent selectivity toward pyrophosphate anion in aqueous organic solvent. The ensemble displays selective displacement of diazophenol indicator upon exposure of pyrophosphate anion. The distinctive color changes from yellow to red was observed only when the supramolecular ensemble was titrated with pyrophosphate anion. We expect that the present work could provide structural foundation for selective sensing of various anions through an naked-eye detection of pyrophosphate anion.

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ORGN.P-834**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

SNSN-Type Thia-Bacteriochlorins : Synthesis and Absorption Properties

황지나 김범식 장태선[1] 김한제[2]

한국화학연구원 환경자원연구센터 [1]한국화학연구원 신화학연구단 [2]공주교육대 과학교육과

Bacteriochlorophylls, the light-absorbing pigments employed by photosynthetic bacteria, contain bacteriochlorin chromophore. The bacteriochlorins are attractive for various photochemical applications (sensors, detector, solar cell, PDT, artificial photosynthesis) due to their strong absorption in the near-infrared (~700 nm) spectral region. Since a concise route to stable bacteriochlorins was developed, various bacteriochlorin derivatives have been prepared and reported. However there was no synthetic effort reported for the core-modified bacteriochlorins despite the potential importance of the compounds. We synthesized the first SNSN-type bacteriochlorins. The compounds were characterized by 1H NMR spectra and Mass data. Also the absorption spectra were obtained and compared to those of NNNN-type bacteriochlorins.

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발표코드: **ORGN.P-835**

발표분야: 유기화학

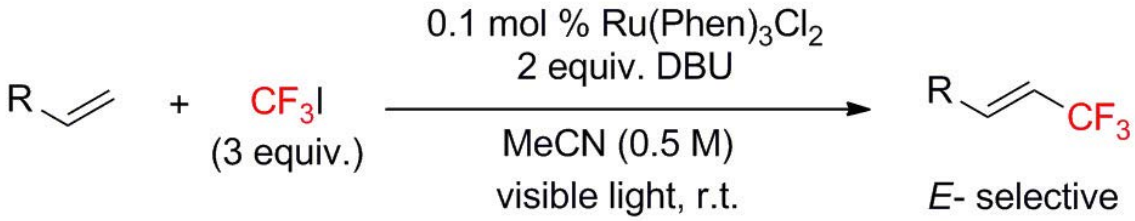
발표종류: 포스터, 발표일시: 수 16:00~19:00

Trifluoromethylation of alkenes by visible light photoredox catalysis

Naeem Iqbal 최성규 조은진

한양대 응용화학과

A method for trifluoromethylation of alkenes has been developed employing visible light photoredox catalysis with CF3I, Ru(Phen)3Cl2, and DBU. This process especially works well for terminal alkenes to give alkenyl?CF3 products with only E-sterochemistry. The mild reaction conditions enable the trifluoromethylation of a range of alkenes that bear various functional groups.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-836**

발표분야: 유기화학

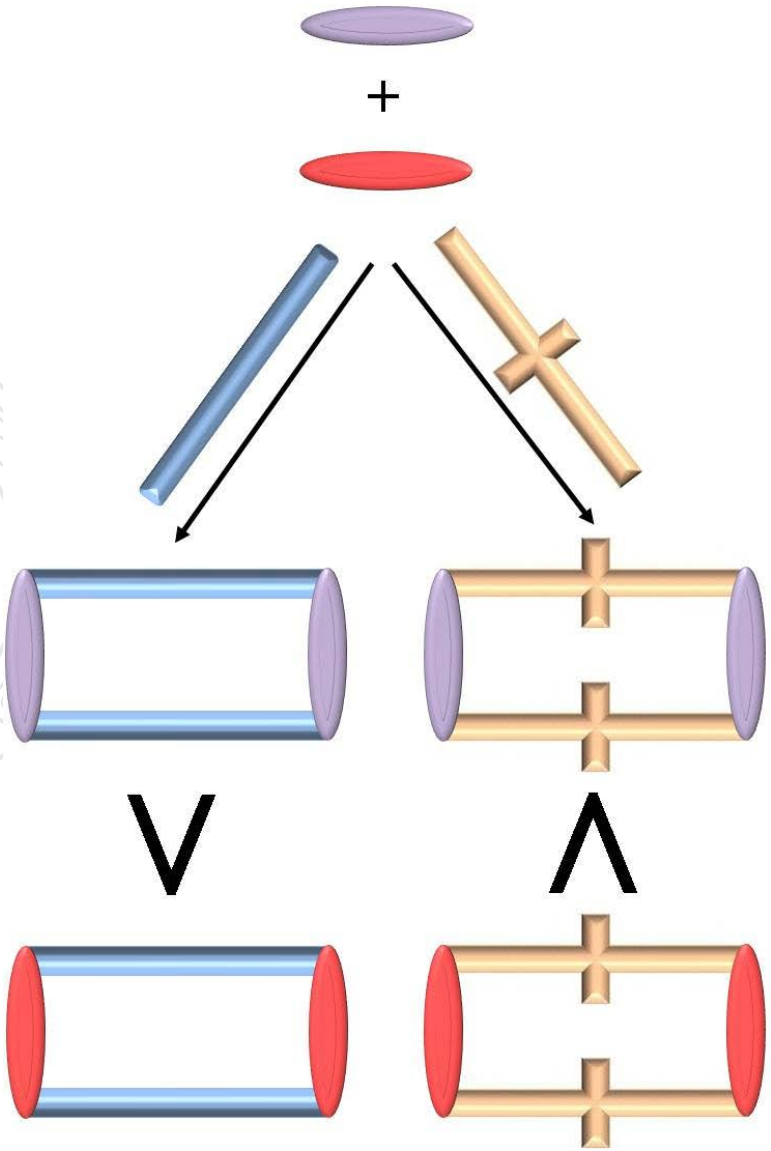
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Selection in the Coordination-Driven Self-Assembly between Octahedral Ru-Acceptors and Dipyridyl Ligands

송영호 민진욱 이승창 지기환

울산대 화학과

Over the past two decades a tremendous number and variety of new cyclic, 2D and 3D architectures have been self-assembled via metal-ion coordination chemistry. Self-assembly is a preeminent process for the formation of ordered structures emerging spontaneously from the precursors in which the overall structure of the final assemblies is controlled by building block.Interest in this field is aesthetic since remarkable high symmetry, high-mass, polymetallic compounds have been obtained via extraordinarily efficient directed-assembly and their versatile applications in chemical sensing, catalysis and molecular hosting.Recently we have reported a variety of [2+2]metalla-rectangles viacoordination-driven self-assembly between octahedralRu(II)-basedacceptors andvarious organic linkers.On continuing the research herein we are reporting for the first time the self-selection in coordination-driven self-assembly betweenoctahedralRu(II)-basedacceptors and dipyridyl ligands.All the complexes were characterized and compared by ^{1}H NMR.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-837**

발표분야: 유기화학

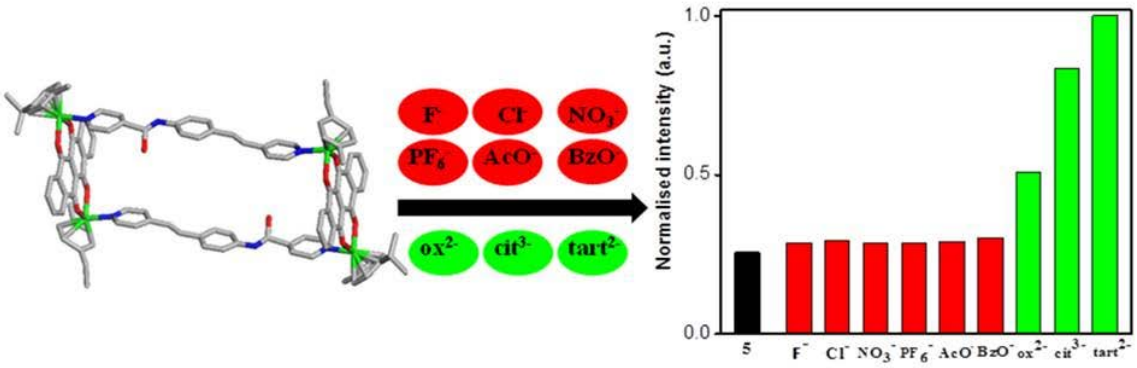
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-Assembled Amide Containing Molecular Metallacycles for Anion Sensing Study

ANURAG MISHRA 이선미 지기환

울산대 화학과

Amide-containing groups are good H-bonding donors, and are used widely to design and synthesize artificial anion receptors. Considerable efforts have been devoted to synthesize new amide ligand as receptor for the selective sensing of anions because of the important roles that they play in various chemical, biological and environmental sciences. Fluorescent sensing of anions has become particularly attractive because of its simplicity and low detection limit. Sensing of multi-carboxylate anions is useful in chemistry as well as in biochemistry. Among multi-carboxylates, oxalate, citrate, and tartrate are widely used for the detection of several diseases, as they occur as intermediates in cellular metabolism. The present work demonstrates the coordination behavior of amide ligands with different Ru-arene acceptors during and after the formation of self-assembled supramolecular metallacycles. These complexes have been characterized by various spectroscopic and X-ray single-crystal structure determination. These self-assembled metallacycles were further explored for anion sensing studies and found turn-on fluorescence response for the multi-carboxylate anions with high selectivity and binding affinity. The poster will address a detail comprehensive account of the mentioned work.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-838**

발표분야: 유기화학

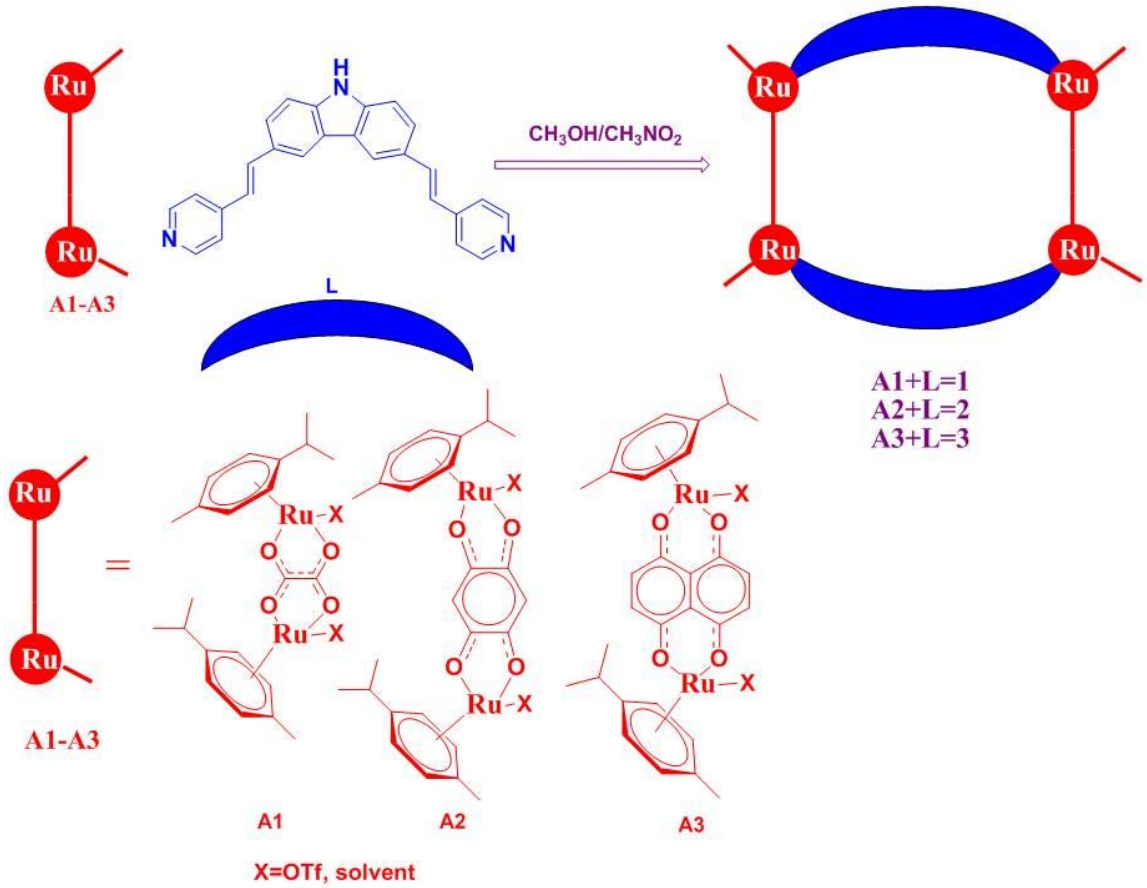
발표종류: 포스터, 발표일시: 수 16:00~19:00

Constructions of 2D-Metallamacrocycles Using Half-Sandwich Ru^{II}_2Precursors: Synthesis and Molecular Structures

DUBEY ABHISHEK 지기환

울산대 화학과

Coordination-driven self-assembly of supramolecular architectures of defined shapes, sizes, and functionality has witnessed rapid growth in the past few years because of their structural diversity as well as their potential applications in host-guest chemistry, catalysis, molecular recognition, biological application. Three new arene-ruthenium [2+2] metalla-rectangles (1-3) were synthesized by the self-assembly approach using arene-ruthenium acceptors (A1-A3) and dipyridyl ligand L, respectively and characterized by NMR and ESI-MS. This new class of metalla-rectangles with extended aromatic π-surfaces holds promise for host-guest properties and can potentially be used to develop new functional materials and sensors.



Scheme 1. Self-assembled arene-ruthenium metalla-rectangles 1-3

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-839**

발표분야: 유기화학

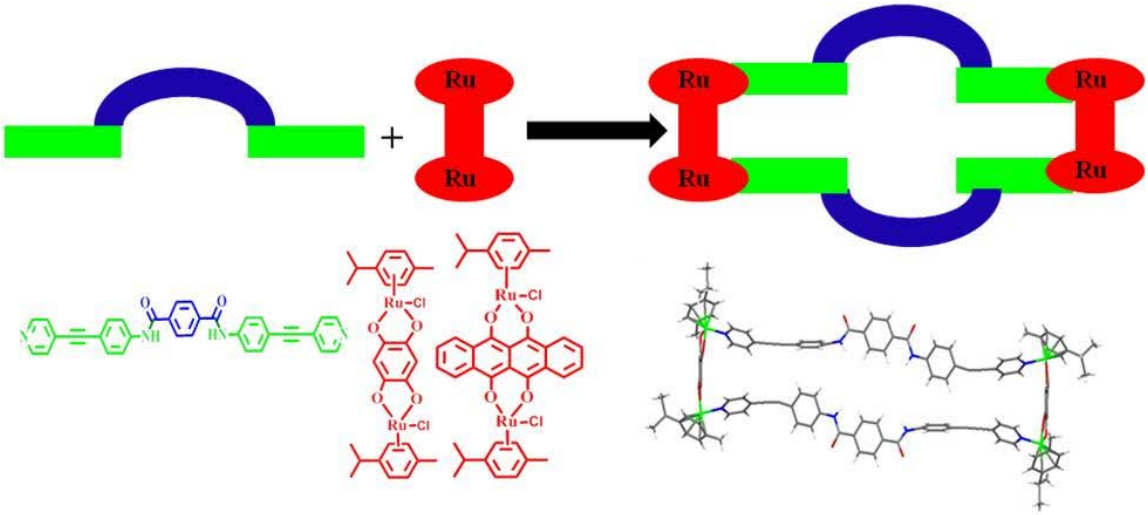
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Self-Assembled Molecular Metallacycles for Fullerene Binding Study

ANURAG MISHRA 정현지 지기환

울산대 화학과

The formations of new metallamacrocyclic entities driven and held together by metal coordination have drawn comprehensive interests in modern supramolecular chemistry. For last two decades, a great number of metallamacrocycles have been synthesized by self-assembly approaches through directional metal-ligand interactions. We present here new large molecular metallacycles by combination of a symmetrically large ethnyl backbone containing N donor and arene-Ru acceptors. These complexes have been characterized by various spectroscopic and X-ray single-crystal structure determination. These self-assembled metallacycles were further explored for fullerene binding study with an amide ligand as a π-electron rich donor and an arene-Ru acceptor as a signaling unit and found that new metallacycles have ability to bind C_{60} and C_{70}, as established by UV-Visible and fluorescence titration.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-840**

발표분야: 유기화학

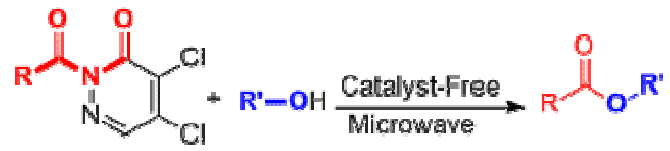
발표종류: 포스터, 발표일시: 수 16:00~19:00

Conversion of *N*-acylpyridazinones into esters under Microwave irradiation

김보람 성기현 윤용진

경상대 화학과

2-Acylpyridazinones are useful acyl sources in synthesis, and also have two carbonyls as 1,3-diketone system. The reactivity of two carbonyls is different due to the delocalization of the lone pair electron of nitrogen in the ring of azinone. According to recent our report, *N*-acylpyridazin-3(2*H*)-one readily forms stable anion, it can also act as a good leaving group. So it can easy removed and/or recycled in organic reactions.Meanwhile, the esterification of carboxylic acid derivatives requires the catalyst and/or additives. Inspired by our report, the esterfication of *N*-acylpyridazinones with alcohol can carry out under the catalyst-free conditions to give the corresponidng esters and recyclable pyridazinones. In this poster, we describe the catalyst-free conversion of 2-acylpyridazinones as *N*-acylpyridazinones into esters under microwave irradiation.



2-Acyl-4,5-dichloro-pyridazin-3(2*H*)-one

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-841**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of tris(4-(9-phenyl-9H-carbazole)phenylamine

백승지 박민규 김보미 이덕희 채규윤[1]

원광대 생명나노화학과 [1]원광대 화학과

tris(4-(9-phenyl-9H-carbazole)phenylamines were synthesised from triarylamine using bromination, alkylation, borination, and suzuki coupling reaction. Products were evaluated for physical properties as an electron transport materials for OLED devices.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-842**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Stereoselective Fridel-Crafts Type Cyclization of Trans- and Cis Vinyl oxiranes via Lewis Acid Catalysis

유찬모 <u>곽진호</u> 양보나

성균관대 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of Lewis acid catalysts are some of the most attractive methodologies. A highly diastereoselective synthesis of trans adduct is achieved from the reaction of trans vinyl oxiranes with 10 mol% of trifluoroborane etherate complex as a Lewis acid catalyst, whereas cis product is formed by tris(pentafluorophenyl)borane as a Lewis acid additive. The method described herein is successful with various substrates in good yields and high levels of diastereoselectivity.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-843**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dehydrogenative amide bond synthesis with amine surrogates

이정빈 홍순혁

서울대 화학부

Amide functional group has attracted considerable attention owing to its great occurrence in modern pharmaceuticals and biologically active compounds. They are the key connection of proteins and also favorable group in all branches of organic chemistry. Despite their popularity, amides have been prepared from carboxylic acid by the use of large amount of coupling reagent or by the prior conversion to its acid derivative, which suffers from poor atom economy. Over the past few years, chemists have extensively addressed the new methodology to amide linkage, aiming at more efficient and environmentally benign pathway, which is based on the use of transition metal catalyst. Dehydrogenative amidation from the reaction between alcohol, instead of carboxylic acid derivative, and amine is the intriguing example. Just as using alternatives to carboxylic acid, chemists also have found the amine surrogates as another N source of amide. Examples include the use of isonitrile, isocyanate, sulphonamide and so on. From the extension of these methods, we have investigated the reaction of different N source for the amide bond formation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-844**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Abnormal N-Heterocyclic Carbene Gold(I) Complexes: Synthesis, Structure, and Catalysis

김승효 홍순혁

서울대 화학과

Two abnormal N-heterocyclic carbene (aNHC) gold(I) complexes [(aNHC)AuCl], were prepared from C2-protected imidazolium salts. The air stable complexes, [1-isopropyl-3-methyl-2,4-diphenylimidazolin] gold chloride (I) and [1,4-diisopropyl-3-methyl-2-phenylimidazolin] gold chloride (I), were synthesized via transmetallation using (SMe2)AuCl and fully characterized spectroscopically and structurally by X-ray crystallography. To investigate the catalytic activity of the aNHC-based Au complexes, sterically similar traditional NHC-based Au complexes [1,3-diisopropylimidazolin] gold chloride and [3-isopropyl-1-phenylimidazolin] gold chloride were prepared from 1,3-diisopropylimidazolium iodide and 3-isopropyl-1-phenylimidazolium iodide. Catalytic activities of the NHC-based Au complexes were screened in the alkyne hydration. On the contrary to our expectation, traditional NHC-Au catalyzed system is more effective in the reaction.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-845**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Completely Atom Economical Amide Bond Synthesis Based on Ruthenium Catalyst

강병준 홍순혁

서울대 화학과

The importance of amide bond in organic synthesis, pharmaceutical science, and polymer science can not be emphasized more. Historically, coupling reagent is the general choice for the amide bond formation. It is one of the most widely used organic transformations of all time, but it bears critical problem - a poor atom economy. Since Milstein's first report in 2007, metal catalyzed coupling of alcohol and amine has been highlighted as a proper alternative with high atom economy. In this case, the only waste is one equivalent of hydrogen gas.With the continuous research on this field, our group realized that the 100% atom economical amide synthesis can be achieved with ruthenium catalysts.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-846**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Correlation of Solvolysis Rates of 3,4,5-Trimethoxybenzoyl Chloride and 2,4,6-Trichlorobenzoyl Chloride

박경호 유찬주[1] 경진범 Dennis N. Kevill[2]

한양대 과학기술대학 응용화학과 [1]한양대 [2]Northen Illinois University

The introduction of methoxy groups into 3- and 5-positions of 4-methoxybenzoyl chloride leads to a reduction in specific rates of solvolysis. An extended Grunwald-Winstein equation for the specific rates of solvolysis of 3,4,5-trimethoxybenzoyl chloride gives sensitivities towards changes in solvent nucleophilicity (l value) of 0.29 and towards changes in solvent ionizing power (m value) of 0.54. The low m value allows specific rates to be determined in highly ionizing fluoroalcohol-water mixtures. A parallel correlation of the specific rates of solvolysis of 2,4,6-trichlorobenzoyl chloride reveals that solvolyses in 100% and 90% ethanol or methanol do not appreciably follow the ionization pathway indicated for solvolyses in the other solvents and it is proposed that, despite the two ortho-substituents, the addition-elimination pathway has become dominant.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-847**

발표분야: 유기화학

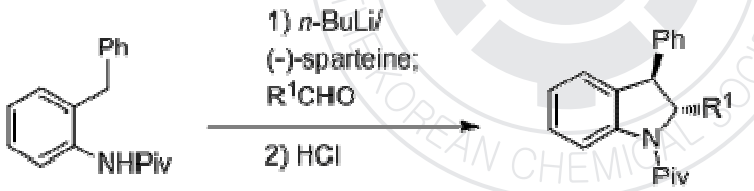
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of trans-2,3-Disubstituted Indoline Derivatives

강경희 박용선

건국대 화학과

A novel method for asymmetric synthesis of trans-2,3-disubstituted indolines has been developed. The strategy involves the (-)-sparteine-mediated electrophilic substitution of 2-benzyl N-pivaloylaniline with aromatic or α,β-unsaturated aldehydes and subsequent acid-catalyzed cyclization. The simple protocol for two-step process can produce highly enantioenriched indolines to 98:2 er



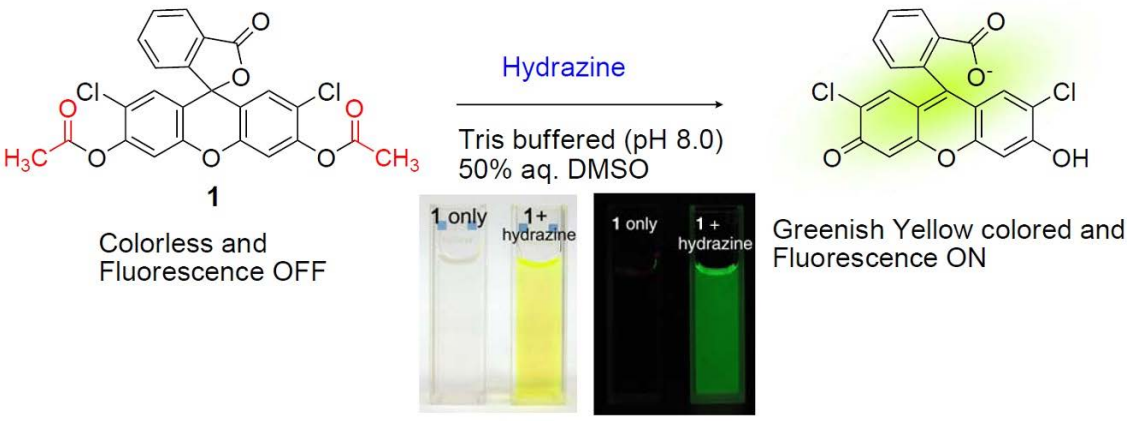
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-848**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric and fluorescent signaling of hydrazine by selective deprotection of dichlorofluorescein acetates

최명길 문정옥 배지희 장석규

중앙대 화학과

The highly selective chemosignaling behavior of dichlorofluorescein acetate toward hydrazine was investigated. Prominent chromogenic and fluorescent turn-on type signalings were realized by hydrazinolysis of the latent dichlorofluorescein acetates. Selective hydrazine signaling was possible by the probe in the presence of commonly encountered metal ions and anions. The detection limit for the determination of hydrazine in 50% aqueous DMSO was 2.9 ppb. The designed probe could be useful for the determination of hydrazine in environmental samples.



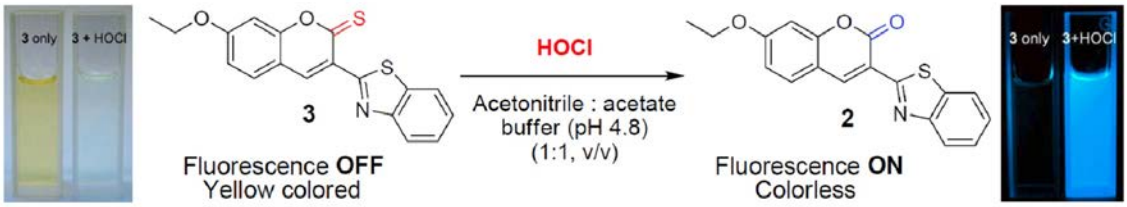
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-849**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual signaling of hypochlorous acid by desulfurization of thiocoumarin

문정옥 이정우 최명길 장석규

중앙대 화학과

The HOCl-selective signaling behavior of thiocoumarin was investigated. The thio derivative of ethoxycoumarin showed selective and efficient colorimetric and fluorogenic signaling behaviors over other commonly used oxidants in an aqueous environment. The signaling is due to the oxidative desulfurization of the thiocarbonyl moiety by HOCl to yield oxocarbonyl function. The interference from Hg^{2+} ions was successfully removed by using bromide ions as a masking agent. HOCl signaling with a detection limit of 8.3 x 10^{-7} M in the presence of common metal ions and anions as background was possible. The designed probe could be useful for the determination of hypochlorous acid in chemical and environmental samples.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-850**

발표분야: 유기화학

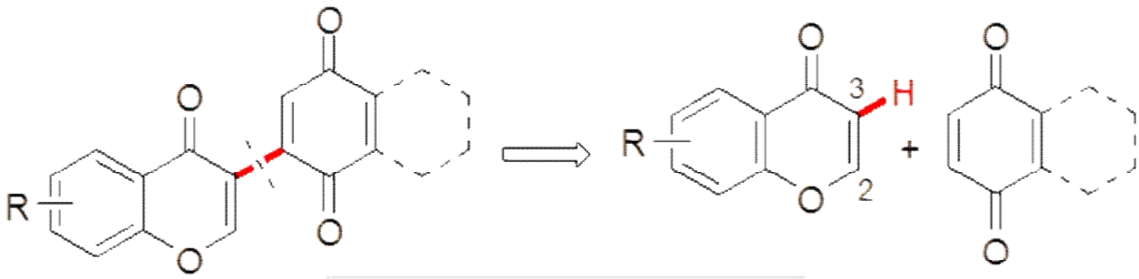
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Facile Route to Isoflavone Quinones via the Direct Cross-Coupling of Chromones and Quinones

문영택 홍승우[1]

KAIST(KAIST) 화학과 [1]KAIST 화학과

The family of isoflavone quinones has been extensively investigated due to its broad range of remarkable biological activities. Isoflavone quinone scaffolds are useful and versatile building blocks and, therefore, provide target systems for synthetic chemists. Despite significant synthetic efforts, existing methods for preparing the scaffolds suffer from multiple steps, and harsh reaction conditions. In view of the high synthetic utility of isoflavone quinone derivatives, the most straightforward method for synthesizing the compounds would involve a direct cross-coupling of chromones with quinones via C-H bond functionalization. We developed an efficient method for preparing isoflavone quinones via a palladium-catalyzed direct C-C coupling reaction. This approach provides facile and affordable access to isoflavone quinone structural motifs, which are privileged and prevalent structures in many biologically active compounds. The beneficial effects associated with the use of AgOAc were clearly observed in this cross-coupling reaction. This method represents an unprecedented example of the direct coupling of chromones with quinones and a significant advance over existing methods.



- *No pre-functionalization*
- *Broad substrate scope*

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-851**

발표분야: 유기화학

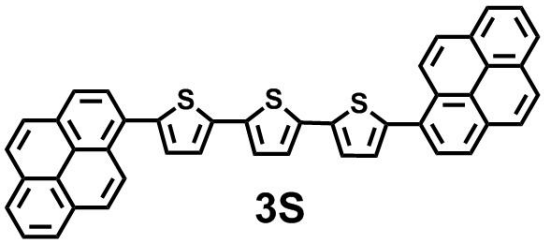
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pyrene end-capped oligothiophene and benzothiadiazole derivatives for heterojunction solar cells

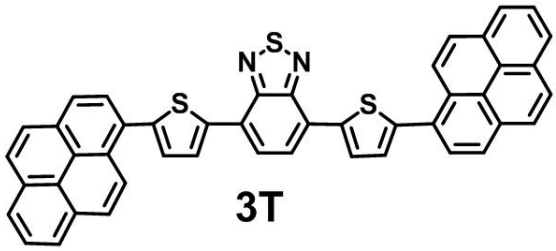
권종철 홍종인

서울대 화학부

Since the first report of organic solar cells (OSCs) by Tang, the development of organic solar cells has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene, benzothiadiazole, and pyrene were commonly used as organic semiconductors due to good charge transport ability. In this study, we report new organic semiconducting materials (3S and 3T), consisting of oligothiophene, benzothiadiazole, and pyrene, as donor materials for OSCs. Fabricated OSC devices based on 3S and 3T exhibited a power conversion efficiency of 1.2% and 1.03%, respectively, under simulated AM 1.5 solar irradiation at 100 mWcm-2.



3S



3T

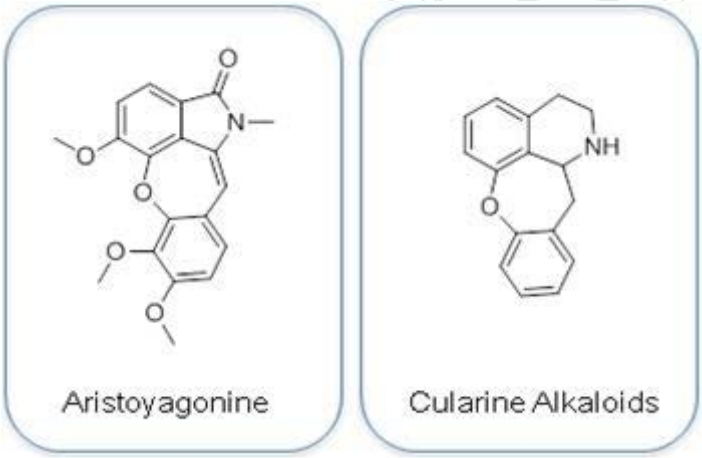
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-852**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Aristoyagonine via a One-Pot Cu-Catalyzed Diaryl Ether Formation and Aldol Condensation.

임혜선 장성연[1] 임환정[1] 박경용 허정녕[1]

충남대 신약전문대학원 [1]한국화학연구원 의약화학연구센터

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 their low natural occurrence in conjunction with their biological activity against various cell lines, several synthetic tactics have been disclosed for the synthesis of these structurally unusual alkaloids. We will describe a strategy for total synthesis of aristoyagonine A via a combination of cu-catalyzed ether formation and aldol condensation reaction for the construction of the 7-membered ring of benzoxepine.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-853**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Facile and Green Protocol for Nucleophilic Substitution Reactions of Sulfonate Esters by Recyclable Ionic Liquids [bmim][X]

LIU YAJUN 채정현

성신여대 화학과

The ionic liquids, [bmim][X] (X = Cl, Br, I, OAc, SCN), were investigated to demonstrate that they are highly efficient reagents for nucleophilic substitution reactions of sulfonate esters derived from primary and secondary alcohols. The counter anions (X^-) of the ionic liquids, [bmim][X], effectively replace the sufonates affording the corresponding substitution products such as alkyl halides, acetates, and thiocyanides in excellent yields. The newly developed protocol is very environmentally attractive because the reactions use stoichiometric amounts of ionic liquids as sole reagents in most cases and do not require additional solvents, any other activating reagents, non-conventional equipments, or special precautions. Moreover, these ionic liquids can be readily recycled without loss of their reactivity, making the whole process “greener”.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-854**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of lactone using Baeyer-Villiger oxidase and chemical reagent for preparing polyester

김규아 송치만[1] 표정인 정규성 정찬성[1]

연세대 화학과 [1]KIST 화학키노믹스연구센터

Polyester is a promising material for the various application fields. In order to prepare this polymer, monomer should be selected very properly. Lactones were used to polymerize as monomers and selected lactones containing chiral center were used for special applications. These monomers were synthesized with heterocyclic ketones using whole cells of recombinant E.coli overexpressing cyclohexanone monooxygenase (CHMO) from *Acinetobacter* sp. NCIMB 9871 strain and *m*-CPBA. The chemoselectivity, regioselectivity and mild condition of this biotransformation, opposite to that observed by chemical oxidation justifies its importance in organic chemistry. These lactones will be polymerized using lipase under the specific condition for further modification to increase potentiality.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-855**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

NHC-Catalyzed Intramolecular Oxidative Cyclization Reactions for the Synthesis of Phthalide Derivatives

송형섭 윤소원

한양대 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 have developed an NHC-catalyzed oxidative lactonization of aldehydes under aerobic conditions involving an unactivated alkyne as an internal electrophile. As part of our continued interest in NHC-catalyzed processes, we investigated an NHC-catalyzed intramolecular oxidative cyclization between aldehyde and unactivated alkene functionalities leading to phthalide derivatives. This process exploits the molecular oxygen in air as a source of an oxygen atom for the oxidation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-856**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Intramolecular Oxidative C-H Amination

강다영 주진혁 윤소원

한양대 화학과

Direct activation and functionalization of C-H bonds in aromatic compounds has attracted the most attention as an efficient, atom-economical, and environmentally friendly synthetic tool. In particular, C-H amination continues to gain prominence as a general and selective method for chemical synthesis. Therefore, we studied transition-metal-catalyzed intramolecular oxidative C-H amination for the synthesis of N-heterocycles. We will demonstrate the effect of nitrogen protecting groups.

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-857**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

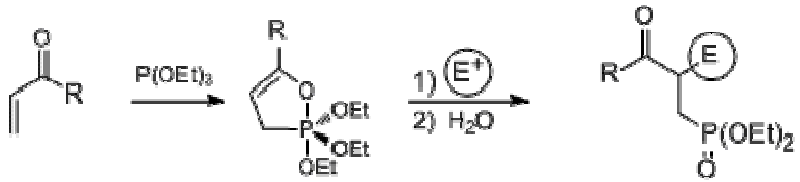
Application of a New Type of Enolate towards the Synthesis of Ketophosphonate Derivativess

김태우 **Tasneem Islam**[1] 정강연

강릉원주대 생명화학공학과 [1]Department of Biological, Chemical and Physical Sciences, Roosevelt University, 1400 North Roosevelt Boulevard, IL, USA

Abstract

Phosphonate analogues have been extensively studied in recent years due to their applications as antibiotics and anti-viral agents as well as insecticides and herbicides. Synthetic methods commonly used for the preparation of phosphonate analogues and mimetics of phosphate esters and carboxylic acids include Arbuzov reaction, Michaelis-Becker reaction, and Abramov reaction, however, all of these methods have some major limitations. Herein, we present our attempt to develop new methodology for the synthesis of biologically active phosphonate derivatives through the use of oxaphospholene intermediates as a new type of enolates.Triethylphosphite was reacted with methyl vinyl ketone to give an intermediate oxaphospholene which was then reacted with a series of carbonyl compounds. We report our preliminarily results on the synthesis of ?-ketophosphonates in good yield which can act as precursors for a range of biologically active compounds through the manipulation of the keto functional group and thus, extend the C-C bond.c



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-858**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-Catalyzed Synthesis of Indole Derivatives

장민정 정은주 윤소원

한양대 화학과

Among the various heterocyclic compounds, indoles are one of the most widely distributed heterocyclic compounds in nature. Indole scaffolds are biologically very attractive and have appeared frequently in the medicinal chemistry literature showing their importance. Recently, we investigated the synthesis of indole derivatives using Pd catalysis. We examined the effect of nitrogen protecting groups in the intramolecular cyclization reaction of *N*-substituted-2-styrylaniline.

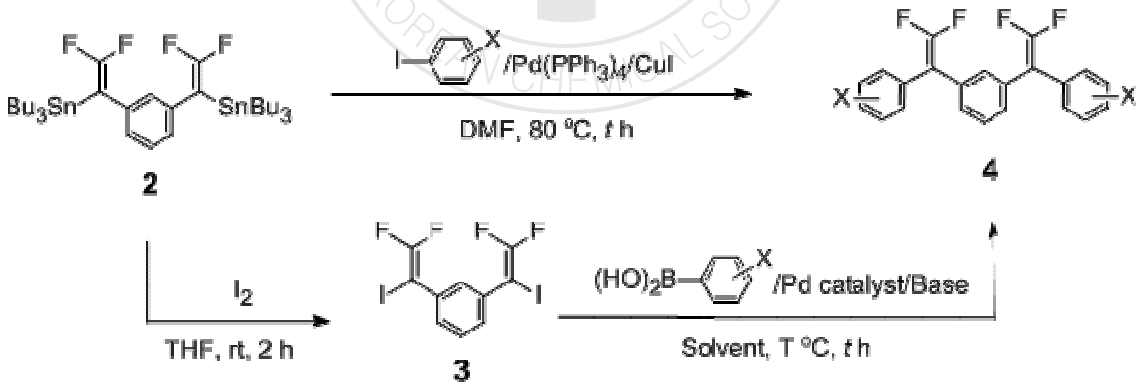
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-859**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of 1,3-Bis(2,2-difluoro-1-tributylstannylethenyl)benzene and its study on the Arylation reactions

최수정 정인화[1]

연세대 화학과 [1]연세대 화학및의화학과

1,3-Bis(2,2-difluoro-1-tributylstannylethenyl)benzene (2) was prepared in a 60% yield from the reaction of 1,1'-(1,3-phenyllene)bis(2,2-difluoroethene-1,1-diyl)bis(4-methylbenzenesulfonate) (1) with bis(tributyltin) (2.2 equiv), LiBr(30 equiv), PdCl2(CH3CN)2 (10 mol%) and X-Phos (20 mol%) in THF at reflux temperature for 6 hours. The cross-coupling reaction of 2 with aryl iodides provided the cross-coupled products 4 in good yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-860**

발표분야: 유기화학

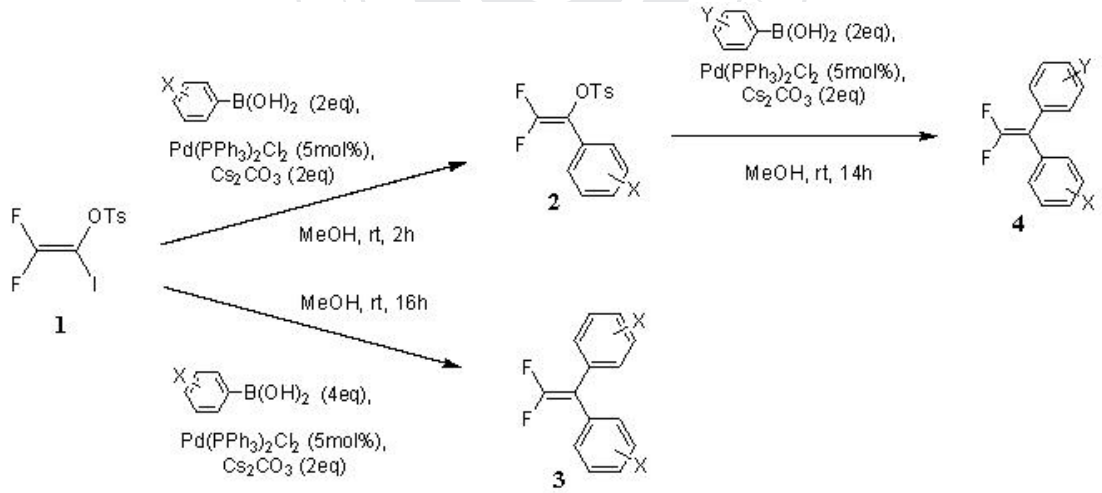
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of 2,2-difluoro-1-iodoethenyl tosylate and its cross-coupling reactions with arylboronic acid

김주희 정인화[1]

연세대 화학과 [1]연세대 화학및의화학과

2,2-Difluoro-1-iodoethenyl tosylate 1 was prepared in 75% yield from the reaction of 2,2,2-trifluoroethyl p-toluenesulfonate with 2.2 equiv LDA at low temperature followed by treatment of I2. Cross-coupling reation of 1 with arylboronic acid provided the mono-aryl 2 and di-aryl difluoroethenes 3 in good yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-861**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of arylamines containing napthyl and fluorenyl sub units

송희정 정진아 송미선 이덕희 채규윤[1]

원광대 생명나노화학과 [1]원광대 화학과

Some arylamines containing naphthyl and fluorenyl sub units were synthesised from napthylamine using bromination, alkylation, borination, and suzuki coupling reaction. Products were evaluated for physical properties as an electron transport materials for OLED devices.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-862**

발표분야: 유기화학

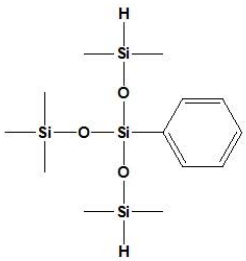
발표종류: 포스터, 발표일시: 수 16:00~19:00

Some siloxane compounds for OLED/LED devices

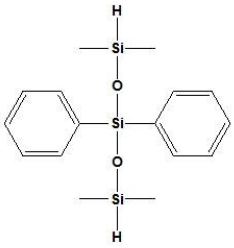
황희민 신세라 송창현 이덕희 채규윤[1]

원광대 생명나노화학과 [1]원광대 화학과

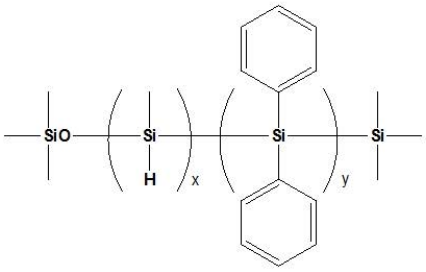
The siloxane compounds containing a silicon-Hydrogen bond, shown below, were evaluated as a cross-linker for manufacturing sealing materials for light-emitting device(LED) and organic light-emitting device(OLED). Refractive Index and hardness of the cured products, and curing time were investigated for each compositions.



structure 1,



structure 2,



structure 3

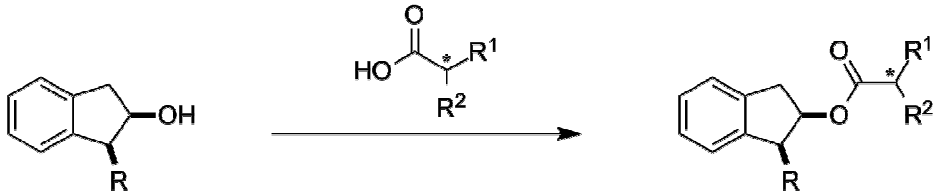
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-863**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Aminoindanol-based chiral derivatizing agents for the determination of the absolute configuration of carboxylic acids

박민정 최기항

고려대 화학과

New chiral derivatizing agents (CDAs), 1a and 1b, for determination of absolute configuration of α-chiral carboxylic acids have been prepared from *cis*-1-amino-2-indanol through efficient and short-step synthesis. Once α-chiral carboxylic acids are derivatized with both enantiomers of the CDA, the ^{1}H NMR signals of the resulting diastereomeric esters show significant chemical shift differences (Δδ). The Δδ values are increased by applying a larger aromatic group (R) to enhance the anisotropic effect of the CDA (1a vs. 1b). These CDAs show the same trend in their Δδ values for various α-chiral carboxylic acids and they provide a reliable NMR spectroscopic method to determine the absolute configuration of α-chiral carboxylic acids.



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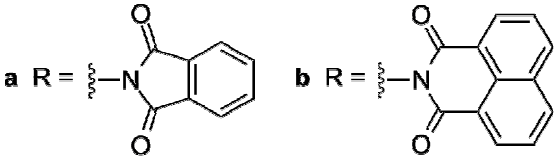


일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-864**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rigid Hydrophobic Group-containing Amphiphiles for Membrane Protein Study

조경호 채필석

한양대 생명나노공학과

Integral membrane proteins (IMPs) serve proper function of individual cells and multicellular organisms by controlling the transfer of information and molecules across lipid barriers. Our understanding of IMP structure and function is hampered by the difficulties associated with handling these proteins. Bringing such proteins into aqueous solution generally requires the use of a detergent to shield the large lipophilic surfaces displayed by IMPs in their native forms from polar solvent medium. Considerable effort has been devoted to the development of new amphiphilic agents for solubilization and stabilization of IMPs, but many proteins remain difficult or impossible to isolate and study because of inadequacies in the biochemical toolbox. Here we introduce a new class of amphiphiles with a rigid hydrophobic group. We show that this new family displays favorable behavior relative to conventional detergents with various membrane protein systems, leading to enhanced structural stability of IMPs in aqueous solution. These results indicate that the new amphiphiles could be promising as tools for membrane science.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-865**

발표분야: 유기화학

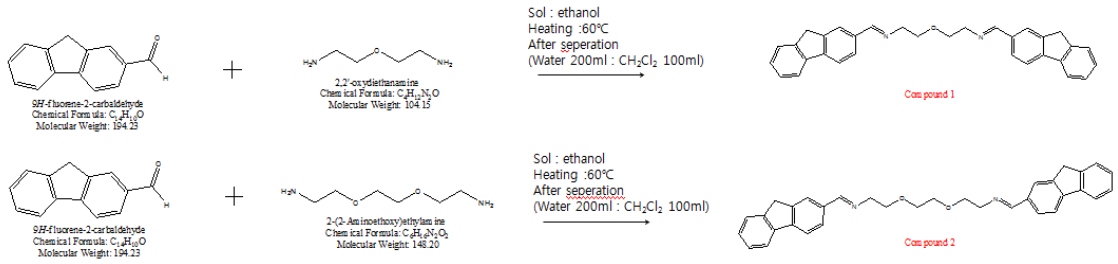
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and recognition properties of new fluorene compounds containing moieties.

김기백 장호 장우식 장승현

대구대 화학과

We synthesized new kinds of bis type of fluorene fluorescent sensors, They were in the ratio of 1 : 2 respectively imine was synthesized by the reaction. *Compound 1* was synthesized from 9H-fluorene-2-carbaldehyde and 2,2'-oxydiethanamine. *Compound 2* was synthesized from 9H-fluorene-2-carbaldehyde and 2-(2-Aminoethoxy)ethylamine. Synthesis, fluorescence properties will be discussed. The structure of *compound 1* and *compound 2* were characterized by ^{1}H NMR, MS and IR spectroscopy.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-866**

발표분야: 유기화학

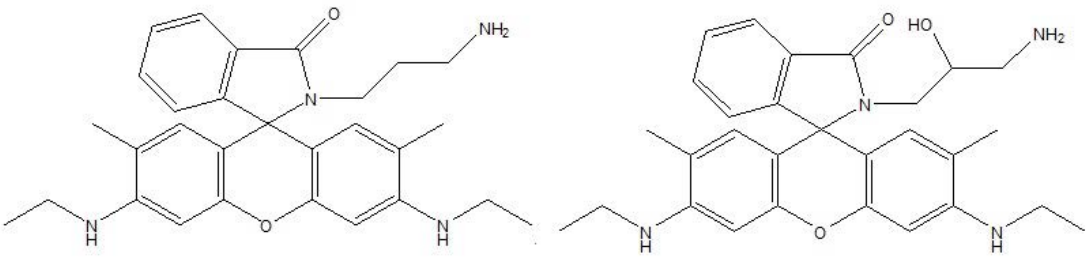
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent chemosensor for the detection of rhodamine 6G compound

장우식 김기백 장호 장승현

대구대 화학과

The on/off fluorescence switching of these chemosensors was based on structure change of the rhodamine moiety between spirocyclic and open/close ring forms. So we synthesized two rhodamine 6G compound by imine reaction. Moreover, synthesized compound confirmed by 1H-NMR, GC-Mass. compared their fluorescent properties.



Scheme 1. Synthesis of rhodamine 6G compound.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-867**

발표분야: 유기화학

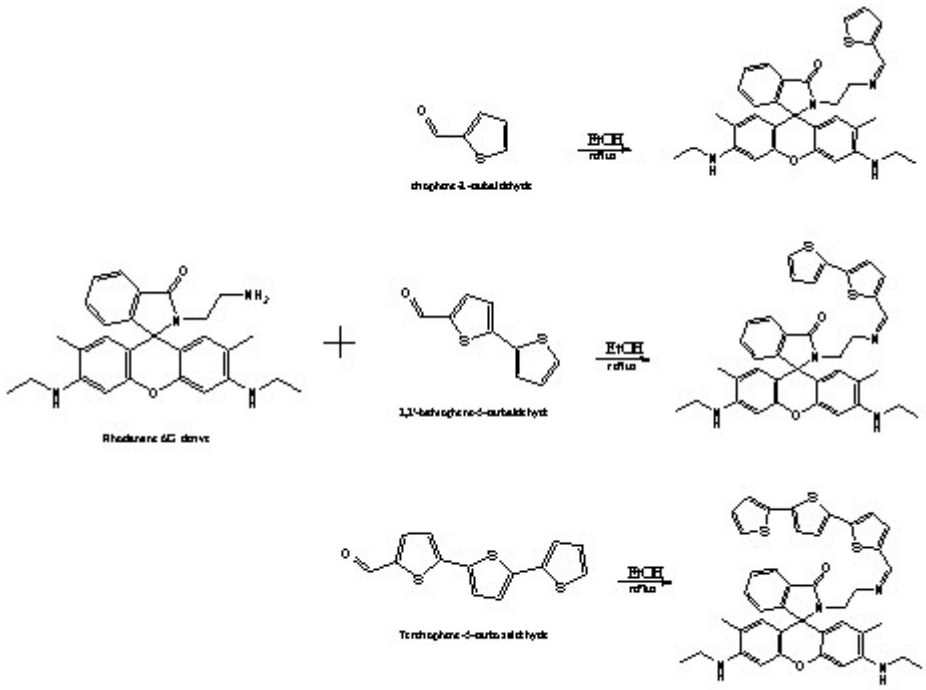
발표종류: 포스터, 발표일시: 수 16:00~19:00

A colorimetric and "turn-on" fluorescent chemosensor for metal ion based on rhodamine derivative

장호 김기백 장우식 장승현

대구대 화학과

The recognition and sensing of biologically and environmentally important species has emerged as a significant goal in the field of chemical sensors in recent years. Fluorogenic methods in conjunction with suitable probes are preferable approaches for the measurement of these analytes because fluorimetry is rapidly performed, is nondestructive, is highly sensitive, is suitable for high-throughput screening applications. Among the fluorophores developed, rhodamines are highly favorable because of their excellent photophysical properties, such as high extinction coefficients, excellent quantum yields, great photosatability, and relatively long emission wavelengths. Rhodamine derivatives are nonfluorescent and colorless, whereas ring-opening of the corresponding lactone gives rise to strong fluorescence emission and a pink color. We synthesized rhodamine derivatives compounds by a Schiff base reaction.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

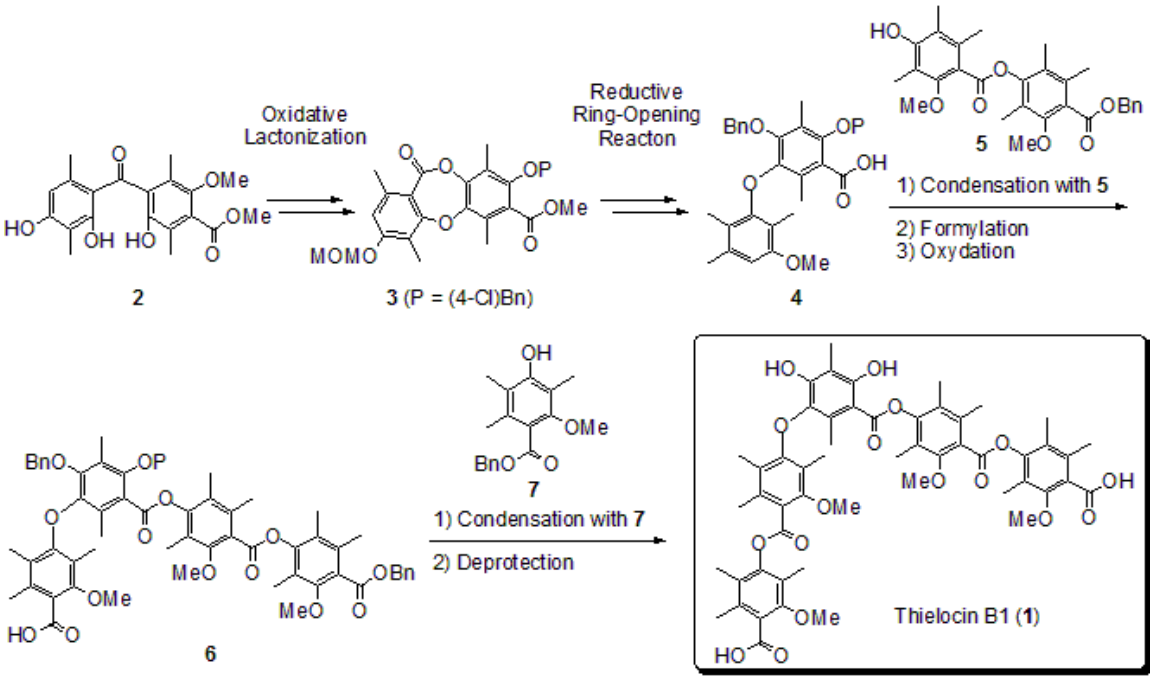
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-868**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Thielocin B1

Kosuke Osawa Masahito Yoshida Motoki Takagi[1] Kazuo Shin-ya[2] Takayuki Doi

Tohoku University [1]Japan Biological Informatics Consortium [2]Advanced Industrial Science and Technology

Thielocin B1 (1) was isolated from the fermentation broth of thielavia terricola RF-143[1] in 1995 and strongly inhibits the formation of PAC3/PAC3 homodimer by interaction in the interface of protein-protein interaction site[2]. 1 is composed of five highly functionalized benzene rings, which are connected by an ether bond and three ester linkages. Especially, 1 contains a 2,2',6,6'-biaryl ether unit, which we have difficulty forming by conventional coupling reactions due to steric hindrance. We are thus interested in the total synthesis and bioactivity of 1. Construction of desired 2,2',6,6'-biaryl ether 4 was achieved by oxidative lactonization of benzophenone 2 and following reductive ring-opening reaction of lactone 3. Condensation of 4 and 5, formylation and oxidation of the resulting aldehyde afforded benzoic acid 6. After coupling of 6 with 7, removal of the benzyl groups by hydrogenation furnished thielocin B1 (1) (Scheme 1), whose spectral data were in good agreement with those of the natural 1.[1] Matsumoto, K.; Tanaka, K.; Matsutani, S.; Sakazaki, R.; Hinoo, H.; Uotani, N.; Tanimono, T.; Kawamura, Y.; Nakamoto, S. and Yoshida, T. J. Antibiot. 1995, 48, 106-112.[2] Hashimoto, J.; Watanabe, T.; Seki, T.; Karasawa, S.; Izumikawa, M.; Seki, T.; Iemura, S.; Natsume T.; Nomura, N.; Goshima, N.; Miyawaki, A.; Takagi, M.; Shin-ya, K. J. Biomol. Screen. 2009, 14, 970?979.



Scheme 1. Total Synethesis of Thelocin B1 (1)

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-869**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Induction and Control of the Helical Sense of an Indolocarbazole Foldamer by Chiral Organic Anions

김단아 석재민

연세대 화학과

We prepared an indolocarbazole trimer that could fold into a helical conformation in the presence of bis(tetrabutylammonium) sulfate. Owing to the enantiomeric relationship, the left- and right-handed complexes were formed in a racemic mixture. Using chiral organic anions such as camphorsulfonates and *c*-AMP, we herein had shown for the first time that one-handed helical folding of an indolocrbazole foldamer can be induced to afford characteristic CD signals. Furthermore, it is also demonstrated that the on/off switching of the chiroptical signal can be reversibly operated by acid and base chemistry, which efficiently governs the association and dissipation of the foldamer and *c*-AMP. Details inculding the binding studies and structural features will be described in the presentation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-870**

발표분야: 유기화학

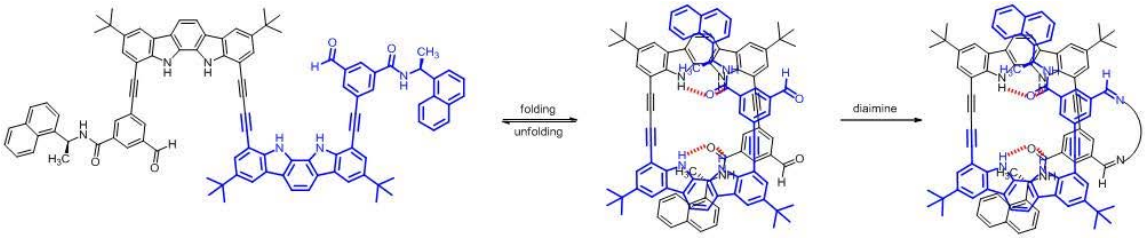
발표종류: 포스터, 발표일시: 수 16:00~19:00

An Indolocarbazole Macrocycle Prepared by Folding Followed by the Post-Imine Bond Formation

김현주

연세대 화학과

Recently, we prepared an indolocarbazole dimer as folded in a helical structure by intra-molecular hydrogen bonds between NH of indolocarbazole and carbonyl oxygen of terminal amide. Chiral segments at ends of the dimer enforce the formation of one-handed helix at least preferentially in solution. Herein, we have prepared another indolocarbazole dimer with the aldehyde appendages that readily react with diamines to afford the corresponding imine macrocycles which adopt helical conformations. The structural and dynamic features of these macrocycles have been revealed by circular dichroic (CD) and ^{1}H NMR spectroscopy. The details of these studies as well as their binding properties of anionic guests will be described in the presentation.



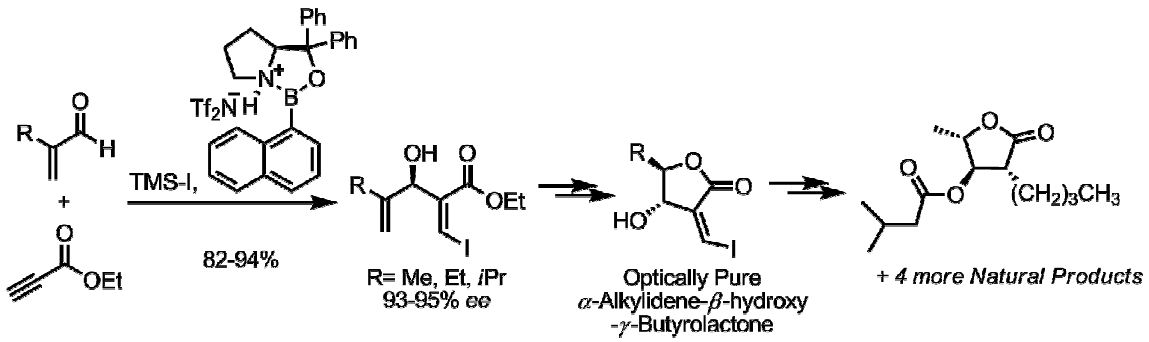
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-871**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of α-Alkylidene-β-Hydroxy-γ-Butyrolactones via Enantioselective Tandem Michael-Aldol Reaction; Total Synthesis of Naturally Occurring γ-Butyrolactones

이성일 류도현

성균관대 화학과

Five membered lactones are core structure in a large number of natural products. Among them, α-alkylidene-β-hydroxy butyrolactone is one of important substructure that shows a wide range of biological activity. Due to the interesting properties and structure, synthetic methods for chiral α-alkylidene-β-hydroxy-γ-butyrolactones are reported during last decade but catalytic enantioselective synthesis of α-alkylidene-β-hydroxy butyrolactone has been rarely reported. In the absence of general procedure for α-alkylidene-β-hydroxy-γ-butyrolactone we anticipated that the optically active (Z)-β-iodo MBH esters could be suitable precursor for producing chiral trisubstituted-α-alkylidene-γ-butyrolactone through a simple transformation. Herein we introduce a general procedure for the optically pure (Z) and (E)-α-alkylidene-β-hydroxy-γ-butyrolactones via highly enantioselective tandem Michael-aldol reaction and its applications to a total synthesis of naturally occurring γ-butyrolactones.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-872**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-Arylbenzo[b]furan Natural Product and its Anti-inflammatory Activity

이재준 전종갑

한림대 화학과, 응용화학연구소

The 2-arylbenzo[b]furan structure is prevalent in a wide variety of biologically active natural and unnatural compounds. Many 2-arylbenzo[b]furan derivatives are well-known to exhibit a broad range of biological activities, including anticancer, antiproliferative, anti-inflammatory, antiviral, antifungal, immunosuppressive, antiplatelet, antioxidative, antifeedent, and insecticidal.The Salvianolic acid C, isolated from water-soluble Salvia miltiorrhiza Bunge (Dan-shen) are considered as the main pharmacological active ingredients for the activities of anti-oxidative, anticoagulant, antithromobotic, anti-HIV, anti-tumor, and so on.We have devised more efficient synthetic route for 2-arylbenzo[b]furan using PPA (poly phosphoric acid) as cyclization reagent starting form 3,4-dihydroxybenzaldehyde and eventually will compare its biological activities with other 2-arylbenzo[b]furan derivatives.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-873**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Stilbene Derivatives for Antioxidant Activity

정세훈 전종갑

한림대 화학과, 응용화학 연구소

Stilbene is one of the long-known aromatic compounds and exists as cis or trans isomer. Phenolic derivatives of stilbene have exceptional antioxidant activity. The antioxidant activity of stilbene derivatives differs from the type of substituents, positions and the structural isomers, respectively. Stilbene derivatives were synthesized according to the existing reductive amination, Horner?Wadsworth?Emmons reaction and Sonogashira coupling method to compare their antioxidant effects. Antioxidant activities including DPPH, ABTS and tyrosinase inhibitory activity of the stilbene derivatives will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-874**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Natural Chalcones and their Derivatives for Biological Activity Tests

김시준 전종갑

한림대 화학과, 응용화학연구소

Chalcones are widespread in plant kingdom and they were reported to have various biological activities such as antitumor, anti-parasitic, anti-leishmanial, anti-oxidative, anti-bacterial, superoxide scavenging, PTP1B inhibitory activity. We synthesized commonly occurring licochalcone D, licochalcone G and their derivatives. Synthesis of this chalcone compounds were prepared through thermal [3,3]-sigmatropic rearrangement and Claisen-Schmidt condensation of protected acetophenone and aldehyde derivatives in basic condition. The whole synthetic procedures of chalcones and their biological activities will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-875**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Benzo[b]furan Natural Product Obovaten

윤현호 전종갑

한림대 화학과, 응용화학연구소

We wish to describe a convenient and general approach to the synthesis of biologically active benzo[b]furan natural product obovaten. This compound was isolated from the persea obovatifolia, which is a small evergreen tree, endemic in the HengChun peninsula of Taiwan. It is also known that they are anticancer constituents of Formosan plant. Benzofuran structure can be synthesized from the Al2O3 mediated coupling reaction between phenol and a-brominated ketone compounds.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-876**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Licochalcone C and Bio-evaluation of Anti-oxidative and Anti-inflammatory Activities.

전제호 전종갑[1]

한림대 천연의약연구소 [1]한림대 화학과

Several chalcone compounds have been extracted and characterized from Licorice, perennial herb which grows in southern Europe, Russia and Turkey. Among these chalcone compounds, licochalcone C is known to have several promising biological activities (antimutagenic, antiparasitic, antileishmanial, anti-ulcer, anti-oxidative and anti-inflammatory effects). But due to low yield of producing this compound through extraction and purifying from natural resources, it is still challenging to prepare sizable amounts of licochalcone C, of which synthesis has not been reported yet, for performing various pharmaceutical studies. The synthetic procedure and results of anti-oxidative anti-inflammatory studies will be described.

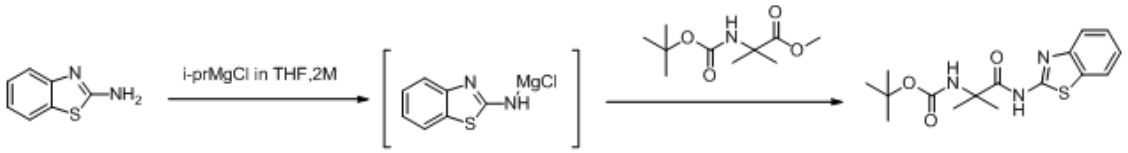
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-877**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a novel amide-coupling strategy for aminobutyric acid with poor nucleophlies.

조민미 여형민[1] 원선우[1] 최민호[2] 곽영신[1] 정재경[3]

충북대 [1]한국생명공학연구원 바이오의약연구소 [2]충북대 약학대학 [3]충북대 제약학과

Amide bond formation by coupling an amine and a carboxylic acid is one of the most popular reactions in synthetic or medical chemistry. However, the reaction can become highly unproductive especially when reactivity of the two coupling partners is challenged sterically or electronically. Aminoisobutyric acid(AIB) is strategically incorporated in molecular design by medicinal chemists since amide bonds bearing AIB often provide favorable metabolic stability profiles or nevel molecular conformations. Despite its utility in medicinal chemistry, amide bond formation with AIB if often troublesome owing to the resistance of its neopentyl carbonyl moiety to coupling with amines. We developed a novel strategy for coupling AIB with poor nucleophlies such as aminothiazoles. The methyl ester of Boc-protected AIB was modified by aminomagnesium chloride species and yielded amidation products under mild condition.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-878**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the synthesis and characterization of various carotenoids as the nanowire.

전선화 구상호[1]

명지대 나노공학과 [1]명지대 화학과

The carotenoids are an important class of organic molecules with delocalized π-electrons, which show electric conductance. We have developed the efficient synthesis of natural carotenoids, which can be extended to the synthesis of unnatural carotenoid wires containing aromatic substituents. The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would offer an extra stability and excellent electronic characteristics compared with those of the natural carotenoids.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-879**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study of synthetic method of efficient units for unnatural carotenoid wire

임보람 구상호[1]

명지대 나노공학과 [1]명지대 화학과

Synthesis of Unnatural carotenoids containing various phenyl substituents has excellent characteristic in terms of stability and Electronics. It is in necessary construction of efficient unit For synthesis of unnatural carotenoids using various routes. First we will construct Chloro allylic sulfone unit containg substituent X. This material can make from Acetophenone derivative depending on the location. According to Indium addition and oxonia- cope rearrangement reaction, The reactions provide high stereoselectivity as well as an absolute regioselectivity. we will make efficient units for synthesis of various Phenyl substituents carotenoids.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-880**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Effective Synthesis of Oxy-carotenoids.

이규상 구상호[1]

명지대 나노공학과 [1]명지대 화학과

Carotenoids such as β-carotene and lycopene are characterized by long conjugated polyene chains that show unique red colors, and are ideally utilized as nonhazardous dyes for foodstuffs.These long conjugated polyene chains react with R.O.S (reactive oxygen species) preventing certain cancers such as pancreatic, oral, bladder cancers and so on. The efficient methods of synthesizing carotenoids have already been reported by our group.The methods are based on the sulfone coupling and double elimination strategy using C20 dialdehyde ((2E,6E,10E,14E)-2,6,11,15-tetramethyl-8-(phenylsulfonyl) hexadeca-2,6,10,14-tetraenedial) and C10 sulfone unit (((2,6,6-trimethylcyclohex-1-enyl)methylsulfonyl) benzene).The synthesizing of oxidized C10 sulfone unit and coupling with C20 dialdehyde to make Oxy-carotenoids was investigated. This study includes the controlled oxidation of C10 sulfone unit along with the methods of coupling, protecting and double elimination with C20 dialdehyde.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-881**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A study of Buchwald amination for palladium catalyzed cross-coupling

김영훈 구상호[1]

명지대 나노공학과 [1]명지대 화학과

Buchwald amination is an efficient method to convert aryl halide into amine compound. This reaction is based on palladium catalyzed cross-coupling of aryl halide with aryl amine. The resulting aryl amine compound can be utilized as a nucleophilie for further transformations. It would be an efficient way of synthesizing carotenoids containing aryl amine substituent by the Buchwald amination of the carotenoids with aryl bromide substituent. We initiated a model study of the Buchwald amination in the carotenoids containing aryl bromide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-882**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of various phosphatidyl choline compounds.

최보슬 구상호[1]

명지대 나노공학과 [1]명지대 화학과

Phosphatidyl choline is a important component that is in every cell membranes and tissues of human body. A general phophatidyl choline is composed of a choline head group that is hydrophilic part and two fatty acids being hydrophobic part. We tried to use α-tocopherol for one fatty group because it is a well known anti-oxidant, which may protect other molecular or cell from reactive oxygen species. Vitamin A which is essential for biological reactivity is another fatty part . In this project, We studied to synthesize the phosphatidyl choline regioselectively containing α-tocopherol and Vitamin A and to identify its characteristics.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-883**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The synthesis of heterocyclic compounds initiated by Manganese acetate from β-ketoester derivatives

Ju Yeming 구상호[1]

명지대 나노공학과 [1]명지대 화학과

Heterocyclic compounds are of great importance in our life, which exhibit anti-cancer, antiseptic, disinfecant, and pesticide properties. The hetero-Diels-Alder reaction is a powerful method for the preparation of heterocyclic compounds considering the increasing number of literatures. We have devised heterocyclic compounds which could be synthesized from isoprenoid chains via intermolecular Hetero-Diels-Alder reactions that are induced by Mn(OAc)3.2H2O and Cu(OAc)2.H2O. In order to increase the stereoselectivity, the introduction of chiral auxiliary is necessary. Based on the methodology we proposed, the application of Mn(OAc)3.2H2O and Cu(OAc)2.H2O could be developed to form various kinds of hetero aromatic containing diverse functional groups that may contribute to the synthesis of nature compounds.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-884**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

synthesis of medium-sized carbocyclic ring compounds.

최정애 구상호[1]

명지대 나노공학과 [1]명지대 화학과

The developement of an efficient cyclization method is very important for the biological and medicinal study.Medium-sized carbocyclic ring systems are ubiquitous present as the structural core in natural products.In this study, We have developed an efficient preparation method of medium-sized carbocyclic compound.We have successfully developed the ring expansion method from 6-membered ring to 7- or 9-membered ring homologues by oxidative ring opening and cyclization strategy.Starting from 1,2-cyclohexanedione, we have synthesised 1,2-cyclohexanediols by the addition of carbo-nucleophiles, and then oxidative ring opening reaction to provide the ring expansion products. Seven and nine membered rings were obtained through the Diels-Alder or the Baylis-Hilman reactions.

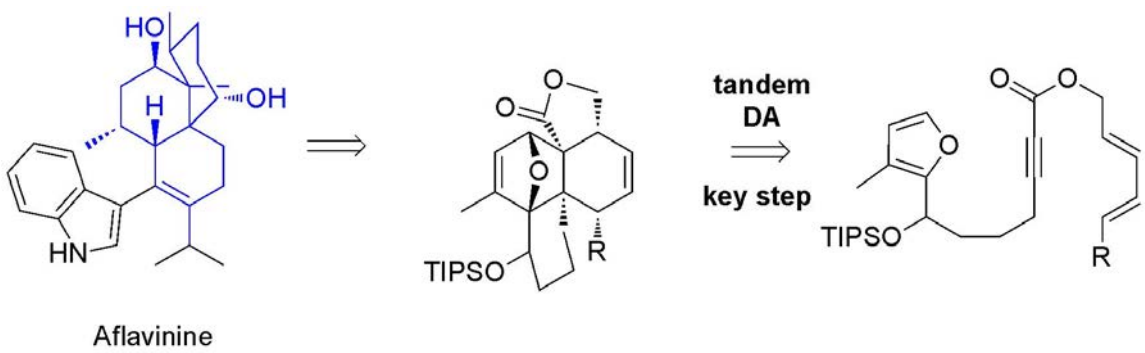
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-885**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic studies toward the total synthesis of aflavinine.

조민미 여형민[1] 원선우[1] 정재경 곽영신[1]

충북대 약학과 [1]한국생명공학연구원 바이오의약연구소

Numerous indole diterpenoids have been discovered from fungal sclerotia and considered as their chemical defense system. Among the indole diterpenoids aflavinines have never yielded the total synthesis to synthetic organic chemists for decades. For the total synthesis of aflavinine, we developed a retrosynthetic plan featuring a tandem Diels-Alder cycloaddition as the key synthetic strategy. We envision developing the tandem reaction strategy would not only provide a rapid access to the core skeleton of aflavinine, but also a useful tool for building compound libraries of high molecular complexity. We report the progress of our synthetic studies toward the total synthesis of aflavinine. Followed by a highly convergent synthesis of the key substrate by combining three easily obtainable fragments, a successful tandem Diels-Alder cycloaddition was demonstrated.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-886**

발표분야: 유기화학

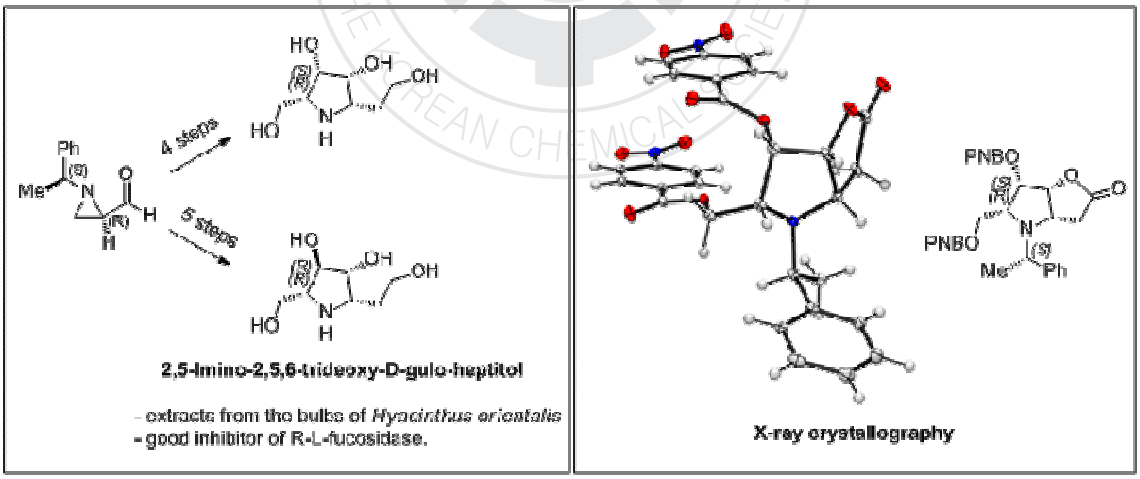
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of polyhydroxylated pyrrolidines, (+)-2,5-imino-2,5,6-trideoxy-gulo-heptitol and its C(3) epimer, from a chiral aziridine and structural evaluation

이호규 장만수 이원구 조재홍[1] 남원우[2] 하현준[3]

서강대 화학과 [1]대구경북과학기술원 신물질과학 [2]이화여대 화학과 [3]한국외국어대 화학과

A stereoselective synthesis of (+)-2,5-imino-2,5,6-trideoxy-gulo-heptitol and its C(3) epimer has been accomplished starting from a chiral aziridine-2-carboxaldehyde. The absolute configurations at the four consecutive carbon centers have been established by X-ray crystallography.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-887**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The efficient synthesis of and L and D-isomers of 18F-FMT

강희원 지대윤

서강대 화학과

18F-fluorinated tyrosine and its analogs were most thoroughly evaluated for their potential to be tumor imaging agents, and O-18Fmethyl tyrosine (FMT) was found to be the best PET agent candidate among investigated analogs. However, the potential of FMT as a PET tracer has been not fully exploited to date due to its complicated synthetic procedure, especially non-direct 18F fluorination step. Here in, we report our effort to synthesize both L and D FMT isomers by utilizing our recent work of one step fluorination between a fluoride ion and the methylhydorxy group attached highly activated triazolium salt leaving group.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-888**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Asymmetric Cascade Reactions of 2-Pyrrolyloxoacetates to α,β-Unsaturated Carbonyl Compounds

이효준 조창우

경북대 화학과

Pyrrolizines have potent cytostatic effects and thus are potentially useful for the development of antitumor and antiviral agents. However, synthesis of chiral pyrrolizines has been sparsely reported. Chiral auxiliary-mediated diastereoselective intramolecular cycloadditions of pyrrole-based nitrone intermediates have been reported only for the synthesis of chiral pyrrolizines. Therefore, recently, we reported the organocatalytic asymmetric cascade aza-Michael-aldol reactions of 2-trihaloacetylpyrroles as the *N*-centered heteroaromatic nucleophiles to α,β-unsaturated aldehydes that provide highly functionalized chiral pyrrolizines in good yields, high enantioselectivities, and excellent diastereoselectivities. This was the first example of organocatalytic cascade reactions in which pyrroles act as *N*-centered heteroaromatic nucleophiles. To make a wide variety of chiral pyrrolizines, we planned to expand the scope of substrates and pyrroles as the *N*-centered heteroaromatic nucleophiles in the organocatalytic asymmetric cascade reaction. Here, we report organocatalytic asymmetric cascade aza-Michael-aldol reactions of 2-pyrrolyloxoacetates as the *N*-centered heteroaromatic nucleophiles to α,β-unsaturated carbonyl compounds that provide highly functionalized chiral pyrroliznes containing three consecutive stereogenic centers.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-889**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Sensitive Detection of Mercury Ions

Nguyen Bao Lam 우한영[1]

부산대 인지메카트로닉스 [1]부산대 나노기술대학 나노정보소재공학과

Mercury is a widespread global pollutant and toxic material to humans even at low concentration. It causes digestive, kidney, and most notably, neurological disorders. Accordingly, sensitive and selective detection of mercury ions is necessary and urgent. In this sense, we have developed a cationic water-soluble fluorescent probe for sensing of mercury ions. The newly developed fluorescent probe showed good solubility, high molar absorption coefficient and quantum yield in water. When binding with Hg^{2+}, absorption and emission of the probe were quenched linearly with the concentration of Hg^{2+}. Narrow dynamic range results in high sensitivity with low limit of detection. This study provides an important guideline for designing efficient chemosensors.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-890**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Chemosensor for Fluoride Based Metal Complex

전남중 조재원 남계춘

전남대 화학과

Platinum(II) complexes have drawn great attention in the last two decades because of the intriguing photophysical properties and the resulting, versatile, potential applications in photonic devices, such as in organic lightemitting diodes (OLEDs), dye-sensitized solar cells, photochemical cells, and optical sensors. These applications are essentially based on the complexes long-lived phosphorescence at room temperature, moderate to strong metal-toligand charge transfer absorption in the visible spectral region, and multiple intramolecular charge-transfer transitions. More importantly, these properties can be modulated by chemical or physical stimuli, such as pH, temperature, cation, anion, and so forth. On account of the important roles of anion in biological, clinical, environmental, catalysis, and chemical processes, the selective and efficient recognition of anion is an area of growing interest in supramolecular chemistry. Fluorescent chemosensors can be effectively used as a tool to analyze and clarify 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 metal complex derivative was obtained successfully by the reaction of bipyridine derivative with $PtCl_2$. The binding properties of metal complex derivative investigated with ^{1}H-NMR and fluorescence titration methods with various anions.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-891**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric Chemosensor for Anions Based on Antraquinone Derivative

윤희상 조재원 전남중 남계춘

전남대 화학과

Design and development of artificial molecular systems for sensing anions in biologically relevant conditions is a challenging task in supramolecular chemistry. In particular, sensing fluoride anion has attracted increasing interest in the molecular recognition community because of its pivotal importance in many areas of biological and chemical sciences. 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. Colorimetric chemosensors can be effectively used as a tool to analyze and clarify such roles of charged chemical species in living system as well as to measure the amount of ions. Among anion receptors, colorimetric 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 bipyridine with antraquinone derivative. The binding properties of antraquinone derivative investigated with ^{1}H-NMR and fluorescence titration methods with various anions.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-892**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient method for purification of cucubit uril[7] by molecular fishing

장은성 이상열[1] 지대윤

서강대 화학과 [1]서강대 PET 방사성의약품융합연구단

Cucutbit[7]uril (CB[7]), a member of the host family cucurbit[n]urils (CB[n], n=5~8, 10), consist a hydrophobic cavity and two identical carbonyl-fringed portals and binds to ferrocene derivatives with high binding constant (K ? 1 x 1012 M-1). However, synthesis of pure CB[7] is a challenging task since all of cucubit urils have similar structure and chemical property. Hence, we report a method to purify CB[7] from other cucubit urils, which capture CB[7] with polymer-bounded ferrocene derivatives and then recover CB(7) by continuous extraction method.

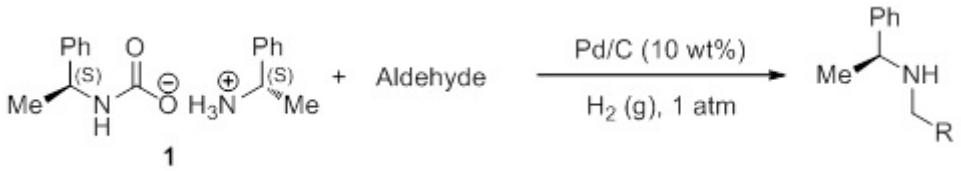
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-893**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent Free Reductive Amination of a solid amine equivalentwith Diversely Substituted Aromatic Aldehydes

강필준 심연수 정미진 이원구 이병노 허남회 이규명[1]

서강대 화학과 [1]한국화학연구원 대사증후군치료제연구그룹

Since many amines are liquid at room temperature and have unpleasant odor, there are some difficulties in handling when we use amines as reagents. Therefore, we transformed a liquid amine to a solid form 1 by using supercritical carbon dioxide to provide a carbamate salt. Since the solid amine equivalent is convenient to quantify, reductive amination can be performed between the solid amine equivalent 1 and aldehydes by 1:1 molar ratio. The reductive amination was initiated with the mixture of 1 and an aldehyde to form the corresponding imine without a solvent then the reduction of the imine was catalyzed by Pd/C and completed in one pot under 1 atm of H2 gas. This solvent free reductive amination reaction is environmentally attractive and solid phase amines can find further application in various chemical reactions.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-894**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

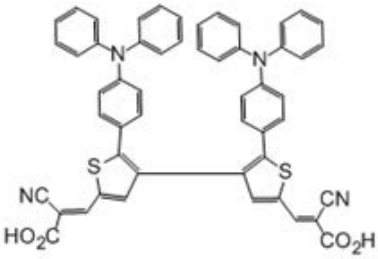
Spiro structured dye induced by bridging of two chromophore : It's photovoltaic performance in DSSC

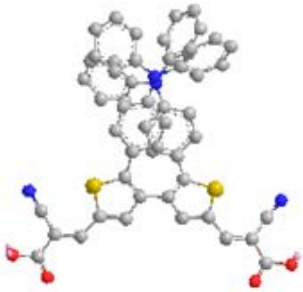
이상희 김가영 신정훈 김동희

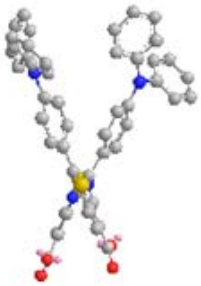
군산대 화학과

Bridging of two planar chromophore molecules induced spiro conformation which can suppress of dyeaggregation. The resulting dye also has two anchoring dgroup which bind to TiO2 efficiently. Binding ability and cell performance of bridged dye will be described.

THE KOREAN CHEMICAL SOCIETY







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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-895**

발표분야: 유기화학

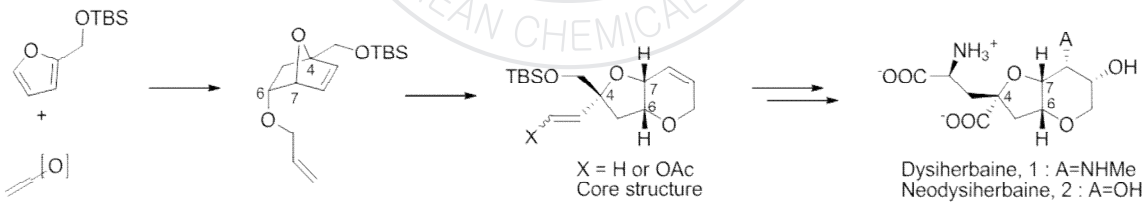
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Formal total synthesis of Dysiherbaine and Neodysiherbaine

이상신 권국태 이희윤

KAIST 화학과

Dysiherbaine and Neodysiherbaine are a novel neurotoxic amino acid isolated from marine sponge *Dysidea herbacea* by Sakai in 1997. Pharmacologically, dysiherbaine is considerably valuable since it was found to be an agonist for glutamate receptors. Dysiherbaine / Neodysiherbaine have unique skeletal structure of *cis*-fused hexahydrofuraopyran ring substituted with alanine amino side chain. By now 6 groups have been researched for its synthesis and showed difficulties for construction of congested stereocenters at C-4, 6 and 7 position. We designed a new strategy in view of the efficiency for setup these stereocenters utilizing diene metathesis pathway.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-896**

발표분야: 유기화학

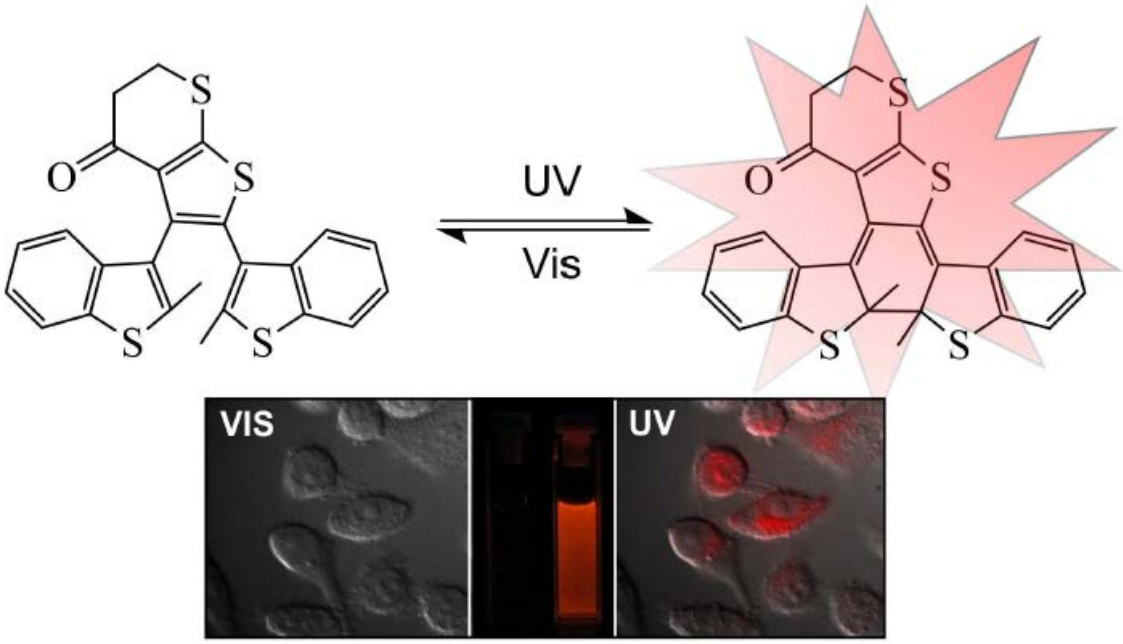
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical properties of novel fluorescence diarylethene and its application on cell

장다은 이민재 강성호 안광현

경희대 응용화학과

A novel fluorescent diarylethene was synthesized through two steps reaction from 2,3-bis(2-methylbenzo[b]thiophen-3-yl)-thiophene (BTT). The new compound emits strong fluorescence in the closed-ring isomer (Scheme 1) and its fluorescence quantum yield was determined to be 0.11, using Rhodamine B (0.70 in ethanol) as the reference upon 510 nm photo-excitation. Photochemical coloration and decoloration cycles were measured and the result showed that the novel compound is an ideal material for photo-induced fluorescence modulation and other applications based on photochromism with high fatigue resistance. The photo-cyclization and photo- cycloreversion quantum yield were found to be 0.25 and 0.17, respectively. Single crystal was obtained by recrystallization from mixed solvents (Hexane/EA = 4:1). The molecule was fixed in an anti-parallel mode and the distance between reacting carbon atoms on the aryl rings is 3.58 ?, which is less than 4.2 ?. Thus the novel compound could undergo photochromism in the crystalline phase during alternating irradiation with 312 nm and visible light. Furthermore, the novel diarylethene-derived photochromic compound, which is noncytotoxic, plasma membranepermeabe and photoswitchable in cells upon alternative UV and visible light irradiation, is appied to live cell imaging. Using a new TIRFM-based detection platform, excellent in vivo photoswitching images were obtained witout photodamage or fatigue effects, which provides a new possibility to use this molecule as a probe for super-resolution microscopy.



대한화학회
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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-897**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic enantioselective decarboxylative Michael addition of β-ketoacids to α,β-unsaturated ketones.

강영구 김대영

순천향대 화학과

The enantioselective decarboxylative Michael addition reaction promoted by chiral primary amine organocatalysts has been developed, allowing facile synthesis of the corresponding chiral 1,5-diketone with excellent enantioselectivity (up to 97% ee). The method reported represents a valuable approach of utilizing β-ketoacids as synthetic equivalents of aryl methyl ketones.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-898**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective electrophilic α-amination of aromatic ketones catalyzed by primary amine organocatalysts.

임영조 김대영

순천향대 화학과

The catalytic enantioselective electrophilic α-amination promoted by primary amine organocatalysts is described. Treatment of aromatic ketones with azodicarboxylats as electrophilic amination reagents under mild reaction conditions afforded the corresponding α-amino aromatic ketones with excellent enantiomeric excesses (93~97% ee). The presence of 4 Å molecular sieves was of great assistance for the high conversions and enantiocontrol.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-899**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic asymmetric Michael addition reaction of 2-hydroxy-1,4-naphthoquinone to β,γ-unsaturated-α-ketoesters.

이지현 김대영

순천향대 화학과

Naphthoquinones have attracted much attention due to the broad scope of their biological activities. There are a few reported examples of the catalytic enantioselective Michael reaction of 2-hydroxy-1,4-naphthoquinone with β,γ-unsaturated-α-ketoesters. In this presentation we wish to report enantioselective conjugate addition reaction of 2-hydroxy-1,4-naphthoquinone with β,γ-unsaturated-α-ketoesters. The process was promoted by bifunctional organocatalyst that is binaphthyl scaffold with H-bonding motif and afforded the chiral adducts in high yields and excellentenantioselectivities (up to 97% ee) under mild conditions.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-900**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly enantioselective conjugate addition of 4-hydroxy coumarin to β,γ-unsaturated α-keto esters.

한태현 김대영

순천향대 화학과

The development of asymmetric methods for the preparation of functionalized coumarin has been of long standing interest to organic chemistry. Coumarin derivatives are an important class of compound found in a variety of natural products and bioactive molecules and are used as versatile intermediates in organic and natural product synthesis. In this presentation, we wish to report the Highly enantioselective Michael addition of 4-hydroxy coumarin to β,γ-unsaturated α-keto esters catalyzed by thiourea-tertiary-amine catalyst.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-901**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium catalyzed asymmetric fluorination of α-chloro-β-ketophosphonates

우샛별 김대영

순천향대 화학과

Fluorine-containing organic molecules are becoming increasingly important in medicinal chemistry. In particular, very few methods for the preparation of α-chloro-α-fluoro-β-ketophosphonates are known. In this presentation, we wish to communicate the catalytic enantioselective fluorination of α-chloro-β-ketophosphonates in the presence of air- and moisture-stable chiral palladium complex. The catalytic electrophilic fluorination of α-chloro-β-ketophosphonates to give the corresponding chiral hetero dihalocompound with excellent enantiomeric excesses. (up to 93% ee).

한국화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-902**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective decarboxylative Michael addition of β-ketoacids to nitroalkenes catalyzed by binaphthyl-derived organocatalysts

이현주 김대영

순천향대 화학과

The catalytic enantioselective decarboxylative Michael addition reaction promoted by chiral bifunctional organocatalysts have been developed, allowing facile synthesis of the corresponding γ-nitro ketones with excellent enantioselectivity (up to 97% ee). The method reported represents a valuable approach utilizing β-ketoacids as synthetic equivalents of aryl methyl ketones.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-903**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic enantioselective bromolactonization of alkenoic acids in the presence of palladium complexes

이현주 김대영

순천향대 화학과

The catalytic enantioselective bromolactonization of alkenoic acids promoted by chiral palladium complexes have developed, allowing facile synthesis of the corresponding γ-lactones with excellent enantioselectivity (up to 97% ee). The method reported represents a practical entry for the preparation of chiral γ-lactones derivatives.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-904**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel (R)-Lipoic acid-Amine compound hybrid molecules for Cholinesterase inhibitor

연고흠 임용배[1] 김재관[2] 김범철[3] 강민석[3] 전병욱[3] 장미 박정호[4]

한밭대 응용화학과 [1]한밭대 응용화학 [2]한밭대 생유기화학실험실 [3]한밭대 생명공학과 [4]한밭대 응용화학생명공학부

Alzheimer's disease (AD) is the most common form of dementia. There is no cure for the disease and eventually leads to death. In the patient's brain and slowly destroys memory and thinking skills. We have developed to find inhibitors for acetylcholinesterase (AChE) and butylcholineasterase (BuChE) which are one of the main targets for Alzheimer's disease. We have synthesized (R)-Lipoic acid-amine compound derivatives and evaluated the inhibition activity against AChE and BuChE. Some (R)-Lipoic acid-amine compounds showed inhibition activity for both AChE and BuChE. The other hybrid compounds had selective inhibition against BuChE.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-905**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regenerative Fluorescence Turn-on Sensor for Biothiols: Cu(II)-Cu(I) Interconversion by Redox Reaction

이경식 신익수 홍종인

서울대 화학부

Biothiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) are implicated in a myriad of vital cellular processes including redox homeostasis1 and cellular growth.2 The alteration of the cellular biothiols is also linked to cancer and AIDS.3 Most of sensing methods for biothiols are reaction based probe systems, which involve specific reactions between probes and thiols, such as Michael addition, cyclization with aldehyde, cleavage of sulfonamide, disulfide and sulfonate ester by thiols.4 The reactions, however, are mostly irreversible and thus provide only single-use assays. Here in, we present a reusable molecular probe where nonfluorescent copper(II) coumarin complex (CuIIL) is converted to the strongly fluorescent copper(I) complex upon the addition of amino acids containing a thiol group (Cys, Hcy, GSH). The probe can be regenerated by chemical (or electrochemical) oxidation, and repeatedly used as the thiol sensor.References1. (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 Company, San Francisco, 2000.2. (a) Duan, Wood, Z. A.; Schroeder, E.; Harris, J. R.; Poole, L. B. TransBiochem. Sci. 2003, 28, 32. (b) Carmel, R.; Jacobsen, D. W. Homocysteine in Health and Disease, Cambridge University Press, UK, 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. USA 1997, 94, 1967.4. (a)Chen, X.; Zhou, Y.; Peng, X.; Yoon, J. Chem. Soc. Rev. 2010, 39, 2120.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-906**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of Hyacinthacine A1 and its analogues

엄희성 하현준 이원구[1]

한국외국어대 화학과 [1]서강대 화학과

Hyacinthacine A1, one of bicyclic-azasugar natural products with interesting biological activities, was synthesized from cis-3-phenylethylaziridin-yl-acrylates with stereoselective dihydroxylation as a key step. Alkylation of acrylate, stereoselective reduction of ketone and cyclization to pyrrolidine were successively achieved in an efficient manner with the concomitant breakage of the aziridine ring to give 2-chloromethyl pyrrolidine with all necessary substituents. Finally, the replacement of the chlorine with various nucleophiles and the subsequent cyclization yielded not only hyancinthacine A1 but its analogues.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-907**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chiral Anion Recognition by Phosphorescent Iridium (III) Complex Containing Glucopyranosyl Group

LIYINAN 안지혜 현명호

부산대 화학과

Cyclometalated iridium (III) complexes have been known to show high phosphorescence efficiency and consequently, they have been utilized as efficient phosphorescent dopants in organic light emmiting diods (OLEDs) and as phosphorescent chemosensors for anions and metal cations. However, the use of cyclometalated iridium (III) complexes for chiral anion recognition is rare. In this study, we prepared iridium (III) complex containing glucopyranosyl group and applied the complex for the recognition various anions including F-, Cl-, Br-, I-, OAc- and H2PO4-. Among various anions, H2PO4- was found to show significant phosphorescence enhancement. In addition, the moderate phosphorescence enhancement for acetate anion prompted us to investigate the chiral anion recognition and we found the two enantiomers of tetrabutylammonium salts of N-t-Boc-a-amino acids and N-(3,5-dinitrobenzoyl)-a-amino acids can be discriminated by the complex. For example, in the case of t-Boc-leucine, the association constant ratio for the complexation of the complex with (D)-enantiomer and with (L)-enantiomer was 3.16. In this poster, the detailed procedure for the synthesis of the iridium complex and its use as a phosphorescent chiral anion sensor will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-908**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Recognition of (D)- and (L)-α-amino Acid Derivatives by Iridium (III) Complex Appended with Chiral Phenylethyluride

LIYINAN 김혜빈 현명호

부산대 화학과

Recently, fluorescence chemosensors have attracted quite attention because of their high sensitivity and selectivity for various anions and metal cations. In addition, fluorescence chemosensors have been successfully utilized for the recognition of the two enantiomers of racemic compounds. Phosphorescent chemosensors are other attractive methods because their emission may be discriminated readily from scattered light and/or shorter-lived background fluorescence normally present in biological and clinical samples. In this study, we prepared a new iridium (III) complex containing chiral phenylethylureide group. The irium (III) complex thus prepared was found to show intense absorption bands at 255 nm and relatively weak absorption bands at 290-450 nm and strong phosphorescence at 570 nm with excitation at 360 nm. The affinity of the complex with simple anions such as $CH_3CO_2^-$, $H_2PO_4^-$, F^-, Cl^-, Br^-, and I^- and chiral amino acid derivatives were investigated. Addition of F^-, $CH_3CO_2^-$ and $H_2PO_4^-$ was found to cause phosphorescence enhancement. When the tetrabutylammonium salts of N-t-Boc-a-amino acids were added, the (L)-enantiomers were found to show greater phosphorescence enhancement than the (D)-enantiomers. In the case of tetrabutylammonium salt of N-t-Boc-valine, the association constant ratio (KL/KD) was 2.68.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-909**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Potassium Aryltrifluoroborates를 이용한 항암활성 천연물의 Naturomimetic Approach Method 개발연구

김태정 Tetsuhiro Ogura[1] Toyonobu Usuki[1] 함정엽

KIST 천연의약센터 [1]Department of Materials and Life Sciences, Sophia University, Japan

최근 자연계에서 발견된 천연물이 인간에게 유용한 생리학적 활성을 나타내어 신약 또는 그의 Lead Compound 로 이어지는 경우를 흔히 볼 수 있다. 그 예로 주목나무의 Taxol, 빙카의 Vincristine, 아편의 Morpine, Codeine 과 같은 천연물 및 그 유도체는 시중에서 항암제, 진통제등으로 널리 이용되고 있다. 특히, 이러한 천연물은 유기합성을 통한 화합물에 비해 독성에 대한 우려가 적어, 신약개발분야에서 크게 주목 받고 있으며 국내뿐만 아니라 전세계적으로 천연물을 이용한 신약개발의 비중은 크게 증가하는 추세에 있다. 이에 본 연구팀은 자연에서 발견된 유용한 생리활성을 가지는 천연물을 시작으로 활성을 나타내는 Pharmacophore (약물특이분자단)의 합성과 더불어 다양한 유도체 합성을 통한 신약개발에 주력하고 있다. 또한 보다 효과적인 천연물의 유도체화 연구를 위해 본 연구팀에서 고안한 Naturomimetic Approach 개념을 도입하여 생리활성 천연물의 활성을 나타내는 Pharmacophore 에 해당하는 모체를 합성한 후, 전이 금속을 이용한 C-C, C-N 등의 결합반응을 통해 효율적인 유도체화 연구를 진행 중에 있다. 본 포스터 발표에서는 Naturomimetic Approach 의 개념과 함께 이를 통해 얻어낸 현재까지의 연구결과를 보고하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-910**

발표분야: 유기화학

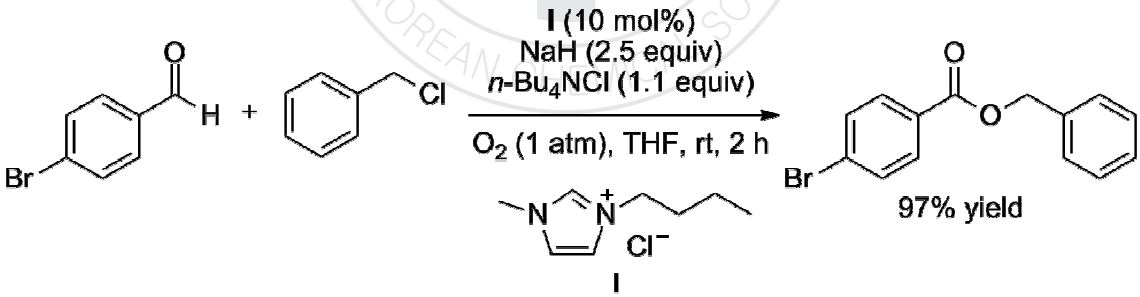
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Esters through a Benzoin Condensation-Oxidative Cleavage-Esterification Triple Cascade Reaction

김미진 김선민[1] 김영석[1] 김동완[1] 양정운[1]

성균관대 화학과 [1]성균관대 에너지과학과

Oxidative esterification of aldehydes with alkyl halides in the presence of catalytic amount of N-heterocyclic carbene catalyst and stoichiometric amount of quaternary ammonium salt as phase-transfer reagent under NaH-O2 system provided moderate to good yields of the corresponding esters. The current oxidative esterification reaction consists of three steps (self-benzoin formation, oxidative cleavage, and esterification) performed in a one-pot manner.



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장소: 부산BEXCO

발표코드: **ORGN.P-911**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Potassium Haloaryltrifluoroborate류의 역결합반응 개발연구

정규혁 김희진[1] 함정엽[1]

강릉원주대 화학신소재학과 [1]KIST 천연의약센터

Potassium organotrifluoroborate (R-BF_3K)류는 일반적으로 Palladium, Nickel, Rhodium, Coppor 등의 금속촉매를 이용하여 탄소-탄소 또는 탄소-헤테로원자 교차반응을 일으키는 것이 알려져 있으며 의약품, 유기 EL, 태양전지 등 다분야에 걸쳐 널리 이용되어 왔다. 본 연구 그룹에서는 R-BF_3K 류가 선택적 조건에 따라 금속촉매에 대해 불활성한 성질을 나타내는 것을 밝혀내었으며, 할로겐원자와 공존하는 출발물질을 이용하여 할로겐원자만을 선택적으로 반응시키는 역결합반응을 연구하여 왔다. 그 예로 아지도화 반응을 통한 Azidoaryltrifluoroboraste 류의 합성, Sonogashira 반응을 통한 Alkynylaryltrifluoroborate 류의 합성, One-pot 1,3-Dipolar Cycloaddition 을 통한 1,2,3-Triazoletrifluoroborate 류의 합성을 통해 지금까지는 구입할 수 없거나 제조에 수 차례의 공정이 필요한 다양하고 복잡한 R-BF_3K 류를 제조하는 연구 결과를 다수 발표하였다.본 포스터에서는 최근 진행중인 금속촉매 하에서의 Potassium Haloaryltrifluoroborate 류의 역결합반응을 통해 유용하고 새로운 R-BF_3K 류의 합성법 개발연구에 대해 발표하고자 한다.

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발표코드: **ORGN.P-912**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Benzoylacetonitriles by Palladium-Catalyzed Carbonylation with $Mo(CO)_6$

표아영 변아름 이선우

전남대 화학과

Benzoylacetonitriles were synthesized by the palladium-catalyzed carbonylation of aryl iodides and trimethylsilylacetonitirle using $Mo(Co)_6$ as a carbon monoxide source. $Pd(PPh_3)Cl_2$ and CuF_2 were employed as the catalyst and activator, respectively. A variety of aryl iodides bearing alkyl, alkoxy, fluoro, chloro, bromo, nitrile, ester, and ketone groups afforded the corresponding benzoylacetonitriles in moderate to good yields.

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발표코드: **ORGN.P-913**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium hydroxysalen-catalyzed coupling reaction of arylboronic acids: Mizoroki-Heck type reaction and decarboxylative couplings

허유미 장화연[1] 이준승 이선우

전남대 화학과 [1]전남대 화학과, 전남대 화순병원

(Salen-OH)Pd (1, salen-OH=N,N'-bis(3,5-di-hydroxysalicylidene)-ethylenediamine) was prepared by a simple one step reaction and fully characterized by 1H and 13C NMR, IR spectroscopy, and X-ray crystallography. This palladium complex showed good activities as a catalyst in the Mizoroki-Heck type reaction and the decarboxylative coupling reaction. In the Mizoroki-Heck type reaction, arylboronic acids and alkenes were reacted at 90℃ for 3 h in the presence of 2.0 mol% of the palladium complex 1 and AgOAc to give the desired coupled product in good yields. In the decarboxylative coupling reactions, the desired coupled products were obtained in good yields when 0.5 mol% of the palladium complex was employed at room temperature.

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발표코드: **ORGN.P-914**

발표분야: 유기화학

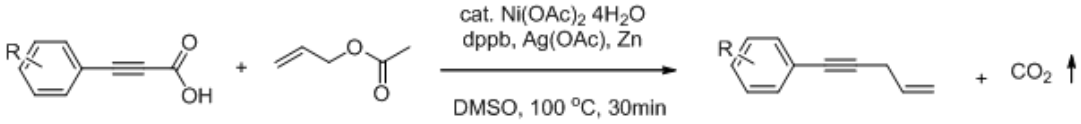
발표종류: 포스터, 발표일시: 수 16:00~19:00

Nickel-Catalyzed Decarboxylative Coupling of Alkynyl carboxylic acids and Allyl acetates

최주석 김원영 이선우

전남대 화학과

Aryl propiolic acids were coupled with allyl acetates using nickel catalyst. We need 10 mol% of cat. Nickel, 10 mol% of silver acetate, and 1 equivalent of zinc powder. We can get products in high yields about most of each reaction. Especially, in case of addition of DBU without Zn powder with same reaction, it was confirmed not alkyl compounds but allene compounds.



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장소: 부산BEXCO

발표코드: **ORGN.P-915**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

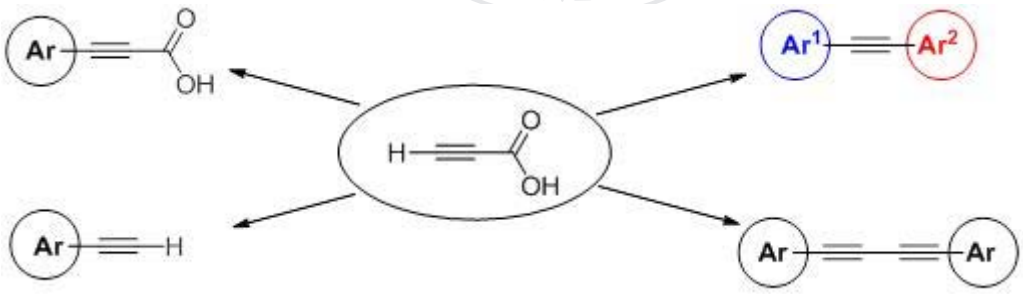
Synthesis of Alkyne Moieties from Propiolic Acid Using Palladium catalyst

박경호 Thiruvengadam Palani manian rajesh kumar 이선우

전남대 화학과

한국화학회 THE KOREAN CHEMICAL SOCIETY

The triple bond of the two carbon is a functional unit often used within synthesis of natural products, pharmaceutical molecules, agrochemicals, the materials encountered conjugated π systems. In this reason, efficient methods for introduction of the alkyne moieties at the target molecules was the one of the hot topics in the synthetic methodologies. Palladium catalyzed coupling reaction of terminal alkynes with aryl halides powerful method for the introduction of the triple bond at aromatic compounds as radily available starting materials. This poster illustrated the method of alkyne moieties from propiolic acid by palladium catalyzed Sonogashira reaction.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-916**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Low Band Gap Planar Polymers based on Naphtho-dithiophenes

강성범

성균관대 화학과

Polymers with planar molecular structures have advantages of rigidity, low band gap, and better chain packing and so on. π-Conjugated and planar polymers are used in bulk-hetero junction solar cells due to facilitated charge carrier transport. We designed naphtho[2,1-b:3,4-b']dithiophene containing a bithienylethene (BTE) moiety. Functionalized BTEs are expected to show photo-responsive properties and packed helical structures. We synthesized monomers using double Suzuki cross couplings and corresponding polymers via electropolymerization. We investigated electrochemical properties of naphto-dithiophene polymers by cyclic voltammetry and spectroelectrochemistry, including photoresponsive properties.

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발표코드: **ORGN.P-917**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Binaphthyl Hinge-Containing Conductive Polymers: Substituent Effects

정동철

성균관대 화학과

Controlling molecular shape and flexibility of conductive polymers is important for designing sensory and stimuli-responsive materials. We report the synthesis of conductive polymers with a hinged molecule 1,1'-binaphthyl. Conformational flexibility around the 1,1' C-C bond was varied with the substituents at the 2,2'-positions: hydroxy, linear alkyl oxy, and macrocyclic alkyl oxy groups. Especially macrocyclic alkyl oxy groups appeared to render the binaphthyl shape-persistent. In addition, the connection patterns of electroactive oligothiophenes to binaphthyls were investigated with 6,6'- and 7,7'-attachments. Electrochemical properties of binaphthyl polymers with varied substituents were examined using cyclic voltammetry, in situ conductivity measurements, and spectroelectrochemistry. We found that the kind of substituents and their connectivity greatly affect the electrochemical properties of conductive polymers. Binaphthyl polymer with hydroxyls and 3,4-ethylenedioxythiophenes exhibited an interesting charge-trapping property. 7,7'-Substitution appeared to give rise to an intra-chain interaction, and linear alkyl chains seemed to promote inter-chain interactions. We believe that the above properties can be applied in developing binaphthyl hinge-containing conductive polymers for use in chiral electroactive sensors, polymer actuators, electrochromic or optoelectronic devices.

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발표분야: 유기화학

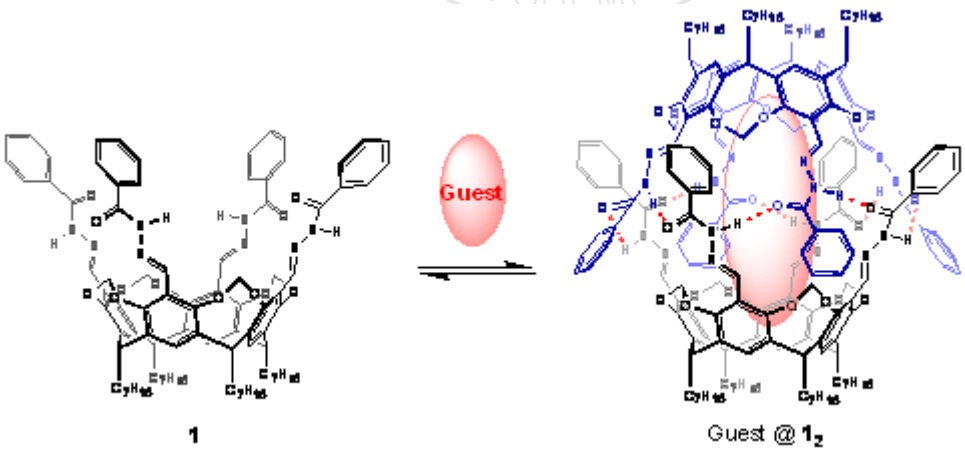
발표종류: 포스터, 발표일시: 수 16:00~19:00

Guest encapsulation of molecular capsule based on tetraamidocavitand

박주완 김가영 박연실 백경수

숭실대 화학과

Self-assembling molecular capsules based on noncovalent interactions have attracted considerable interest due to their potential as molecular storage, sensor, catalysts, or reaction chambers in the field of supramolecular chemistry. Imino-cavitand 1 having four benzamide moieties self-assembles into molecular capsule 1_2 through the eight intermolecular amide N-H···O=C hydrogen bonds when suitable guests are present in the noncompeting solvent. Molecular capsule 1_2 encapsulates neutral molecules such as toluene, p-xylene, 4-iodotoluene, adamantane, or heptanes to form complexes G@1_2 which are highly stable thermodynamically and kinetically. The properties of molecular capsule 1_2 were studied by ^{1}H, 2D EXSY, 2D-DOSY NMR, and crystal structure analyses.



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발표코드: **ORGN.P-919**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembled Barrier Materials for Phosphoric Acid Poisoning of Pt in HT-PEMFC

이혜경

성균관대 화학과

High temperature-proton exchange membrane fuel cell (HT-PEMFC) is an environmentally friendly energy source and has various advantages such as large current density, tolerance to impurities in hydrogen gas and carbon monoxide gas, absence of humidification and etc. In phosphoric acid-doped polybenzimidazole membrane systems, phosphoric acid poisoning is one of the factors that degrade the Pt catalytic activity. Barrier materials which can block the access of phosphoric anion were introduced to prevent phosphoric acid poisoning of Pt. Smaller oxygen is easy to pass through the barrier molecules, so that it can react on Pt surface, but bigger phosphoric anions are blocked by the barrier before they reach on the Pt. Here in, we focused on the synthesis of barrier materials based on a binaphthyl moiety and confirmed that the resistance to phosphoric acid poisoning of Pt catalyst increase. The increased resistance to the poisoning was further analyzed in terms of alkyl chain length, binding strength and structural rigidity.

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

Synthesis of Glycoconjugates having Bioactivities

정지은 신인재

연세대 화학과

Carbohydrates have various functions like energy source and composition of cell scaffold. Carbohydrates are found on the cell surface and interior of the cell. Most Carbohydrates are existed in the form of glycoconjugates, proteoglycans, glycosphingolipids. Recently, importance of carbohydrates related with biological functions becomes known. Nowadays, the carbohydrate field has achieved a series of significant advances. Carbohydrates have been known to play biologically important roles such as cell adhesion, cell recognition, fertilization, embryogenesis, immune through the interaction with proteins. Also, interactions between carbohydrates and proteins cause metastasis of tumor cells, infections caused by bacteria or viruses, etc. In this study, carbohydrates related with Helicobacter pylori and cell recognition were synthesized. At first, the oligosaccharide using detection of H. pylori which is well known as gastric pathogen causes chronic inflammation, stomach ulcer and gastric cancer and so on. Developing another way to detect H. pylori have become important to human health. On the surface of H. pylori exist two proteins are BabA and SabA which interact with glycoconjuagates on stomach wall. In this research, sialyl Lewis X was synthesized for study about the interactions between the SabA. Also Lewis X and Lewis Y are synthesized to study about the interactions between carbohydrates. These interactions are related to cell recognition and adhesion.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 3-amino-1-quinoxalin-2 (1H)-one library: A preliminary solution-phase test

이상협 RAMACHANDRAN[1]

대구가톨릭대 생명화학과 [1]대구가톨릭대 화학과

Combinatorial solid-phase organic synthesis (SPOS) provides the main driving force for the preparation of small organic molecules libraries for application in lead discovery and high-throughput medicinal chemistry research within the pharmaceutical industry. Our research program has focused on the application of polymer-bound α-diazo-β-ketoesters as key building blocks for the diversity-oriented synthesis of a series of a nitrogen-containing heterocyclic compound libraries, including oxazoles, indoles, imidazolones, pyrazines and pyrazines, etc.In continuation of this work, we are developing the solution and solid-phase synthesis of 3-amino-1-quinoxalin-2 (1H)-one library by using ethyl 2-chloro-2-oxoacetate as a key building block. Quinoxaline derivatives exhibit a wide range of biological functions including various antibiotics such as Echinomycin, Levomycin and Actinoleutin that are known to inhibit growth of gram positive bacteria and are active against various transplantable tumours. Initially, ethyl 2-(2-azidophenylamino)-2-oxoacetate, which was previously obtained from the coupling reaction between ethyl 2-chloro-2-oxoacetate and azidoaniline was subjected to N-alkylation with various alkylating agents in presence of LiHMDS.Then, these alkylated products were cyclized by the treatment of TPP to yield corresponding 3-amino-1-quinoxalin-2 (1H)-ones via Staudinger reaction followed by aza-Wittig reaction, which can be finally derivatized by Lewis acid mediated smart cleavage.

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발표코드: **ORGN.P-922**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Galectin inhibitor using carbohydrate derivatives library

권다은 신인재

연세대 화학과

Galectins are a family of soluble lectins that bind β-galactoside-binding containing glycans, until now, were discovered 15 kinds. Natural small saccharides such as β-galactose, D-lactose and N-acetyllactosamine bind to galectins and can inhibit their biological activity. But natural ligands are difficult to synthesize since they are sensitive to hydrolysis and generally too polar to be used as drugs.N-acetyllactosamine is the most effective natural ligand for galectin-3, but it showed low inhibition potency. So we will synthesis development of new inhibitors with higher affinity for galectin-3, modification of N-acetyllactosamine galactose 3-OH position. After making carbohydrate chips by synthetic LacNAc derivatives library, we will find new inhibitors of galectin-3 in a close relationship development of anti-anti inflammatory and anticancer drug. If we find galectin inhibitor using carbohydrate chips in this study, carbohydrate chips are an important means of excavation disease-related inhibitors and lectins.

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

Total solid phase synthesis of an amide analogue of Coibamide A

임동렬 박재관 Ganesh Sable

세종대 화학과

Coibamide A is a cyclic depsipeptide isolated from marine filamentous cyanobacterium Leptolyngbya sp.Synthesis of amide analougues of Coibamide A included key changes such as N-Me-Threonine to Diamino propionic acid and Hydroxy Valeric acid to Valine. The strategy comprises resin attachment of the first amino acid via the side chain free hydroxyl handle of Tyrosine residue, stepwise solid phase synthesis of the linear peptide analogue, and cyclization. followed by N,N-dimethylation. After resin cleavage, O-methylation on the side chain of tyrosine residue was performed to yield desired product.All couplings were monitored by RP-HPLC and LC-MS analysis and final two compounds have been characterized by 2D- NMR.

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장소: 부산BEXCO

발표코드: **ORGN.P-924**

발표분야: 유기화학

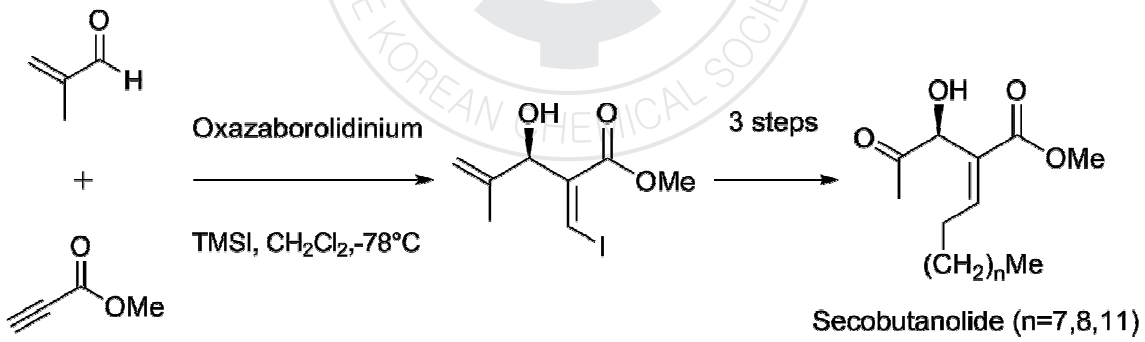
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric total synthesis of cytotoxic secobutanolides

남동국 정현실

성균관대 화학과

A stereoselective synthesis of (Z, R)-β-iodo Morita-Baylis-Hillman ester has been developed through a three-component coupling reaction using oxazaborolidinium catalyst and TMS-I. Iodine catalyzed photo reaction provided a geometric isomer, (E, R)-β-iodo Morita-Baylis-Hillman ester without racemization. The syntheses of cytotoxic secobutanolides; secoisolancifolid (n =7), secoaggregatalactone (n=8), secosubamolide (n=11) were accomplished after organocuprate coupling reaction and ozonolysis.



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장소: 부산BEXCO

발표코드: **ORGN.P-925**

발표분야: 유기화학

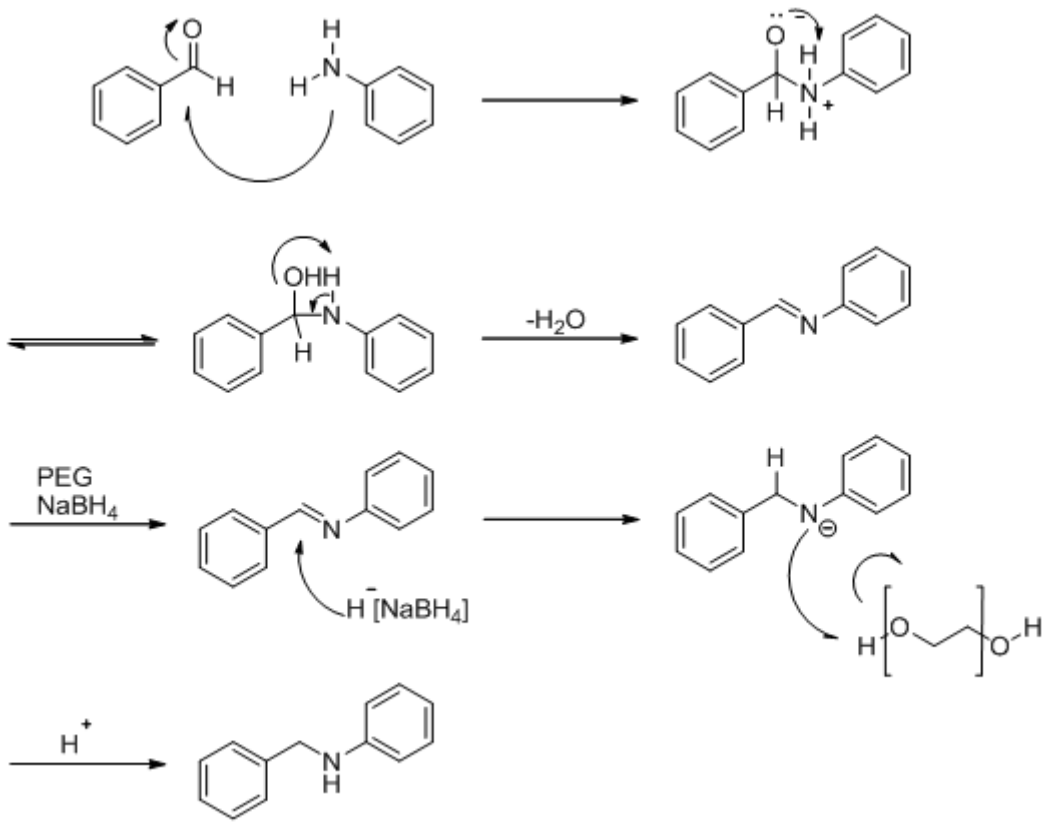
발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct reductive amination of aldehydes and ketones with sodium borohydride and polyethyleneglycol 200under solvent-free conditions

이란 이종찬

중앙대 화학과

In biological and chemical systems, direct and indirect reductive amination of aldehydes and ketones is an important transformation, which allows the direct conversion of carbonyl compounds into amines using simple operations. We will describe the procedure for the preparation of amines from aldehydes and ketones with sodium borohydride and polyethyleneglycol (PEG) 200 under solvent-free conditions. A variety of aromatic aldehydes, ketones and amines when mixed with NaBH4/ PEG 200 at room temperature for 5 minutes, afforded excellent yield of the corresponding amines.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-926**

발표분야: 유기화학

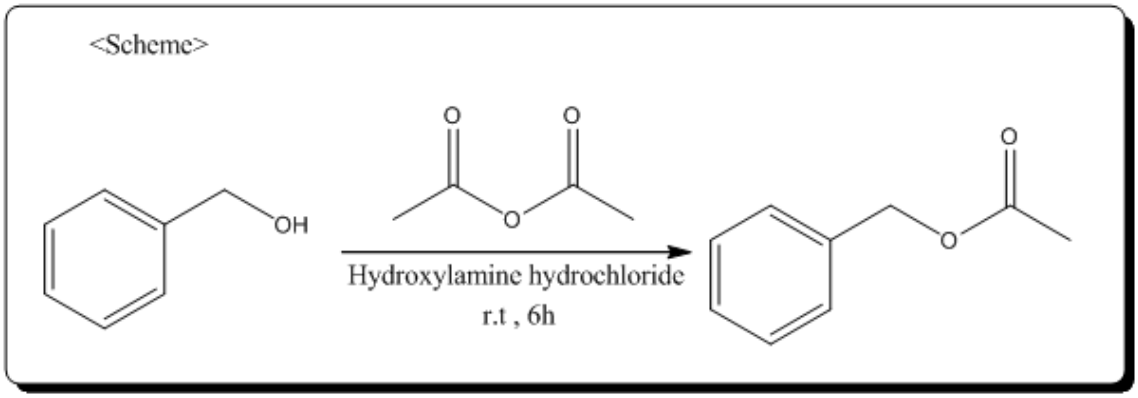
발표종류: 포스터, 발표일시: 수 16:00~19:00

Mild and simple method for acetylation of alcohols, phenols and amines with acetic anhydride using hydroxylamine hydrochloride.

이승배 이종찬

중앙대 화학과

Hydroxyl groups are present in number of compounds of biological and synthetic interest, including nucleosides, carbohydrates, steroids, macrolides. During various reactions of these compounds, protecting hydroxyl groups is often necessary. In the present work, we have developed a mild, simple and efficient method for versatile acetylation of alcohols, phenols and amines with acetic anhydride using hydroxylamine hydrochloride at room temperature.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-927**

발표분야: 유기화학

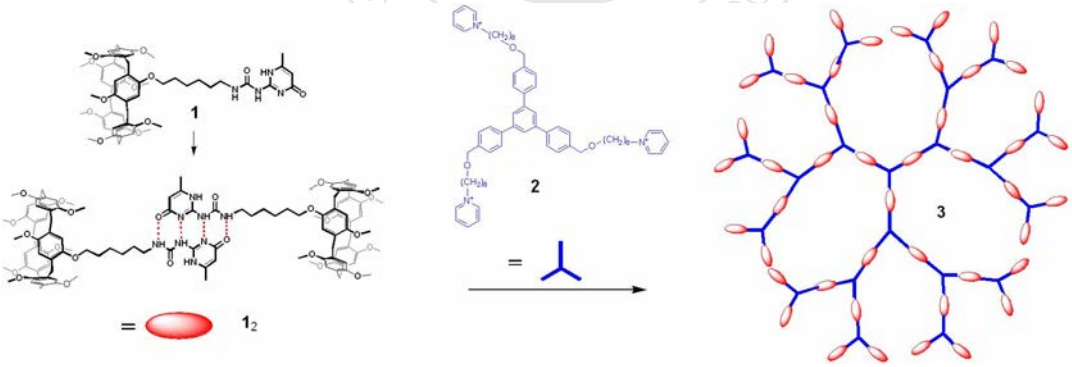
발표종류: 포스터, 발표일시: 수 16:00~19:00

Applications of copillar[5]arene with ureidopyrimidone unit

황성민 이서현 박연실 백경수

숭실대 화학과

Dendrimers which are polymeric architectures possessing generations of branches emanating from a central core have been received considerable attentions in the past decade due to their unique properties such as catalytic, optical, magnetic, biomedical and electrical properties. The copillar[5]arene 1 mono-substituted with ureido-4[1H]-pyrimidone forms a stable dimer 1_2 by quadruple hydrogen bonding, and the dimer 1_2 was applied to form a self-assembled supramolecular dendrimer 3 through cation-π interactions with a tri-cationic core guest 2. Their synthesis and characteristics will be presented.



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장소: 부산BEXCO

발표코드: **ORGN.P-928**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study on trehalose based macromolecules with potential application in pharmaceutical field

Ashrafuzzaman MD 표정인[1] 정찬성[2]

과학기술연합대학원대 Green Chem. & Env.BT [1]연세대 화학과 [2]KIST 화학키노믹스연구센터

The use of trehalose based molecules has created tremendous impact in cryobiology, biomedical and pharmaceutical fields during the past decades. Trehalose has been applied as a cryopreservation agent to a variety of biologicals, including mammalian cells, various tissue, proteins, viruses, bacteria, and yeasts. Trehalose based polymers can be applied in drug delivery systems, as scaffolds for tissue engineering, repair and gene delivery. These applications have led to an increasing demand of well-defined trehalose macromolecules and polymers as novel biomaterials. We have synthesized trehalose-sucrose combined molecules with enzymatic process using divinyladipic esters. We found superior enzyme during screening among several enzymes and have immobilized this enzyme using Sol-Gel methods. Trehalose-sucrose molecules used for further modification by polymerization and tested for cryobiology evaluation. Such modifications of trehalose based molecules are of significance in the development of new functional materials in the biomedical and pharmaceutical field with potential application.

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발표코드: **ORGN.P-929**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence PET sensor for the detection of water content in organic solvent

김강현 김대영 김형진

전남대 응용화학공학부, 기능성나노신화학소재 사업단

Water in organic solvents is considered as impurity. Measurement of water in organic solvents is therefore an important technology in various scientific and industrial fields. Many fluorescent water sensors show that the fluorescence intensities decrease with an increase of water content in organic solvents, and the water detection ranges are narrow. In this study, in order to find a fluorescence-based chemosensor for detecting the wide range of moisture content in polar organic solvents, we designed and synthesized new photo-induced electron transfer (PET) fluorescence protocols possessing a 1,8-naphthalimide group as a fluorophore linked with proton-donating and proton-binding sites within the molecular framework. Emission properties have been investigated in various water-miscible organic solvents such as methanol, ethanol, acetone, acetonitrile, and dimeyhylformamide. The fluorescence intensities of these dyes were significantly increased with increasing the wide range of water in common polar organic solvents. Synthesis, detection limits and detection ranges for the new fluorescent PET water sensors will be presented.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent and colorimetric ICT chemosensors for pH detection in highly acidic media

김대영 김강현 김형진

전남대 응용화학공학부, 기능성나노신화학소재 사업단

Not much is known fluorescent pH sensors that operate at low pH values. In this study, we synthesized new push-pull (D-π-A) conjugated pyran derivatives possessing an aniline moiety as a proton acceptor, and investigated their absorption and emission properties responding to pH changes in solution. In acidic condition below pH 3, there were remarkable changes in fluorescence intensities of the dyes. They also exhibited reversible color changes between pH 1 and 3; large red-shifts (ca. 66 nm) were observed in absorption with the pH increase, which is attributed to an internal charge transfer (ICT). We will present the structures of the dyes and the sensing properties as pH indicator in the pH range 1-3.

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발표코드: **ORGN.P-931**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Polyimide-siloxane copolymer

황남익 타쿠오 와타나베[1] 윤호규[2]

고려대/도레이첨단소재(주) 연구소 [1]도레이 연구소 [2]고려대 그린스쿨대학원

Polyimides have recently been applied to a variety of industries due to their superior thermal stability.In adhesive industry, Many researchers have used polyimide with low glass transition temperature(Tg) to improve a processability of polyimide.We have conducted a copolymerization of polyimide and siloxane content for this improvement. And we have investigated the change of Tg and characteristic of polyimide-siloxane copolymer as siloxane content and processing condition.In this investigation, We have found that Tg's behavior of polyimide-siloxane copolymer is decreased with increase of siloxane content for various polyimide system.We have investigated adhesion characteristic and Tg's behavior as heat treatment conditions.

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발표코드: **ORGN.P-932**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a "convergent" synthetic strategy to prepare nonactic acids.

이재은 김현석 송운영 김학중

고려대 화학과

Nonactic acids are structural components of a natural product, nonactin, and have been of great interest in organic synthesis community due to their intriguing structures featured by densely populated stereogenic centers within a compact architecture as well as the presence of 2,5-cis-tetrahydrofuran motif, frequently found in polyketide-type natural products. Thus far, there have been more than fifty publications regarding their syntheses. Yet, almost all syntheses are relying on the "linear" synthetic sequences and, therefore, they are presumably ineffective in generating a library of structurally diversified nonactic acid analogues. As an effort to overcome such limitation, we report our progress on the development of a "convergent" synthetic strategy to prepare nonactic acids, based on the triple tandem reaction sequence involving metathesis, substitution, and hydrogenation. The established methodology is anticipated to enable the expedited generation of nonactic acid analogues and, thereby, to contribute our future studies on the mechanistic investigation of the nonactin biosynthesis as well as discovery of novel nonactin derivatives with improved activity.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation, photochromic reaction, solvatochromic study of Spiropyran-PAMAM

신은주 허대영

순천대 화학과

Dendrimers have attracted much attention because of their fascinating structure and unique properties. They show the most appealing characteristics such as globular macrocyclic architecture, size monodisperse, peripheral functional density, ample interior voids, and amphiphilicity, thermal stability, flexibility, high biocompatability, and low viscosity, pH-dependent contraction and swelling. Thus, dendrimers have inspired active research activities in material science, nanoreactors, sensors, biomaterials, green catalyst supports, and drug delibery systems.On the other hand, spiropyran(SP) is well-known photochromic compound that have been studied widely for application in optical memory and switch. Colorless SP can be photochemically transformed by UV irradiation into colored merocyanine(MC), and then the colored form MC returns to the colorless form SP by ring closure thermally or on irradiation of visible light.Incorporating a photochromic molecule into dendrimer could lead to a variety of photoresponsive systems, the properties of which can be manipulated by light. In this study, SP-PAMAM consisting of SP and PAMAM dendron was prepared and reversible photochromic reaction and solvatochromic behavior in a variety of solvents was investigated using absorption spectroscopy.

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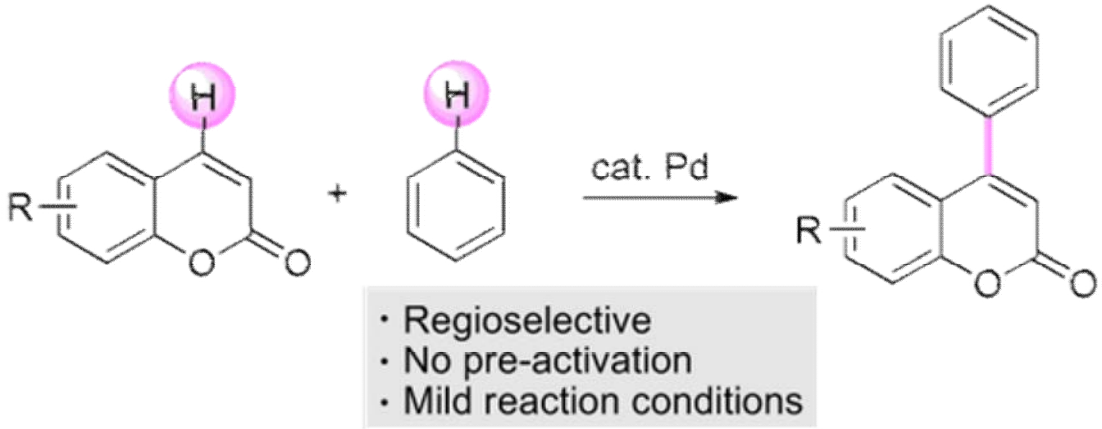
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Synthesis of Biologically Active Chromenone Derivatives via Pd-Catalyzed Twofold C-H Functionalization

민민식 홍승우[1]

KAIST(KAIST) 화학과 [1]KAIST 화학과

Chromenone derivatives such as flavones and neoflavones constitute a major class of naturally occurring compounds and privileged medicinal scaffolds that exhibit a broad range of biological and pharmaceutical properties, including anti-HIV, anti-tumor, anti-hypertension, anti-arrhythmia, anti-inflammatory, anti-osteoporosis, antiseptic, analgesic and anti-coagulant activities. Although many strategies for the synthesis of the flavones and neoflavones have been developed, the scope of such condensation reactions has been somewhat limited due to the harsh conditions, multistep synthesis, poor substituent tolerance, or low chemical yield, and therefore, the synthesis of some derivatives continues to pose a challenge. Herein, we report the general and atom-economical synthesis of chromenone derivatives for the efficient identification of biologically active compounds.



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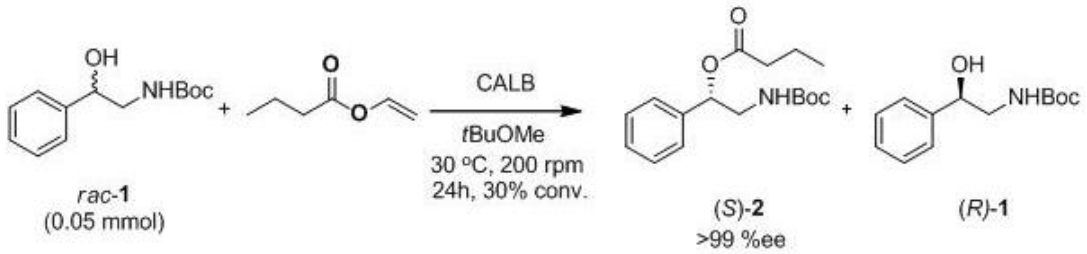
장소: 부산BEXCO
발표코드: **ORGN.P-935**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Kinetic Resolution of Aminoalcohols by Lipase-catalyzed enantioselective transesterification

박아름 민보라[1] 손훈영[2] 이혁[3]

과학기술연합대학원대 의약 및 약품화학 [1]성균관대 화학과 [2]한국화학연구원 의약화학/성인병 치료제 [3]한국화학연구원 의약화학 연구 센터

Enzymatic kinetic resolution of racemic alcohols via transestericifation has been broadly studied as one of the most effective methods for the preparation of optically active alcohols. Candida Antarctica lipase (CALB) has been widely used for enantioselective kinetic resolutions of secondary alcohols. Since the reaction pocket in CALB has been known relatively narrow for substrates, the scope of secondary alcohols is limited. Recently we have investigated the kinetic resolution of amino alcohol moieties. Among them, enantioselective transesterification of tert-butyl(2-hydroxy-2-phenylethyl)carbonate was screened by diverse enzymes. Themomyces lanuginosa lipase with a large reaction pocket showed the best activity with high enantioselectivity. In addition, CALB also exhibited high enantioselectivity for this screening, although the reaction rate was slow. This result is noteworthy because the width of reaction pocket in CALB is not sufficient for this substrate by computational calculation. We will discuss the further experiment of this phenomenon.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-936**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Spectroscopic Properties of Rhodamine-Spiropyran Dyad

신은주 하종운

순천대 화학과

Artificial sensors for sensing and recognition of various metal ions have received considerable attention. Especially, the design and synthesis for colorimetric and fluorimetric detection of metal ions is a challenge to many chemists. Nonpolar, colorless, UV-absorbing spiropyran(SP) is well-known photochromic compound accomplishing reversible molecular structural changes to polar, colored, VIS-absorbing merocyanine(MC). SP carries out the photochemical ring opening on UV irradiation, and in turn, MC is reversed to SP by ring closure thermally or on irradiation of visible light. Reversible photochromic SP-MC interconversion is one of subjects of active research on molecular switch, on the basis of significant difference in color and polarity between two forms. Spiropyran itself is chemosensor for CN- anion. Rhodamine(Rh)-based chemosensors have been extensively studied because of their vivid color change enabling detection with the naked eye and a turn-on fluorescence changeIncorporating SP into Rh might should lead to excellent light-controlled ion sensing system. In this study, SP-Rh dyad, a rhodamine derivative with spiropyran unit, was prepared and their spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

3D Molecular Architectures by the Self-Assembly of α/β-Peptide Foldamer

엄재훈 이양호[1] 이희승

KAIST 화학과 [1]KAIST(KAIST) 화학과

The self-assembly of peptide-based building blocks into nano/microstructures is an attractive method for the preparation of materials for biological applications. Various types of self-assembled nano/microstructures by natural or synthetic building blocks have been reported. However, the morphologies are limited to simple shapes such as spheres, tubes, and rods. Recently our group reported unprecedented 3D molecular architectures having shapes of a windmill, rod, and molar tooth by the self-assembly of 12-helical β-peptide. In this presentation, we report another example of highly sophisticated and homogeneous 3D molecular architectures by the self-assembly of α/β-peptide foldamer which is an artificial oligomer that adopts stable 11-helical secondary structure in solution. The 3D shapes of polyhedral structures could be easily controlled by simple experimental process.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Synthesis of alpha-Alkyl-beta-keto Esters: Asymmetric Roskamp Reaction Catalyzed by Oxazaborolidinium Ion

강병철 gaolizhu[1]

성균관대 화학 [1]성균관대 화학과

We have developed a novel, catalytic asymmetric Roskamp reaction of alpha-alkyl diazoesters with both aromatic and aliphatic aldehydes, which produces alpha-alkyl-beta-keto esters in high yields and excellent enantioselectivities. The absolute configuration of the major reaction product was the same as predicted by the transition-state model. This methodology was successfully applied to a concise two-step synthesis of sitophilate.

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

Thermally Reversible Property of Thermoresponsive Polydiacetylenes

이민지 이송이 이재연[1] 김명화[2] 윤주영[3]

이화여대 바이오융합과학과 [1]이화여대 화학·나노과학과 [2]이화여대 화학 나노과학과 [3]이화여대 화학-나노과학과

Fluorescent and colorimetric sensors are powerful tools to monitor biologically relevant and environmentally important species due to simplicity and high sensitivity. Among them, conjugated polymers based chemosensors appear to be particularly attractive due to their unique changes in absorption, emission, and redox properties are sensitive with environmental perturbations. Polydiacetylenes (PDAs), a family of conjugated polymers, are a colorimetric polymer owing to a brilliant blue-to-red color transition that takes place in response to environmental perturbations. Also, it already has been known that “blue-phase” PDAs are nonfluorescent while their “red-phase” counterparts fluorescence. Owing to the color (blue-to-red) and fluorescence (non-to-fluorescent) changes, PDAs are an ideal choice for use as a chemosensor. The stimulus-induced apparent blue-to-red transition of the PDAs has led to the development of a variety of PDA-based chemosensors for temperature, Pb^{2+}, Zn^{2+}, K^{+}, Hg^{2+}, Cu^{2+}, cationic and anionic surfactants, ATP/pyrophosphate, toxin/bacteria, melamine, fatty acids, etc. Thermochromism is also one of the beneficial properties of PDAs. Thermochromic reversibility of PDA material has been achieved by increasing the attractive intramolecular interaction among their side-chains. In this work, we synthesized the thermoresponsive polydiacetylenes. And this new polymer displays colorimetric reversibility in some range of the temperature.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel spin-bearing π-conjugated organogel for exploring spintronic responses

남해림 권지언 박수영

서울대 재료공학부

Spintronics, which utilizes not only the charge but also the spin of an electron, has received much attention because of its potential applications in next-generation electronics systems. So far materials studied for spintronics have been dominated by conventional metallic/inorganic compounds and semiconductors. However, recent studies have found that the excited states and charge transport experience significant spin interactions in organic functional materials. Our research objective is exploring novel spintronic responses from advanced functional organic materials comprising π-conjugated molecular framework with spin-radical moieties to give a variety of optoelectronic properties. To this end, we synthesized novel π-conjugated torsion spring molecules, CN-TFFP and IN-CN-TFFP, intramolecularly bearing spin-polarizable radicals, nitronyl nitroxide and imino nitroxide, respectively. The nitroxide molecules were ESR-active and formed organic gels in organic solvents.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Multicolor Tunable Fluorescence Emission from Energy Transfer-Free Organic Nanoparticles

권지언 박수영

서울대 재료공학부

During the past decades, fluorescent nanoparticles have received considerable attention in biological imaging applications. Multicolor Tunable fluorescent nanoparticles are more attractive because they can decipher multiple biological events simultaneously. Here, we report a set of three primary color-emitting amphiphilic molecules that form self-assembled nanoparticles in water with excited-state intramolecular proton transfer (ESIPT). The whole range of emission colors enclosed within the color triangle is conveniently reproducible from mixed assemblies containing two or more different amphiphiles based on additive color theory due to the absence of energy transfer between dyes.

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발표분야: 유기화학

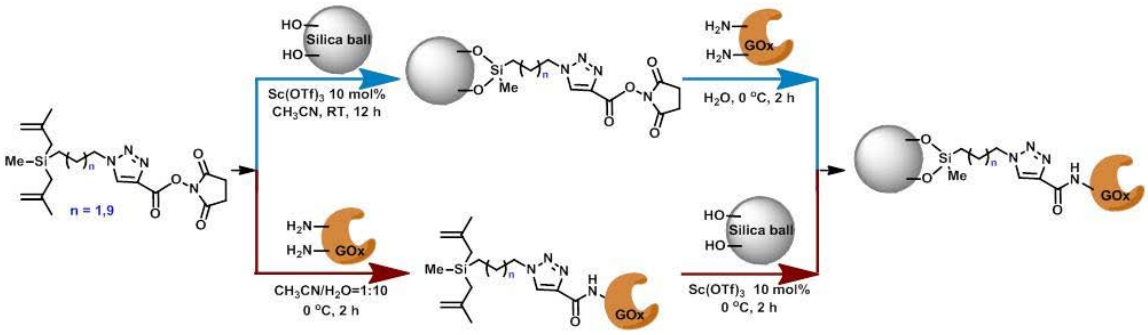
발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Immobilization of GOx onto Silica Surface by Chemical Modification Method.

김보형 심용균 전철호

연세대 화학과

Recently we successfully developed catalytic grafting method for immobilizing organic functional group onto solid surface using organomethallylsilane derivatives. Among various organic molecules for immobilization, Glucose Oxidase (GOx) can be readily immobilized onto silica surface under very mild conditions by this grafting method. However, this grafting method requires a large quantity of NHS-ester functionalized methallylsilane precursors. To reduce the amount of NHS-ester functionalized methallylsilane, we newly developed chemical modification method. To do this, amine of a lysine residue in GOx is chemically modified with NHS-ester functional group by reacting with NHS-ester functionalized methallylsilane. And then unreacted excess NHS-ester functionalized methallylsilane is removed by addition of amino group immobilized silica. After the chemically modified GOx is purified by this protocol, GOx is immobilized onto silica surface by addition of $Sc(OTf)_3$ catalyst at room temperature. As a result, we developed new immobilization method of GOx onto silica surface with high-efficiency.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-943**

발표분야: 유기화학

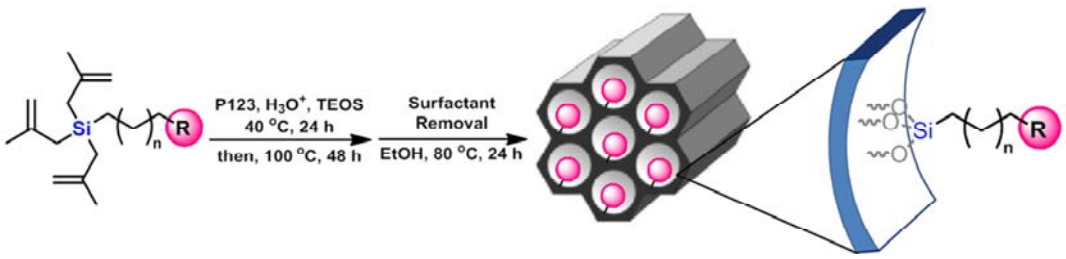
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Functional Group Modified SBA-15 Mesoporous Material Using Methallylsilane Derivatives

한예리 김한일 전철호

연세대 화학과

SBA-15 mesostructure containing various functional groups has been synthesized by one step co-condensation method. In this reaction methallylsilane derivatives are used as a substitute of alkoxysilane because of the stability. The stable methallylsilane having various functional group such as azido- and pyrenyl, amino groups has a merit to be purified by column chromatography. Methallylsilane derivatives and TEOS are used as co-condensation reagents to form a frame of mesoporous material while triblock copolymer surfactant P123 is used as a structure directing reagent in an acidic condition.



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-944**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Heterojunction organic solar cells based on pyrrolo[3,2-*b*]pyrrole-2,5-diones and carbazole

박혜지 송수희 심주영 진영웁[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

Organic p-conjugated polymers and small molecules constitute an important class of functional materials. Solution-processable small molecules have recently received great attention for both OPVs. Small molecules do not suffer from batch to batch variations, broad molecular-weight distributions, end-group contamination, or difficult purification methods, which can be significant problems for polymeric materials. These considerations make small molecules a promising class of donor material for BHJ solar cell applications. Pyrrolo[3,4-c]pyrrole-1,4-diones (DPP) has advantage because of Low band gap and strong π-π interaction, but there is disadvantage; poor solubility and film forming ability. So we were synthesized novel acceptor small molecule based on pyrrolo[3,2-*b*]pyrrole-2,5-diones. Pyrrolo[3,2-*b*]pyrrole-2,5-diones is expected to improve solubility, changed atoms position and extending π-conjugation. And Recently, poly(2,7-carbazole) derivatives have proven to be good candidates for the design of high hole carrier mobility with optimized HOMO and LUMO energy levels allowing to reach for the first time a certified PCE close to 6%. Therefore novel acceptor small molecule based on pyrrolo[3,2-*b*]pyrrole-2,5-diones and carbazole was synthesized by stille coupling.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-945**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

α-Aminoallylation of aldehydes with benzoyl hydrazine and allyl bromides

이범석 장두옥

연세대 화학과

Three component reactions of carbonyl compounds, nitrogen nucleophiles, and carbon nucleophiles that assembles both nitrogen-carbon and carbon-carbon bonds are useful and convenient methods for the synthesis of protected or unprotected secondary amines. We have developed a one-pot α-aminoallylation of aldehydes with benzoyl hydrazine and allyl bromides in the presence of indium and $Zn(ClO_4)_2 \cdot 6H_2O$. The protocol affords mild, efficient, chemoselective reaction conditions for the synthesis of protected secondary amines.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-946**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective allylation of α-ketoesters with organocatalyst

이정진 장두옥

연세대 화학과

The use of α-hydroxy ketones and their derivatives as chiral synthons in organic synthesis has grown collaterally with advances in methodology for their asymmetric synthesis. If the reaction can be performed in a catalytic fashion, small amounts of chiral catalyst are needed to give large amounts of enantiomerically enriched products. The α-hydroxy carbonyl unit is found in many biologically active natural products such as sugars and antibiotics. Enantiomerically pure α-hydroxy carbonyl compounds are also important synthons for the asymmetric synthesis of natural products. Consequently, efficient methods for the construction of enantiomerically pure, or at least enriched, α-hydroxy carbonyl derivatives are in demand. We present a highly enantioselective indium-mediated allylation of α-ketoesters using indium/allylbromide in the presence of a chiral ammonium salt.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-947**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Elimination Reactions of (E)-2,4,6-Trinitrobenzaldehyde O-Benzoyloximes Promoted by $R_2NH/R_2NH_2^+$ in Aqueous MeCN(aq). Effects of β - Aryl Group and Leaving Group on the Nitrile-Forming Transition-State

변상용 류은미

부경대 화학과

Nitrile-forming eliminations from (E)-2,4,6-$(NO_2)_3C_6H_2CH{=}NOC(O)C_6H_4X$ (1) promoted by $R_2NH/R_2NH_2^+$ in 70mol% MeCN(aq) have been studied kinetically. The reactions produced only elimination products and exhibited second-order kinetics. The β and $|\beta_{lg}|$ values remained nearly the same within experimental error regardless of the ability of the leaving groups and the base strength variation. The results can be described by a negligible p_{xy} interaction coefficient, $p_{xy} = \partial\beta/\partial pK_{lg} = \partial\beta_{lg}/\partial pK_{BH}$? 0, which describes the interaction between the base catalyst and the leaving group. The negligible p_{xy} interaction coefficient are inconsistent with the E2 mechanism for which $p_{xy} > 0$ is expected, but provide a strong evidence for the $(E1cb)_{irr}$ mechanism.

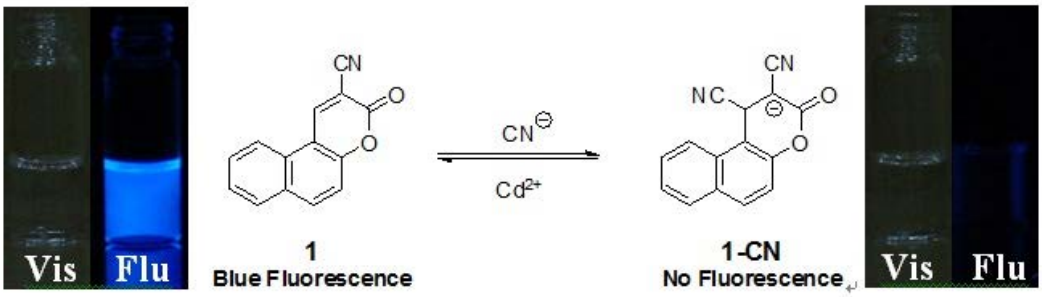
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-948**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reversible Dual Chemosensor for Cyanide and Cadmium Ions

박석안 김해조

한국외국어대 자연과학대학 화학과

Cyanide is toxic to mammals to such an extent that it can severely damage or inhibit their respiratory systems by absorption through the lungs, gastrointestinal tract, or skin.[1] Cadmium(II), a congener of Zn(II), can occupy Zn-binding sites in many enzymes and proteins, forming Cd(II)-proteins that cannot function as well as the corresponding Zn(II)-proteins and can severely weaken human bones in Itai-itai disease.[2] We study a reaction-based probe that can reversibly recognize both aqueous cyanide and cadmium ions. A naphthocoumarin-based chemosensor 1 capable of sensing both cyanide anion and mercuric cation was designed through a reversible reaction with the two toxic chemicals. The probe exhibited a rapid fluorescence response to cyanides through the Michael reaction and to cadmium ions through the metal-induced elimination reaction, whose cycle was reversibly operable in aqueous buffer.[3] (figure)References[1] (a) Warburg, O. Hoppe-Seyler's Z. Physiol. Chem. 1911, 76, 331. (b) Kellin, D. Proc. R. Soc. London, Ser. B 1929, 104, 206. (c) Vennesland, B.; Comm, E. E.; Knownles, C. J.; Westly, J.; Wissing, F. Cyanide in Biology, Academic Press: London, 1981.[2] (a) Crichton, R. R. Biological Inorganic Chemistry: An Introduction, Elsevier, 2008. (b) Ochiai, E. Bioinorganic Chemistry: A Survey, Elsevier, 2008.[3] Park, S.; Kim, H.-J. Sens. Actuators B. 2012. 161. 317.



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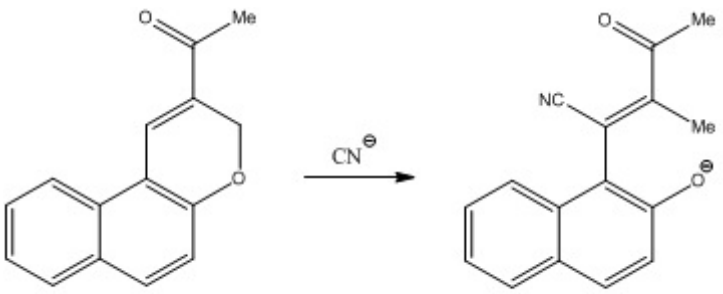
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-949**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ratiometric Fluorescent Probe for Cyanide in Aqueous Solvent

이희진 김해조

한국외국어대 자연과학대학 화학과

Currently, the development of molecular probes for anions such as cyanide has been a subject of intense research interest, because anions play important roles in biological systems and also constitute some pollutants in our environment.[1] Cyanide is an extremely toxic anion and can affect many functions in the human body, including the vascular, visual, central nervous, cardiac, endocrine, and metabolic systems.[2] Nevertheless, cyanide is widely used in many chemical processes, such as electroplating, plastics manufacturing, gold and silver extraction, tanning, and metallurgy.[3] Herein we report a benzochromene-based ratiometric fluorescence probe which is activated by cyanide anions. The chemodosimeter has shown a selective response to cyanide anion over other various anions through the Baylis-Hillman condensation reaction. The dramatic optical changes of 1 allowed us to detect toxic cyanide anions even by the naked eye in aqueous solution.Fig 1. Probe 1 and its reaction with cyanide anionReference[1]. Xu, Z.; Kim, S. K.; Yoon, J. Chem. Soc. Rev. 2010, 39, 1457?1466. [2]. Way, J. L. Annu. Rev. Pharmacol. Toxicol. 1984, 24, 451?481[3]. Qian, G.; Li, X.; Wang, Z. J. Mater. Chem. 2009, 19, 522?530



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-950**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Eliminations from (E)-2,4-Dinitrobenzaldehyde O-Aryloximes Promoted by R_3N in MeCN. Effects of β-Aryl Group and Base-Solvent on the Nitrile-Forming Transition-State

변상용 류은미 조봉래[1]

부경대 화학과 [1]고려대 화학과

Nitrile-forming eliminations from (E)-2,4-$(NO_2)_2C_6H_2CH{=}NOC_6H_4$-2-X-4-$NO_2$ promoted by R_3N in MeCN have been studied kinetically. The reactions are second-order and exhibit Br?nsted β = 0.83 - 1.0 and $|\beta_{lg}|$ = 0.41 - 0.46. The results have been interpreted in terms of highly E1cb-like transition state with extensive $C_ß$-H bond cleavage and limited N_α-OAr bond cleavage. Comparison with exiting data reveals that the structure of the transition state changes from E2-central to highly E1cb-like either by the change of the β?aryl group from Ph to 2,4-dinitrophenyl under the same condition or by the base-solvent system variation from EtO^--EtOH to Et_3N-MeCN for a given substrate.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-951**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Application of Biocompatable Materials for Efficient siRNA Delivery

박정우 김병현

포항공과대 화학과

Small interfering RNA (siRNA) has been applied for gene therapy as a powerful tool. siRNA can recognize and silence complementary sequence of target mRNA in the cell and inhibit the target protein expression. Even though siRNA has great therapeutic potential, application of siRNA still has several problems such as cytotoxicity, low cellular uptake, poor target specificity, and weak nuclease resistance. Among various factors, the most interesting siRNA delivery system is peptide-based gene delivery systems. In general, peptide-based delivery exhibits no or low toxicity because peptides are constituent part of our body and rarely induce immune responses. To overcome the obstacles of siRNA therapy, we compare two types of delivery systems. One is peptide-siRNA conjugation method. In this method, various peptides are introduced to the end position of siRNA by using covalent bonds such as a disulfide bond. The other is peptide-siRNA complexation methods using electrostatic interaction between siRNA and peptide. We will discuss the physical and biological properties of both systems and their transfection activities towards various cells. Meanwhile, the integration of nucleoside and peptide into a single molecule results in a novel class of supramolecular hydrogelators. Hydrogels have investigated as an important class of biomaterials under intensive attention and show the similar morphology to extracellular matrices (ECMs) in tissues. Therefore various hydrogels have been applied to biomedical applications such as tissue engineering and drug or gene delivery. We are interested in developing chemically modified nucleosidebased hydrogelators that will behave as delivery systems or media for cell culture. we have investigated the preparation of effective hydrogelators based on nucleobase-modified nucleoside monomers and dipeptide, L-Phe-L-Phe (FF; L-Phe=L-phenylalanine), and also describe their application of gene delivery and cell cultures. Reference1.Park, J. W.; Bang, E.-K.; Jeon E. M.; Kim, B. H.,

Complexation and conjugation approaches to evaluate siRNA delivery using cationic, hydrophobic and amphiphilic peptides. *Org. Biomol. Chem.*, 2012, *10*, 96.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-952**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses of Glycosyl Nucleoside-Based Lipids as siRNA Delivery agent

박유진 김병현

포항공과대 화학과

Gene therapy has gained attention as a potentially powerful method for curing disease, but there are still some difficulties to deliver genes into the cells. Therefore, the clinical success of gene therapy is critically dependent on efficient and safe gene delivery. For this reasons, it is necessary to use delivery agents. As non-viral transfection agent, glycosyl nucleoside-based lipid (glycosyl nucleolipid) have been developed and have some advantages.: low cytotoxicity compared to viral transfection agents, a natural amphiphilic character to the molecules to induces the formation of self-assemlY similar to cell membrane, recognition and favorable interactions with negatively charged gene and cell membrane. Owing to presence of the nucleoside, the glycosyl nucleolipids present additional H-bonding and π-stacking capability. The novel glycosyl uridine-based cationic lipid has been synthesized for the delivery of therapeutic gene, siRNA. The 5’ position of uridine was conjugated with glucose, β-glucopyranoside. The 5 position of uridine was combined by Sonogahira reaction with basic amino acid, arginine and lysine. To make diverse length and kink on tails, octyl, dodecyl, and oleyl alkyl chain were linked at 2’ and 3’ positions by carbamate group.

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장소: 부산BEXCO

발표코드: **ORGN.P-953**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Indium Tri(isopropoxide)-Catalyzed Selective Meerwein-Ponndorf-Verley Reduction of Aliphatic and Aromatic Aldehydes

류태규 박상준 이필호

강원대 화학과

Indium tri(isopropoxide)-catalyzed Meerwein-Ponndorf-Verley reduction of aliphatic and aromatic aldehydes in 2-propanol gave selectively the corresponding primary alcohols in good to excellent yields at room temperature. A wide range of functional groups including alkene, ether, ketone, ester, nitrile, and nitro were tolerated under the optimum reaction conditions. Chemoselective reductions were also achieved not only between aromatic aldehyde, aromatic ketone, and epoxide but also between aliphatic aldehyde and alkene.

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발표코드: **ORGN.P-954**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New Synthetic Method of Substituted Coumarins via Bronsted Acid-Mediated Condensation of Allenes

박상준 류태규 이필호

강원대 화학과

Coumarins were obtained from the condensation of electron-rich arenes with allenes in the presence of TfOH in good yield. Depending on the substituent pattern of allenes employed, the general synthetic method of 4- and 3,4-di-substituted 3-arylcoumarins has been developed. Readily available allenes were employed as the three carbon atom sources constituting the coumarin skeleton for the first time.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-955**

발표분야: 유기화학

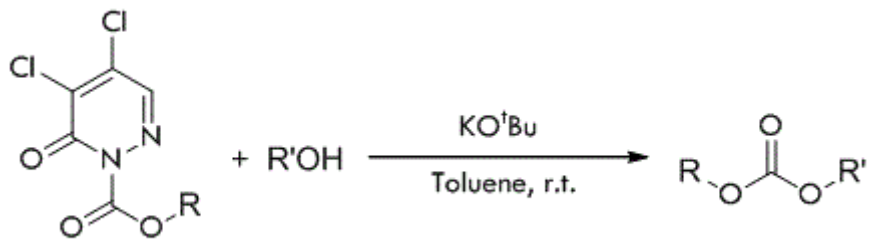
발표종류: 포스터, 발표일시: 수 16:00~19:00

Convenient Synthesis of Organic Carbonates from Alcohols Using 2-alkoxycarbonyl-4,5-dichloropyridazin-3(2*H*)-ones

성기현 김보람 윤용진

경상대 화학과

Organic carbonates are very important compound as the synthetic intermediates, solvents of Li-ion battery, reaction solvent and reagents. Although some prepared methods reported, these require toxic and/or gaseous carbonyl source such as phosgene, CO_2 and CO. These have also some drawbacks such as use of specific additives and side reactions. Inspired by recent other report of the conversion of N-phenylcarbamate to unsymmetric urea, we investigated to develop facile synthesis of carbonates. Herein, we present a convenient method of symmetric and unsymmetric carbonates from alcohols using 2-alkoxycarbonyl-4,5-dichloropyridazin-3(2*H*)-ones.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-956**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Copper-Catalyzed Intramolecular Hydroalkoxylation

김상혁 박상준 이필호

강원대 화학과

2,5-Dihydrofurans are important heterocycles that are widely used in pharmaceuticals and as flavor and fragrance compounds and found in naturally occurring and biologically important molecules. Accordingly, substantial attention has been given to developing efficient methods for the synthesis of 2,5-dihydrofurans. Consequently, the development of synthetic approaches of functionalized 2,5-dihydrofurans is major interest. Herein, we developed an efficient and selective copper-catalyzed intramolecular hydroalkoxylation of α-hydroxyallenes for the synthesis of highly functionalized 2,5-dihydrofurans through a 5-endo mode that eliminates the need to use an expensive catalyst. This method provides a valuable new way to synthesize a wide range of functionalized 2,5-dihydrofuran derivatives.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-957**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrosilyloxylation Driving Tandem Aldol and Mannich Reactions Catalyzed by Gold

강동진 박상준 류태규 이필호

강원대 화학과

The chemoselective formation of an enolate from alkyne in the presence of a carbonyl and imine group was realized, which constructed a variety of structural motifs under exceedingly mild reaction conditions in a tandem process. Reaction driving tandem hydrosilyloxylation/aldol reactions was achieved through the formation of enol silyl ethers catalytically generated in situ from readily available alkynes. These reactions were expanded to obtain β-amino enol silyl ethers in good yields via the tandem hydrosilyloxylation/isomerization/Mannich reaction.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-958**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 4-(4-([1,2,4]Triazolo[4,3-a]pyridin-3-yl)-3-phenyl-1H-pyrazol-1-yl)thieno pyrimidine Derivatives using Vilsmeier-Haack Reaction

김성민 송양헌

목원대 화학과

Synthesis of a new thienoipyrimidine compounds containing pyrazole ring is described. The thienopyrimidinyl hydrazones were treated with mixture of POCl3 in DMF to give 3-phenyl-1-(thieno[3,2-d]pyrimidin-4-yl)-1H-pyrazole-4-carbaldehyde. These compounds on treatment with various hydrazines in refluxing EtOH gave (E)-4-(3-phenyl-4-((2-(pyridin-2-yl)hydrazono)methyl)-1H-pyrazol-1-yl)thienopyrimidine which on further reaction with [bis(acetoxy)iodo]benzene afforded 4-(4-([1,2,4]triazolo[4,3-a]pyridin-3-yl)-3-phenyl-1H-pyrazol-1-yl)thienopyrimidine derivatives via cyclization process.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-959**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 5-(4-Ethylpiperazin-1-yl)-2-(methylthio)-8-phenylthiazolo[4,5-e][1,2,4]triazolo[1,5-c]pyrimidine compounds as A3AR Agonist.

이혁주 송양헌

목원대 화학과

A3AR agonist have been evaluated for the treatment of autoimmune inflammatory diseases such as rheumatoid arthritis, psoriasis, and for live cancer. We have synthesized some of new thiazolo thiazolopyrimidine compounds as A3AR agonist candidate. Reaction of carbohydrazide with ethyl 4-cyano-2-(methylthio)thiazol-5-ylcarbamate gave 2-(methylthio)-8-phenylthiazolo[4,5-e][1,2,4]triazolo[1,5-c]pyrimidin-5(4H)-one, which converted to 5-chloro-2-(methylthio)-8-phenylthiazolo[4,5-e][1,2,4]triazolo[1,5-c]pyrimidine using POCl3. The corresponding chloronated derivatives 5-chloro-2-(methylthio)-8-phenylthiazolo[4,5-e][1,2,4]triazolo[1,5-c]pyrimidine underwent substitution with piperazine to afford final compounds, 5-(4-ethylpiperazin-1-yl)-2-(methylthio)-8-phenylthiazolo[4,5-e][1,2,4]triazolo[1,5-c]pyrimidine.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-960**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Conia-Ene Cyclization of 2-Alkynic 1,3-Dicarbonyl Compounds

박영철 정연석 이필호

강원대 화학과

A cheap, simple, and effective $FeCl_3$-catalyzed Conia-ene cyclization of 2-alkynic 1,3-dicarbonyl compounds was stereospecific to afford alkylidenecyclopentanes in (*E*)-isomers via the 5-*exo*-dig pathway. The 5-*endo-dig* and 6-*exo-dig* cyclizations were also possible, depending on the structure of the substrates.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ORGN.P-961**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inter- and Intramolecular Pd-Catalyzed Allyl Cross-Coupling Reactions

이구연 이의철[1] 이필호[1]

강원대 생명건강공학과 [1]강원대 화학과

The development of efficient synthetic methods for C-C bond formation is an important continuing research subject in organic synthesis. Transition metal-catalyzed cross-coupling reactions of organometallic reagents with a wide range of electrophilic coupling partners represent one of the most useful methods to form C-C bonds. In this poster, we report in full the novel intermolecular and intramolecular palladium-catalyzed cross-coupling reactions of a wide range of allylindium reagents generated in situ from allyl halides and indium with organic electrophiles such as aryl and vinyl halides and aryl and vinyl.

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

Synthesis of Cyclic Vinyl Phosphates Catalyzed by Gold

오수성 전인철 이필호

강원대 화학과

Gold-catalyzed nucleophilic additions to alkynes have attracted a great deal of attention in recent years. These nucleophilic additions include hydroamination, hydration, hydroalkoxylation, hydrocarboxylation as well as the use of other oxygen- or nitrogen-containing nucleophiles such as ketones and imines or even carbon nucleophiles such as C-C double bonds in enols or arenes. Recently, we reported the gold-catalyzed addition of diphenyl phosphate to alkynes to yield vinyl phosphates through the Markovnikov addition. Although the Markovnikov addition is usually observed for termial alkynes, for unsymmetrical alkynes, there is a regioselectivity issue, which is difficult to resolve. In this regard, we have been interested in utilizing alkynyl hydrogen phosphates as temporary phosphate tethers, not only to control the regioseletivity of the cyclization but also to utilize the cyclic phosphate products as coupling partners in transition metal-catalyzed cross- coupling reaction.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Synthetic Method of Trisubstituted Alkenes via Gold(I)-Catalyzed Hydrophosphoryloxylation of Haloalkynes

엄다한 서정민 이필호

강원대 화학과

Synthesis of stereodefined trisubstituted alkenes is very important in organic synthesis and many ingenious approaches have been devised. Among various approaches, one of the most attractive approaches is to utilize the transition metal-catalyzed cross-coupling reactions of stereodefined alkenyl derivatives and depends very much on the regio- and stereospecific synthesis of alkenyl derivatives from alkynes. Herein, we described a new stereoselective synthesis of trisubstituted alkenes, which is based on Au(I)-catalyzed regio- and stereoselective hydrophosphoryloxylation of haloalkynes and subsequent transition metal-catalyzed cross-coupling reactions.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hybrid System of Metal/Brønsted Acid Relay Catalysis for the Double Hydroarylation and Cationic Cyclization

모준태 김철의 이필호

강원대 화학과

Transition metal-catalyzed intramolecular hydroarylation of alkynes, alkenes, and allenes by the addition of an aryl C-H bond across a π-bond has received considerable attention for its highly useful synthetic applications. This reaction has been demonstrated to be one of the most effective green chemistry because of its ideal atom economy. Recently, we developed Pt-catalyzed hydroarylation of benzyl allenes through a 6-*endo* mode for the preparation of 1,4-dihydronaphthalenes. Because tandem reactions have long been established as efficient methods for the rapid synthesis of complex compounds in relatively short steps starting from simple and readily available substrates, we envisioned that a tandem process involving transition metal-catalyzed intramolecular hydroarylation of diyne diether and diamine followed by Brønsted acid-catalyzed cationic cyclization of diene in one-pot would provide structurally diverse heterocycles. Herein, we describe the development of tandem intramolecular Au-catalyzed double hydroarylation of 2,4- diyne-1,6-diethers or diamines followed by cationic cyclization in one-pot.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Isomerization of Kinetic Enol Derivatives to the Thermodynamically Favored Isomers

김진식 신서현 이필호

강원대 화학과

Considerable attention has been focused on the selective synthesis of enol derivatives due to their usefulness in various synthetic transformations. The major issue in these transformations is selectivity (kinetic vs. thermodynamic). In particular, the more substituted thermodynamic enol derivatives from unsymmetrical ketones normally predominate under thermodynamic conditions but do not form exclusively, which is a serious problem in organic synthesis. Herein, we report trifluoromethanesulfonic acid catalyzed isomerization of kinetic enol derivatives to the thermodynamically favored isomers. Under the present conditions, kinetic enol phosphates, enol acetates and benzoates, and enol sulfonates were smoothly isomerized to produce the corresponding thermodynamically favored isomers in good to excellent yields.

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

Protein Immobilization via Schiff base Formation by UV irradiation

여세원 김재희 이윤식

서울대 화학생물공학부

Protein microarray chip has been commonly utilized for an easy diagnosis of diseases. First of all, immobilization of protein on a chip is an important and critical step for successful bio-analysis on a microarray chip. For preparing the protein microarray chip, printing method has been commonly used so far. However, the printing method has a limitation to make integrated spots, so it is difficult to fabricate efficient microarray. In this presentation, we tried to overcome this problem by using photo-lithography method. For this, we prepared a photo-reactive molecule which has *ortho*-nitrobenzyl alcohol group for the immobilizing of proteins via Schiff base formation. The photo-reactive molecule was selectively modified by UV irradiation and the protein was immobilized in specific sites via Schiff base formation.

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발표분야: 유기화학

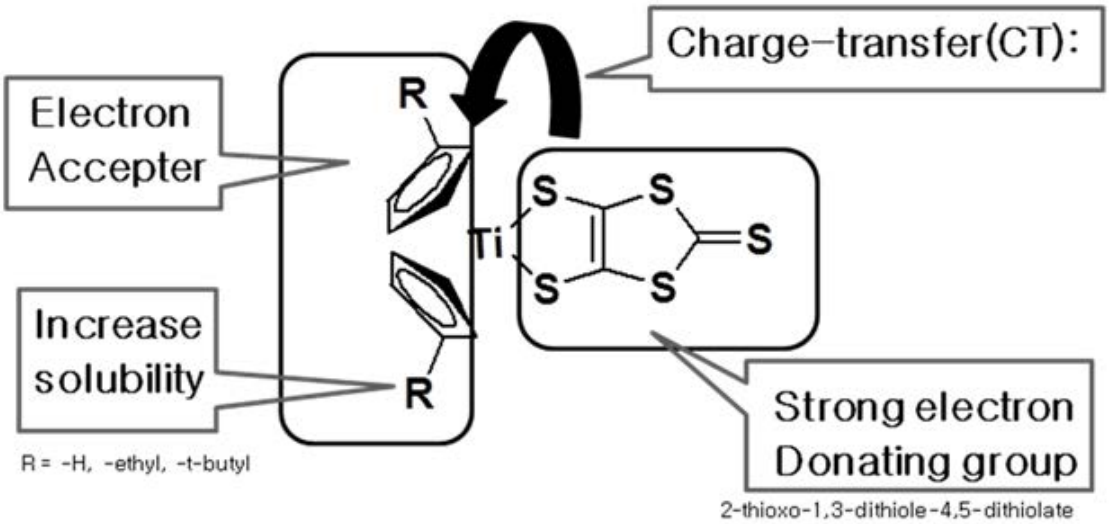
발표종류: 포스터, 발표일시: 수 16:00~19:00

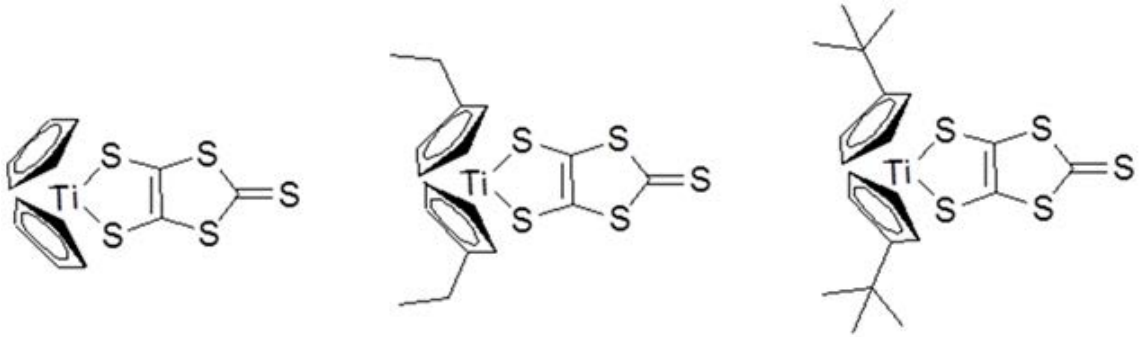
Synthesis and Characterization of Titanium metal Complex with a Dithiolate Ligand for Green LCDColor Filter Dyes

신환규

가톨릭대 화학과

Three green compounds for color filter dyes based on bis(cyclopentadienyl)Titanium complexes including dithiolate ligand were synthesized. Physical properties by the change of the substitution groups of the synthesized materials were systematically examined. UV-visible absorption spectrum of the synthesized materials showed maximum absorbing wavelengths of about 427~430 nm, 632~635nm in solution state and 434 ~ 438 nm, 637~651nm in film state, indicating green and black color. It was observed that the extinction coefficient values (log ε) of all the synthesized materials are very high at 4.0 or above. In addition, it was shown that since the Td values of three synthesized materials show thermal stability higher than 240 °C, they possess high potential to be applied as dyes for LCD color filter and black matrix additive.





•**Figure. 1**

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일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-968**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A low band-gap polymer based on dimethyl-2*H*-benzimidazole for photovoltaic applications

심주영 송수희 박혜지 진영읍[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

One of the most successful approaches to obtain high efficiency OSCs is development of low band-gap conjugated polymers. Low band-gap polymers based on internal donor?acceptor interaction have special advantages because their absorption ranges can be extended to longer wavelengths to absorb more photons, and their electronic property can be easily tuned by an appropriate combination of donor and acceptor units. The application of fused-ring monomers planarizes the copolymer backbone, enabling efficient π-stacking and higher charge carrier mobilities. We report conjugated polymers for OPVs device utilizing a new type of acceptor, 2,2- dimethyl-2*H*-benzimidazole. New copolymers were synthesized by stille coupling to generate PFDTMBIs and PFBBTMBIs. The solid films of PFBBTMBIs show absorption bands with two maximum peaks at about 443?452 and 643?652 nm which is red-shifted about 20 nm as compared to PFDTMBIs. The device with PFBBTMBI5:$PC_{61}BM$ blend demonstrated a V_{OC} value of 0.68 V, a J_{SC} value of 3.10 mA/cm^2, and a *FF* of 0.35, leading to the efficiency of 0.74%.

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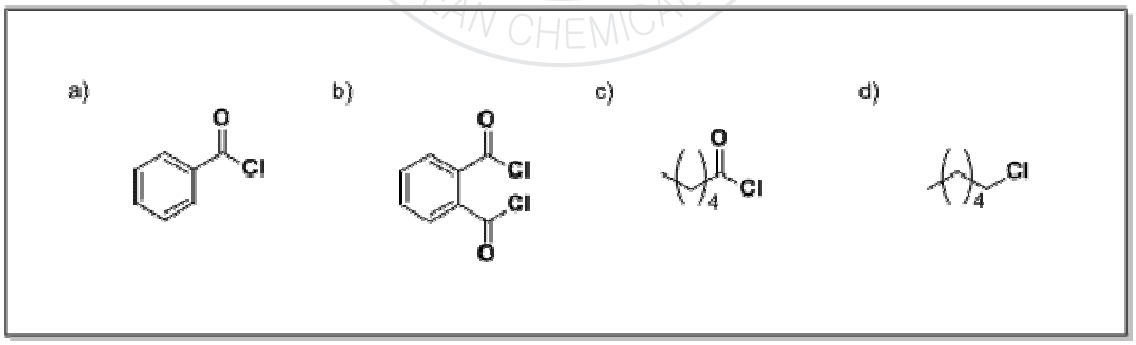
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Functionalization of Porous-Alumina for Luminence Organic-Inorganic Hybrid Material

김기우 안철진

창원대 화학과

The functionalization of porous alumina with organic compounds is developed to prepare the organic-inorganic hybrid luminescent material. The convenient preparation and characterization of organic-inorganic hybrid luminescent material will be discussed.



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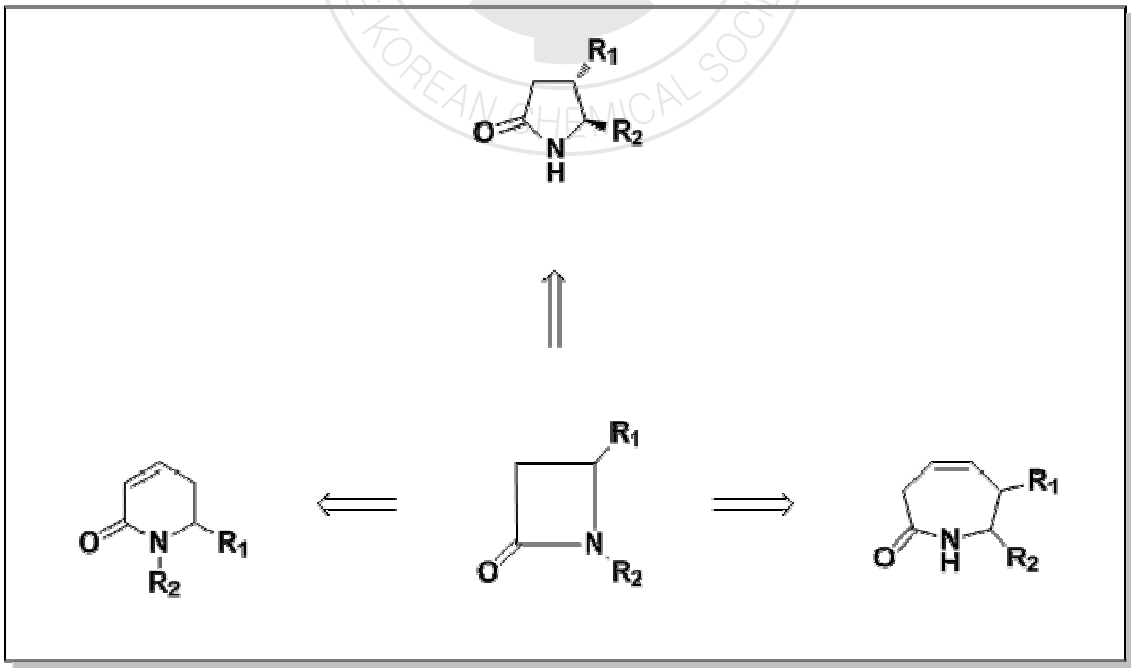
장소: 부산BEXCO
발표코드: **ORGN.P-970**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis of various Lactam Derivatives through the Ring Expansion of β-Lactam Derivatives

장지성 안철진

창원대 화학과

Various lactam derivatives have been prepared stereoselectively via ring expansion from the corresponding β-lactam derivatives. The stereochemistry of γ-lactams with aryl and alkyl substituents on C-3 has been investigated systematically. The regiochemistry of δ-lactam over ε-lactam derivatives with vinyl substituents on C-4 has been investigated too.



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장소: 부산BEXCO

발표코드: **ORGN.P-971**

발표분야: 유기화학

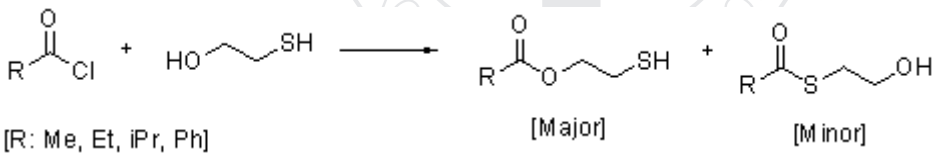
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Convenient Preparation of Thiol Ester using Mercapto Ethanol and Acid Chloride

김은선 안철진

창원대 화학과

The micelle structure of the gold nano particle(GNP) is commonly used for cell recognition. In order to form this micelle structure, GNP and the thiol derivatives need to connect effectively. For this connection, a thiol group needs to be linked to a pre-existing functional group efficiently before it combines with the GNP. In our lab, the thiol ester derivatives as major product are prepared unexpectedly by coupling mercapto ethanol with acid chloride derivatives.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-972**

발표분야: 유기화학

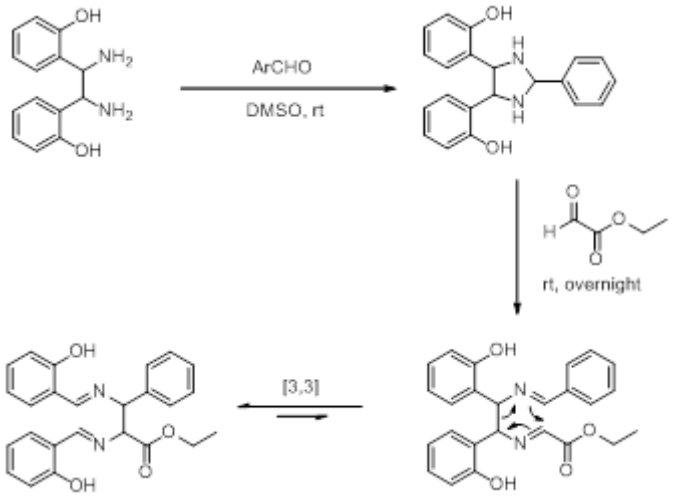
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Synthesis of Chiral α,β-diamino Acid Derivatives Using Diaza-Cope Rearrangement

변상문 권순호 김병문

서울대 화학부

Chiral vicinal diamine derivatives are important starting materials not only for chiral ligands of novel catalysts, but also for diverse chiral drug intermediates. Therefore, many interesting chiral vicinal diamine derivatives have been synthesized through oxidation, reduction, reductive coupling, C-C bond forming reactions and chiral resolutions. We developed a stereospecific synthesis of chiral vicinal α-β-diaminopropanoic ester derivatives using our previously developed diaza-Cope rearrangement reaction.1-3 References (1)Kim, H.; So, S. M.; Chin, J.; Kim, B. M. Aldrichimica Acta 2008, 41, 77. Kim, H.; So, S. M.; Chin, J.; Kim, B. M. Aldrichimica Acta 2008, 41, 77.(2)Kim, H.; Nguyen, Y.; Yen, C. P.; Chagal, L.; Lough, A. J.; Kim, B. M.; Chin, J. J. Am. Chem. Soc. 2008, 130, 12184.(3)Kwon, S. H.; Lee, S. M.; Byun, S. M.; Chin, J.; Kim, B. M. Org. Lett. 2012, 14, 3664.



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발표코드: **ORGN.P-973**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Cysteine-Selective Fluorescent Probe for the Cellular Detection of Cysteine

정효성 한지혜[1] 김수연 동방선 김태영 박나영 강철훈[2] 김종승

고려대 화학과 [1]경희대 동서의학대학원 의과학전공 [2]경희대 동서의학대학원

We have synthesized a series of coumarins that can emit fluorescence in a turn-on manner through a Michael-type reaction with thiol-containing compounds. The only difference among the coumarins is the position of a carboxyl group on its benzene ring moiety near the double-bond conjugated coumarin. Their selectivity for Cys, GSH, and Hcy as well as the associated fluorogenic mechanism were illustrated by fluorescence spectroscopy, DFT calculations, and kinetic studies. All isomers prefer Cys over GSH in the reaction from 48.6 (probe 3) to 111-fold (probe 1) as demonstrated in a second order kinetics. The high selectivity of probe 1 to Cys might be achieved since the ortho carboxyl group on its benzene ring prefers a less negatively charged nucleophile. During intracellular Cys detection using probe 1, a possible interference by a large amount of GSH in the HepG2 cells was evaluated. The cells were treated with L-buthionine sulfoximine (BSO), an inhibitor of glutamylcysteine synthetase, providing an experimental condition where the cells could not synthesize GSH from Cys or other species. Then, the fluorescence intensity of probe 1 in HepG2 cells under BSO-H_2O_2 treatment was strongly enhanced by N-acetylcysteine (NAC), a precursor of Cys, implicating that the fluorescence signal from the cells is mainly associated with changes in intracellular [Cys] rather than that in intracellular [GSH].

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발표분야: 유기화학

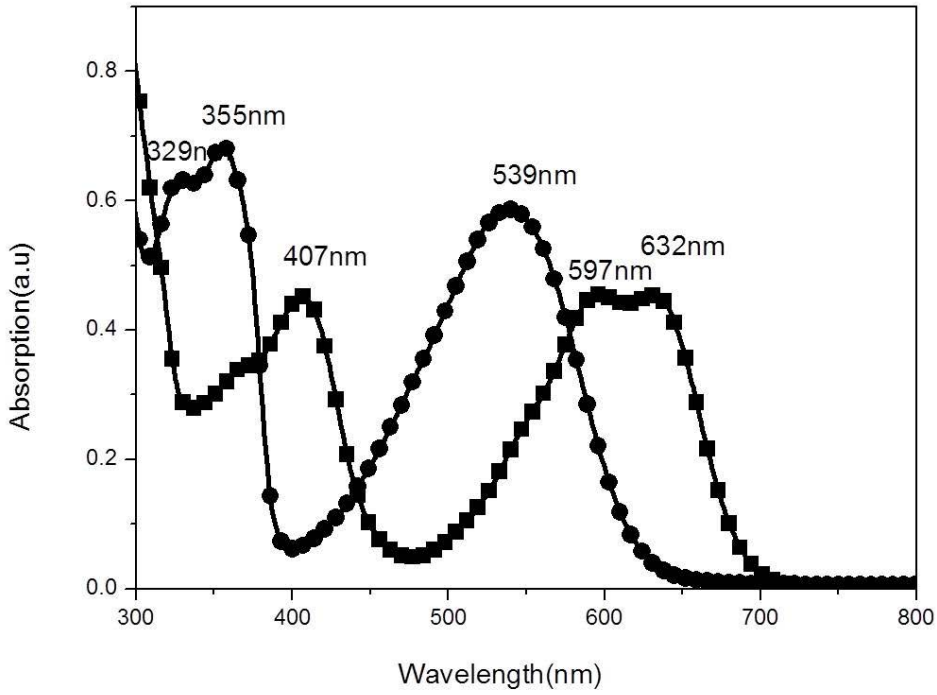
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Dyes Based on Anthraquinone Derivatives for Color Filter Colorants

박수연

가톨릭대 화학과

Display information industry recently showed rapid development in liquid crystal displays (LCD). Especially dyes and pigments have been widely used as core materials for color filter (CF), which is used to make full color spectra in LCD device.In CF of LCD, the role of dyes and pigments is to express full color by reflecting or absorbing light at specific wavelengths using red, green and blue pigments when white-backlight is passing through.Therefore, optical characteristics of colorants used in CF must allow light with wanted or unwanted wavelength to pass through and filter remaining wavelengths. Such colorants are thus required to have wanted absorption spectrum and high molar extinction coefficient value.In this study, two compounds for new CF dyes bearing quinoline group at 1,4-position and 1,8-position of anthraquinone were synthesized, and the changes of physical properties by the change of the respective substitution position of the synthesized materials were also examined. Two compounds are 1,4-Bis-(quinolin-3-ylamino)-anthraquinone (1,4(3QL)AQ) and 1,8-bis(quinolin-3-ylamino) anthraquinone (1,8 (3QL)AQ).In figure 1, the synthesized material, 1,4(3QL)AQ exhibited UV-visible maximum values of 407, 597 nm, and 632 nm and blue color in solid state. Molar extinction coefficient values of 407, 597, and 632 nm of 1,4(3QL)AQ were 18,200, 18,100, and 18,100 L/mol?cm, respectively. 1,8(3QL)AQ showed UV-visible maximum value at 355 and 539 nm and violet color in solid state. Molar extinction coefficient value of 1,8 (3QL)AQ was 27,400 and 23,400 L/mol?cm.All these compounds exhibited purer colors based on higher molar extinction coefficient. Good thermal stability on higher decomposition temperature(Td) was achieved in all synthesized compounds.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of C_{3V}-Symmetric Anion Sensor with Urethane Ligands on Trindane Molecular Backbone

박진오

경북대 응용화학과

아마이드기, 요소기와 우레탄기의 NH 수소는 우수한 수소결합 주게로 작용하여 음이온 수용체의 리간드로 널리 활용되고 있다. 많은 음이온들은 C_{3V}-대칭 요소를 가지고 있어 호스트 수용체가 C_{3V}-대칭으로 상호작용할 수 있으면 선택성과 안정성이 뛰어난 분자인식이 가능할 것이다. 본 연구실에서 개발한 trindane-tricarboxylate 화합물은 C_{3V}-대칭성을 가지고 있어, 이 화합물의 carboxylate 기를 알콜기로 환원하고 형광체나 발색체를 갖는 isocyanate 와 반응하여, 새로운 C_{3V}-대칭의 urethane 리간드를 갖는 음이온 분자 광센서를 합성하고, 이의 구조적 특성과 음이온과의 광학 특성을 연구하였다. 선택적 음이온 인식에 대한 NMR 적정 및 분자모델링 연구결과를 분석 토론하였다. Keyword: Urethane Ligand, Anion Molecular Sensor, Trindane tricarboxylate

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Disulfide-based probes for thiols in various organelles

한지혜 이민희[1] 정효성[1] Le Thi Hoa[2] 김태우[2] 김종승[1] 강철훈[2]

경희대 동서의학대학원 의과학전공 [1]고려대 화학과 [2]경희대 동서의학대학원

Recently, several fluorogenic naphthalimide derivatives have been synthesized to be guided to various organelles and to detect ithiol. Each probe has a unit to guide it to be delivered to its designated intracellular location. The unit may be a galactose, butyl, RGD or triphenylphosphonium group for delivering the probe to endoplasmic reticulum, random hydrophobic locations or mitochondria. Although these probes' reactivity toward biological thiols such as glutathione, cysteine, or thioredoxin in vitro are similar to each other, its in vivo selectivity inside the cells may be different since the dominant thiol species may vary according to the intracellular locations. We present evaluation of in vivo selectivity of the probe regarding the types of thiols.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Diversification of Heterocycle by microwave-assisted O,S-arylation

강희성 염을균

충남대 화학과

Heterocycles are widely used for drugs, agrochemicals, and other chemical substances. Diversification of heterocycles are very important for the biological applications. Specially, O, S-arylation of heterocycles are very difficult to obtain common synthetic methods. In this study, we examined microwave assisted organometallic approach to obtain diarylated ether and thio ethers in short reaction time. Particularly we focused optimization of C-O and C-S bond formation with catalytic Cu and organic ligands. We will discuss the reaction conditions and diversification of variety heterocycles under microwave reaction.

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ORGN.P-978**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of furo heterocycles by heterogeneous Pd catalyst annulation with alkynes.

김지은 염을균

충남대 화학과

Furo-heterocycles have shown diverse biological activities and commercial utilities.Therefore these compounds are synthesized by various synthetic method. However, synthesis of pyridine containing furohetrocycles are very difficult due to totaumerization of hydroxy pyridines. In this study, we examined Pd catalyzed heteroannulation with terminal alkynes to synthesize biologically active furo heterocycles. Specially, heterogeneous catalysis is very useful for the industrial purpose. In this study, various catalyst have been examined for recovery of catalyst and suitable support. We also examined diversification of furo pyridines.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표코드: **ORGN.P-979**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of largely conjugated oligothiophene derivatives for OPVs

김재미 윤주영[1]

이화여대 화학나노과학과 [1]이화여대 화학-나노과학과

Organic photovoltaic cells (OPVs) have been the focus of cost-effective solar cells in recent years. Contrary to other solar cells like silicon-based solar cells OPVs have light-weight, low-cost, and flexibility advantages. Especially, small molecular semiconductors for OPVs are very attractive due to their well-defined molecular structure, definite molecular weight, and high purity.Oligothiophenes one of the largest families of organic semiconductors are widely used in OPVs. Because of their long conjugated system, they can have high charge-carrier mobility. In addition, they are facile to synthesis to tune energy levels. To achieve high efficiency OPVs based on oligothiophenes, introducing highly polarizable π-electron system is important. Accordingly, we introduced highly conjugated group to oligothiophene. It can contribute to extend the absorption spectrum of the donor toward long wavelength. Furthermore, for solution process, we made long alkyl chain derivatives.

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장소: 부산BEXCO

발표코드: **ORGN.P-980**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric alkylation reations using non-cross-linked polystyrene-supported 2-imidazolidinone chiral auxiliaries

강병선 김택현[1]

전남대 신화학소재공학과 [1]전남대 응용화학공학부 광바이오사업단

Asymmetric alkylations using chiral auxiliar are now important and general methods for asymmetric carbon-carbon bond formation. Chiral 2-imidazolidinone has been used to be a versatile auxiliary for asymmetric syntheses, exhibiting excellent levels of stereocontrol, greater stability, and recyclability. Soluble polymer supports allow expeditious transfer of solution-based synthetic protocols. After the addition of an appropriate poor solvent, the polymer support can be precipitated, allowing its effective recovery. In this study, asymmetric alkylation reactions using the non-cross-linked polystyrene-supported 2-imidazolidinone chiral auxiliaries will be introduced with high stereoselectivity and yields. In addition, the good recycling of our chiral auxiliaries will be discussed.

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발표코드: **ORGN.P-981**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Aldol Reactions Catalyzed by the Combination of (S)-Proline and Isothiouronium Salt

조은 김택현[1]

전남대 신화학소재공학과 [1]전남대 응용화학공학부 광바이오사업단

The direct catalytic aldol reaction is a well-studied and broadly applicable C-C bond forming reaction, which provides enantiomerically enriched β-hydroxy carbonyl compounds. The (S)-proline-catalyzed version has attracted much attention and there have been a significant number of successful attempts to improve the efficiency and selectivity of the original proline-catalyzed aldol process. Considering the probed ability of isothiouronium salts in anion recognitions, we examined the function of using isothiouronium salts as new additives in the aldol reactions. Herein, we will discuss the results of the proline-catalyzed intermolecular direct aldol reactions between ketones and aromatic aldehydes using isothiouronium salts as additives.

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장소: 부산BEXCO

발표코드: **ORGN.P-982**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent- and catalyst-free direct reductive amination of aldehydes and ketones with Hantzsch ester: synthesis of secondary and tertiary amines

N.P.B.Quynh 김택현[1]

전남대 신화학소재공학과 [1]전남대 응용화학공학부 광바이오사업단

A green, facile and rapid method for the parallel synthesis of a series of secondary and tertiary amines by the direct reductive amination of aldehydes and ketones with Hantzsch ester at elevated temperature has been developed. Solvent- and catalyst-free as well as mental- and acid-free conditions, considerably short reaction time, and broad scope of substrates with high yields and excellent chemoselectivity are the key points of this method.

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-983**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Including Nitrogen and Fused Heterocyclic Molecule for OLEDs

정은빈 황민지 이상경

경상대 화학과

Organic light-emitting diodes (OLEDs) are promising materials such as next generation flat-panel displays and solid state lighting etc. The development of new electron transport materials with optimum properties are needed for next generation OLEDs. Nitrogen rich heterocyclic molecules capable of high electron mobility are of increasing interest in the development of electron transporting materials (ETMs) and hole-blocking layers (HBLs).Incorporation of nitrogens into aromatic organic semiconductors provide many advantages, including increase in electron affinity, improved photo-oxidative stability, and processbility from both aprotic and protic organic solvents. So, many researchers are studied including nitrogen molecules.So, we want to prepare and test for physical properties of a new heterocyclic molecule as a new ETMs and the results reported in this poster

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

Designed and Synthesis of New Organic Electronic Materials

황민지 정은빈 이상경

경상대 화학과

Organic semiconductors have seen significant development in the past two decades owing to their potential application to future-generation ultrathin, large-area, and flexible devices consisting of, for instance, organic thin film transistors (OTFTs), organic light-emitting diodes (OLEDs), and organic photovoltaics (OPVs), which can be fabricated by low-cost and low-energy processes and thus offer novel features that are different from those of conventional silicon technologies. However, the field effect mobility of OTFTs is still lower than those of the inorganic thin film transistor. The introduction of fused ring compounds such as pentacene, bis(dithienothiophene), benzodithiophene, and anthradithiophenes into OTFTs has been shown to result in improved TFT performance due to enhanced intermolecular ordering and ??? stacking. To date, the high field effect mobility values for OTFTs have been achieved with vapor-deposited purified pentacene films. But, to minimize manufacturing costs, the TFT fabrication process should ideally include solution-based methods such as spin-coating, stamping, or ink-jet printing. Therefore, we designed and synthesized a series of alkylated fused ring compound for solution-processable.In this presentation, we will report the synthesis and physical properties of a new organic semiconductor.

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장소: 부산BEXCO

발표코드: **ORGN.P-985**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Non-cross-linked polystyrene supported 2-imidazolidiones chiral auxiliaries for asymmetric alkylation reactions

N.P.B.Quynh 김택현[1]

전남대 신화학소재공학과 [1]전남대 응용화학공학부 광바이오사업단

Solid phase synthesis has emerged as a versatile and powerful technique in organic synthesis to prepare chemical libraries. However, several limitations were shown because of non-linear kinetic behavior. Soluble polymer supports have been studied as a way to overcome the problems of insoluble supports. In this study, we wish to report the preparation of non-cross-linked polystyrene supported 2-imidazolidiones chiral auxiliaries and the preliminary results of our investigations concerning the asymmetric alkylation reactions on these chiral auxiliaries.

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장소: 부산BEXCO

발표코드: **ORGN.P-986**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Highly Selective Pyrene Derivated Fluorescent sensor for homocysteine

이혜연 윤주영[1]

이화여대 바이오융합과학 [1]이화여대 화학-나노과학과

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. Homocysteine has been implicated in various types of vascular and renal diseases. Elevated Hcy in the blood (>12 mm) is a well-known risk factor for cardiovascular and Alzheimers disease, neutral tube defects, complications during pregnancy, inflammatory bowel disease, and osteoporosis. 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. In addition, despite the interesting biological importance of Hcy, only few fluorescent Hcy sensors were reported compared to Cys sensors. Herein, we developed the pyrene derivated fluorescent sensor which showed an excellent selectivity and sensitivity toward Hcy.

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장소: 부산BEXCO

발표코드: **ORGN.P-987**

발표분야: 유기화학

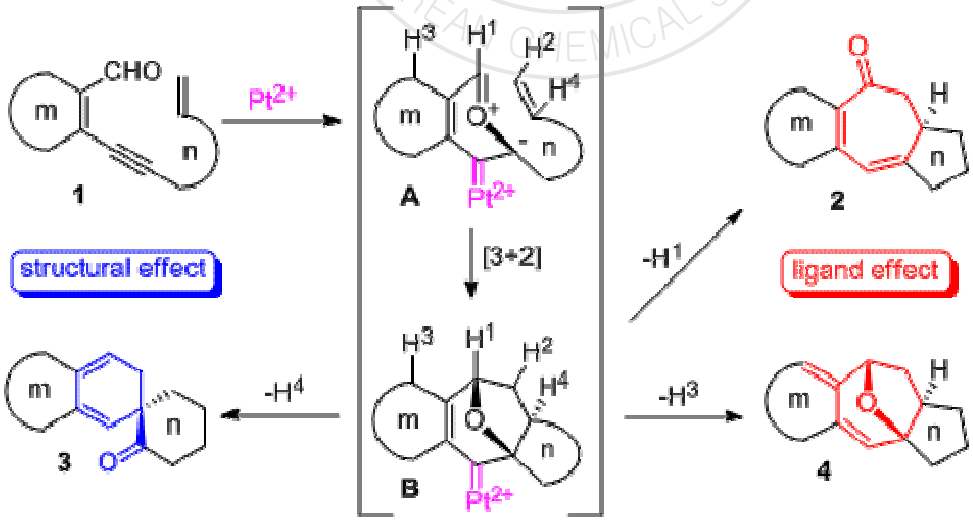
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of aliphatic polycycles via intermolecular [3+2] cyclization of platinum-bound pyrylium with alkenes

이지호 박종률 오창호

한양대 화학과

We have developed an efficient method for the selective construction of aliphatic polycycles through Pt-catalyzed cyclization of the 2-alkynylcycloalkenecarboxaldehydes 1 by considering electronic (ligand) and structural (olefinic tether) effect. The presence or absence of ligand and the length of olefinic tether determine the course of the reaction after the formation of an Pt-carbene complex B, so that three type of aliphatic polycycles can be formed selectively. This is able to provide us with a convenient route to medium-sized heterocyclic ring systems in synthetic methods for various natural products.



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장소: 부산BEXCO

발표코드: **ORGN.P-988**

발표분야: 유기화학

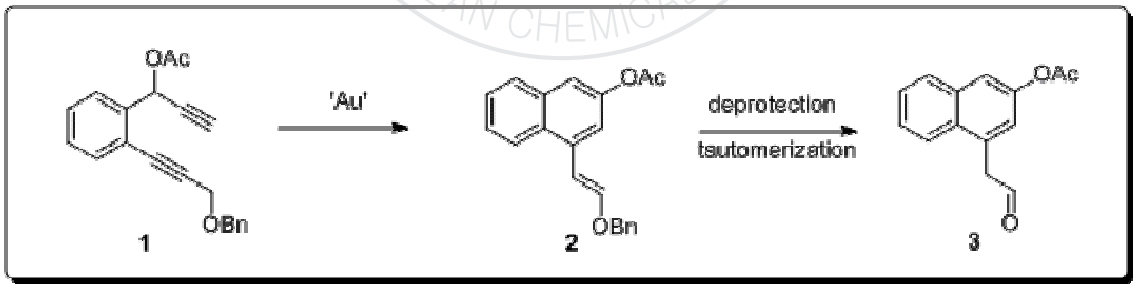
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold-catalyzed cyclizations of 1-(2-(3-(benzyloxy)prop-1-ynyl)phenyl)prop-2-ynyl acetate to 4-(2-oxoethyl)naphthalen-2-yl acetate and their related benzene derivatives

PIAOLANHUA 김지희 오창호

한양대 화학과

We developed a Au-catalyzed cascade reaction of 1-(2-(3-(benzyloxy)prop-1-ynyl)phenyl)prop-2-ynyl acetate and its derivatives to the corresponding 4-(2-oxoethyl)naphthalen-2-yl acetate in excellent to good yields. Propargylic carboxylate and triple bond in a same substrate 1, through activation of triple bonds gave resulting compound 2 and subsequent deprotection and tautomerization gave nephthalenyl final product -(2-oxoethyl)naphthalen-2-yl acetate.



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-989**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

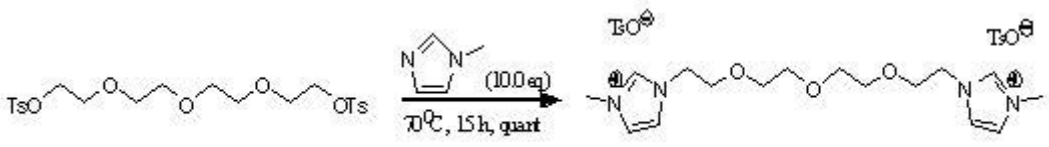
Synthesis of ionic liquids based-alkylimidazolium salts and their efficient coal dissolution and dispersion

김진원 강미숙[1] 나춘섭[1]

영남대 이과대학/화학 [1]영남대 화학과

A series of ionic liquid (three types; 1,1'-(2,2'-oxybis(ethane-2,1-diyl))bis(3-methyl-1H-imidazol-3-ium) 4-methylbenzenesulfonate, 1,1'-(2,2'-(ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl))bis(3-methyl-1H-imidazol-3-ium) 4-methylbenzenesulfonate, and 1,1'-(2,2'-(2,2'-oxybis(ethane-2,1-diyl)bis(oxy))bis(ethane-2,1-diyl))bis(3-methyl-1H-imidazol-3-ium) 4-methylbenzenesulfonate) containing alkylimidazolium-based cations and tosylate anions were successfully synthesized with excellent yields. A certain ionic liquid can be used to fragment, disperse, and partially dissolve coal to such an extent that good contact can be made with commercially obtained, micrometer-size coal particles by simply mixing these particles with the ionic liquid/coal dispersion. Good liquefaction yields under standard conditions are obtained using this approach. In this study, the length of oxygen chains between imidazolium rings with tosylate anion were considered, and the synthesized ionic liquids were used to the most popular chain of a typical hydrogen donor in this study. Their own ability to dissolve coal and thermal performance due to the dissolution of coal are analyzed. As the results, the dissolution performance of coal was enhanced over ionic liquid depends on oxygen chain number between imidazolium rings, and more light hydrocarbons were produced.

Fig. 1. synthesis of 1,1'-(2,2'-(2,2'-oxybis(ethane-2,1-diyl)bis(oxy))bis(ethane-2,1-diyl))bis(3-methyl-1H-imidazol-3-ium) 4-methylbenzenesulfonate



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-990**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Alkyne기를 포함하는 Potassium Organotrifluoroborate의 유도체화 연구

송중호 김태정[1] 김희진[1] 함정엽[1]

강릉원주대 화학신소재학과 [1]KIST 천연의약센터

Alkyne 화합물은 수소화반응, Diels-Alder 반응, 1,3-Dipolar Cycloaddition 등을 통해 손쉽게 작용기 변환이 가능하여 의약품, 고분자 소재 및 천연물의 전합성 분야에서 이용가치가 높아 다분야에 걸쳐 널리 이용되고 있다. 그럼에도 불구하고 Alkyne 화합물은 제조의 어려움과 시판되는 종류의 제한성 때문에 이를 활용한 다양한 반응에 어려움이 있었다. 최근에는 Suzuki-Miyaura 교차반응에서 Potassium Organotrifluoroborate 류가 반응기질로써 많이 사용되고 있다. 더욱이 Organotifluoroborate 가 특수한 반응조건에서 안정하다는 사실이 알려지면서 기존의 Boronic acid (ester)로 만들 수 없었던 새로운 Organotrifluoroborate 유도체화 연구가 증가하고 있다. 본 연구진은 Aryl halide 를 출발물질로 전이 촉매를 이용한 탄소-탄소 결합 반응을 통해 Alkyne 기를 포함하는 Organotrifluoroborate 의 손쉬운 합성법 개발에 성공하여 이에 대한 내용을 발표하고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ORGN.P-991**

발표분야: 유기화학

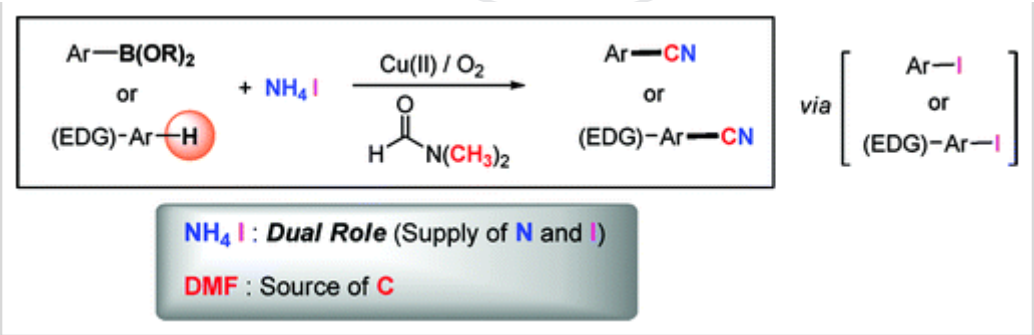
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Mediated Sequential Cyanation of Aryl C-B and Arene C-H Bonds Using Ammonium Iodide and DMF

김진호 장석복[1] 최지호[1] 신광민[1]

University of Wisconsin-Madison [1]KAIST 화학과

The cyanation of aromatic boronic acids,boronate esters, and borate salts was developed under copper-mediated oxidative conditions using ammonium iodide and DMF as the source of nitrogen and carbon atom of the cyano unit, respectively. The procedure was successfully extended to the cyanation of electron-rich benzenes, and regioselective introduction of a cyano group at the arene C?H bonds was also achieved. The observation that the reaction proceeds via a two-step process, initial iodination and then cyanation, led us to propose that ammonium iodide plays a dual role to provide iodide and nitrogen atom of the cyano moiety.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-992**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photovoltaic Properties of Small Molecules Utilizing DTMBI and Various Donor

박혜지 송수희 심주영 진영웁[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

As the acknowledgement of energy crisis is driven serious all over the world, another energy source including low cost, lightweight, flexibility and other attractive sources has been researching. Among other energy source, solar cells are more suitable. Solar cells based on organic semiconductor donor/acceptor (D/A) interfaces have advantages for providing a cost-effectively alternative photovoltaic technology for power industry. Small molecules do not suffer from batch to batch variations, broad molecular-weight distributions, end-group contamination, or difficult purification methods, which may be significant problems to polymeric materials. These properties help small molecules promising unit of donor material for BHJ solar cell applications. The new type of donor was synthesized in 5-hexyl-2,2'-bithiophene and DTMBI. Three small organic molecules, 5-hexyl-2,2'-bithiophene (HS-5431), 5-benzo[*b*]thien-2-yl-2-thienyl (HS-5458) and 2,2-dimethyl-2*H*-benzimidazole-4,7-diyldi-5,2-thiophenediyl (HS-5439) with 2,2-dimethyl-2*H*-benzimidazole type as new electron-deficient type, were synthesized using Suzuki coupling reaction.

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장소: 부산BEXCO
발표코드: **ORGN.P-993**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Low Band-gap of Conjugated Polymer Containing Benzimidazole and Various Thiophene for OPVs

박혜지 송수희 심주영 진영웁[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

Thermal annealing or solvent annealing is a excellent nanomorphology control on polymer-based bulk heterojunction (BHJ) organic photovoltaics (OPVs). The most outstanding break through for high-performance OPVs was based on the concept of a bulk-heterojunction (BHJ) structure in the organic active layer, which comprises a blend of a π-conjugated polymer as an electron rich donor (p-type) and a fullerene derivative as an electron deficient acceptor (n-type). Compared to conjugated homopolymers (such as P3HT), donor?acceptor (D?A) conjugated polymers, with electron-rich and electron-deficient units on the polymer backbone, are demonstrated to be an effective approach to make low bandgap polymers. The thin films of PCBBTMBIs show two absorption peaks at about 450 and 640~650 nm. The polymers with bithiophene units were red-shifted about 20 nm as compared to PCDTMBIs with thiophene units. In case of the most efficient polymer PCBBTMBI3, the device annealed at 100 ^{o}C for 10 min proved a V_{oc} value of 0.60 V, a J_{sc} value of 4.31 mA/cm^2, and a *FF* of 0.35, leading to the efficiency of 0.91%. Using a annealing temperature of 100 ^{o}C for 10 min, PCBBTMBI3:PCBM device efficiency can be improved from an initially low efficiency of 0.69% before annealing to 0.91% after annealing.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-994**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Water-Soluble Borondipyrromethene (BODIPY) Derivatives

김철용 이정태

한림대 화학과

BODIPY is a well-known fluorescnet dye. and has recently been studied as a solar cell. Usually a fluorescnet reporter moiety has not a lot of difference between λ_{ab} and λ_{em}, given that, it has relatively a large stokes-shift between λ_{ab} and λ_{em}. Water-soluble BODIPY could be used as an imaging agent in the human body. The introduction of various functional groups, especially water solubilizing moeities, to the bodipycore can be achieved. Our goal is the design, synthesis and characterization of the water-soluble BODIPY dye suitable for in vivo imaging in physiological condition.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-995**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Hierarchical Structure of Amphiphilic Tetrathiafulvalene Liquid Crystal

김대윤 이종훈[1] 이상아 이명훈 정광운[2]

전북대 고분자나노공학과 [1]전북대 유연인쇄전자공학과 [2]전북대 고분자.나노 공학과

A novel amphiphilic tetrathiafulvalene molecule (amph-7TTF14) was newly designed and synthesized. The morphological observations using transmission electron microscopy, atomic force microscopy, and polarized optical microscopy indicated that the amph-7TTF14 formed not only flat ribbons but also scrolls and helices. The face-to-face π-π interaction between TTF groups and the nanophase separation between rigid TTF groups and flexible hydrophobic alkyl and hydrophilic ethylene oxide tails were the main driving forces for the self-assembly of amph-7TTF14. It was realized that the scrolls and helices were induced by the unbalanced surface stresses generated during the crystallization process. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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장소: 부산BEXCO

발표코드: **ORGN.P-996**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Antioxidant Activity Evaluation of Hinokiresinol Derivatives by ABTS and DPPH assay

김미정 유지숙 이정태 김인수[1]

한림대 화학과 [1]성균관대 약학대학/약학과

Hinokiresinol is a well-known natural product that has antioxidant activity. Therefore, various hinokiresinol derivatives have been newly synthesized to enhance antioxidant activity. In general, antioxidant activity trend of these derivatives was dependent on the type and position of the substituents. The antioxidant activity of the newly synthesized compounds has been measured by ABTS and DPPH assay. As a result, IC_{50} values of these compounds were obtained.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Phase Identification of Board-Shaped Tetrathiafulvalene Liquid Crystal

김대윤 이종훈[1] 이상아 이명훈 정광운[2]

전북대 고분자나노공학과 [1]전북대 유연인쇄전자공학과 [2]전북대 고분자.나노 공학과

A board-shaped tetrathiafulvalene molecule (symTTF11) with four flexible alkyl chains chemically attached to the peripheries of mesogens was newly synthesized. The phase transitions and physical properties were investigated by the combined experimental technique. Based on the thermal, microscopic and scattering experiments and analyses, molecular packing 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, symTTF11 showed good charge carrier mobility. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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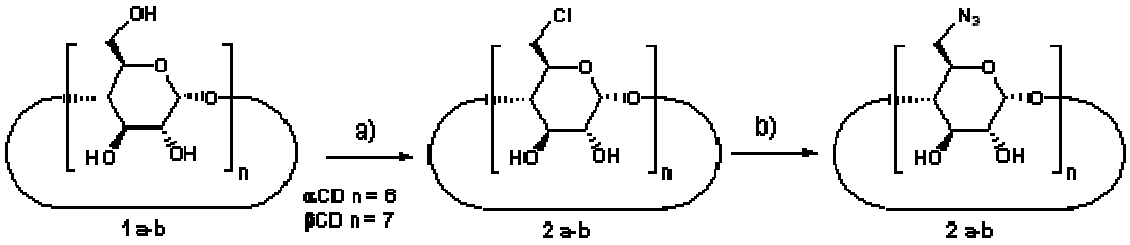
발표코드: **ORGN.P-998**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile synthesis of 6-azido-6-deoxy-cyclodextrin via 6-chloro-6-deoxy-cyclodextrin through microwave-assisted reaction

김태우 임춘우 **Le Thi Hoa**

경희대 동서의학대학원

Several synthetic approaches have used the copper(I)-catalyzed azide-alkyne cycloaddition (click reaction) to make cyclodextrin click clusters (CCCs). All perfunctionalized CCC synthesis starts from 6-azido-6-deoxy-cyclodextrins. Thus the easy way to synthesize highly pure, gram-quantity 6-azido-6-deoxy-cyclodextrins is essential as a first step of successful CCC application development.The conventional synthesis of 6-azido-6-deoxy-cyclodextrin has been based on SN2 reaction of 6-bromo/iodo-6-deoxy-cyclodextrin. For the preparation of 6-bromo/iodo-6-deoxy-cyclodextrin, the Vilsmeier-type reagents arising from interaction of bromine or iodine with triphenylphosphine and N,N-dimethylformamide, used in situ was originally reported by Gadelle, A. and Defaye, J. However, the removal of the resulting triphenyl phosphine oxide makes the work-up tedious and time consuming in practice. In this poster we report the facile synthesis of 6-azido-6-deoxy-cyclodextrin via 6-chloro-6-deoxy-cyclodextrin. The method can be easily scale-up up ~ 20 g without any trick work-up. The purity of 6-azido-6-deoxy-cyclodextrin was determined by 300/600 M Hz 1H NMR.



Scheme . Reactions and reagents. a) Methanesulfonyl chloride, DMF, 65 C; b) NaN3, DMSO, MW.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-999**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Acceptor : pyrrolo [3,2-*b*]pyrrole-2,5-dione Based Novel Alternating Polymers for Efficient OPVs

박혜지 송수희 심주영 진영웁[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

The DPP unit has a well-conjugated structure, which leads to strong π-π interaction, and the lactapart makes the DPP unit exhibit a high electron-withdrawing effect, and hence the DPP unit has high electron affinity. In our study, new conjugated novel materials containing electron donor-acceptor pairs for OPV device utilizing a new type of materials pyrrolo[3,2-*b*]pyrrole-2,5-dione, are reported to show good solubility at room temperature in organic solvents. So The new type of materials was poly(*N*-9-heptadecanyl-2,7-carbazole-alt-1,4-bis(4-butylphenyl)-3,6-bis{5-[4-(diphenylamino)phenyl]-2-thienyl}pyrrolo[3,2-*b*]pyrrole-2,5-dione) (PCDTPPDB), poly(*N*-9-heptadecanyl-2,7-carbazole-alt-3,6-bis{5-[4-(diphenylamino)phenyl]-2-thienyl}-1,4-diphenylpyrrolo[3,2-*b*]pyrrole-2,5-dione) (PCDTPPDH), poly(*N*-9-heptadecanyl-2,7-carbazole-alt-3,6-bis{5-[4-(diphenylamino)phenyl]-2-thienyl}-1,4-bis(4-methylphenyl)pyrrolo[3,2-*b*]pyrrole-2,5-dione) (PCDTPPDM). Under white light illumination (100 mW/cm^2), the cell based on PCDTPPDB/$PC_{71}BM$ as the active layer has a short circuit current density (J_{sc}) of 5.31 mA/cm^2, an open circuit voltage (V_{oc}) of 0.71 V, and a fill factor (*FF*) of 35 %. The power conversion efficiency (PCE) is 1.33 %. Under the same white light illumination, for PCDTPPDH J_{sc} is 4.23, V_{oc} is 0.65 and *FF* is 34%. PCE is 0.93 %. Under the same white light illumination, for PCDTPPDM J_{sc} is 4.61, V_{oc} is 0.66 and *FF* is 35%. PCE is 1.06 %.

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발표코드: **ORGN.P-1000**

발표분야: 유기화학

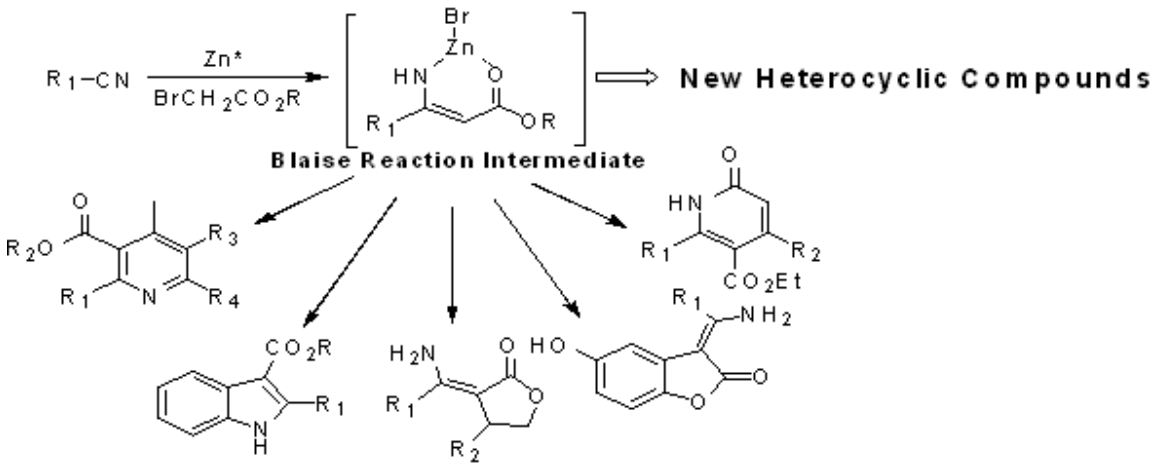
발표종류: 포스터, 발표일시: 수 16:00~19:00

Tandem Synthesis of Heterocyclic Compounds Using the Blaise Reaction intermediate.

전유성 이상기

이화여대 화학/나노과학과

The heterocyclic compounds are the core structure of many biologically active compounds, which are considered to be an important chemical synthon of various physiological significance and pharmaceutical utility. Although numerous synthetic methods have been developed, synthesis of heterocyclic compounds still remains a significant challenge for synthetic chemists. Recently, we have demonstrated that the Blaise reaction intermediate, a zinc bromide complex of?β-enaminoester, could react with various electrophiles to afford heterocyclic compounds, which are important components in various natural products, pharmaceuticals, and functional materials. We present here our recent results on the development of tandem one-pot methods for the synthesis of heterocyclic compounds using the Blaise intermediate.



대 한 화 학 회
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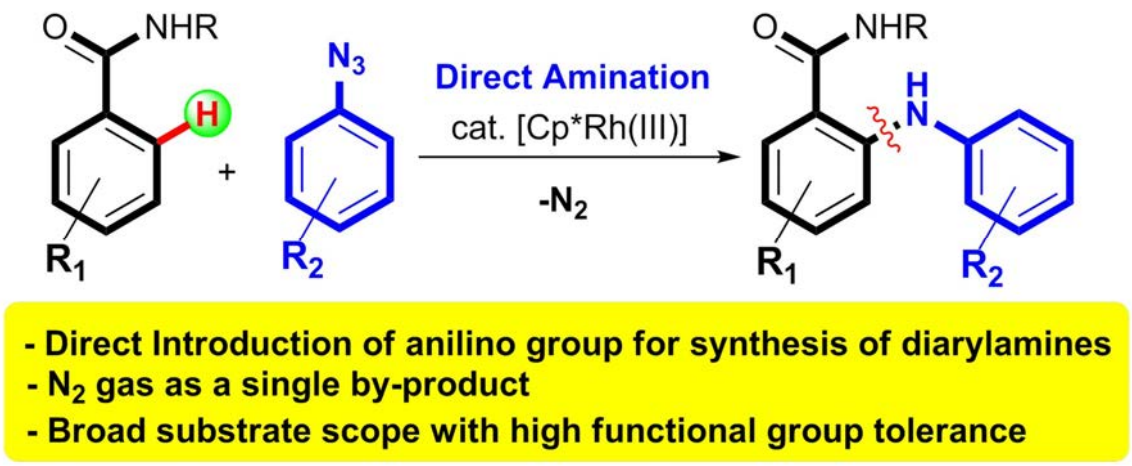
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1001**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium-Catalyzed Direct C-H Amination of Benzamides with Aryl Azides: A Novel Synthetic Route to Diarylamines

유재윤 신광민[1] 박세흠 김지영 장석복

KAIST 화학과 [1]KAIST 화학과

The rhodium-catalyzed intermolecular direct C-H amination of benzamides and ketoximes has been developed for the first time using aryl azides as the amino source. Diarylamines are obtained in high yields over broad substrate scope with excellent funcational group tolerance. Direct and selective C-2 amination of indole was also subsequently achieved with the same catalyst system using a pyrimidyl group as an easily intallable and readily removable directing group. The aminaton requires no external oxidants to release only nitrogen gas as the single by-product, thus offering an environmentally benign procedure. Synthetic utility of 2-anilinobenzamides, readily obtainable through the present study, was demonstrated in the preparation of carbazoles and biologically important compounds.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1002**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Environmentally-friendly efficient oxidation of benzylic alcohols using UHP/DBDMH in water

정연진 이종찬

중앙대 화학과

The oxidation of alcohols to the corresponding carbonyl compound has been recognized as a fundamental organic transformation in organic chemistry.In general, various methods have been achieved using toxic reagents , intractable method and transition metal containing oxidation.Therefore, we need development of eco-friendly and simple oxidative methodology.We have accomplished green and efficient oxidation of benzylic alcohols using water which is ideal solvent in green chemistry. The generality of this reaction was shown by the successful oxidation of benzylic alcohols with UHP(1.0eq) and DBDMH(0.5eq) in water(1ml) at 60℃ for 30~60min giving the corresponding aldehydes and ketones in high yields. Depending on solubility of water, the reaction was carried out on water condition. In conclusion, we have developed a green and efficient protocol for the oxidation of a variety of alcohols with the reagent combination of UHP and DBDMH in water.

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장소: 부산BEXCO

발표코드: **ORGN.P-1003**

발표분야: 유기화학

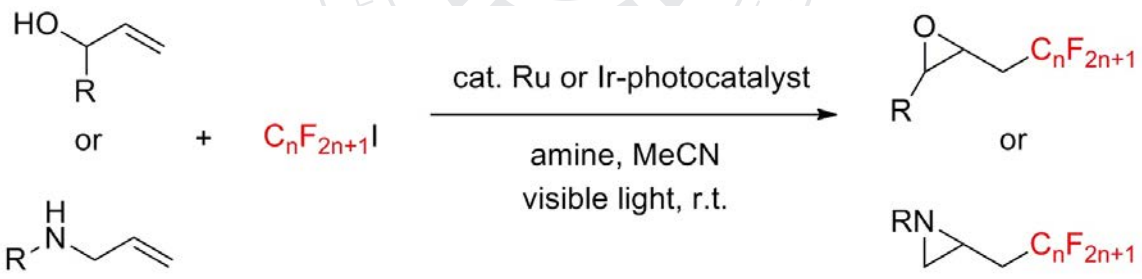
발표종류: 포스터, 발표일시: 수 16:00~19:00

The generation of perfluoroalkylated oxiranes and aziridines by visible light photocatalysis

김은진 최성규 조은진

한양대 응용화학과

An efficient method for the generation of perfluoroalkylated oxiranes and aziridines has been developed. A variety of allylic alcohols and allylic amines with perfluoroalkyl iodide were transformed into the corresponding perfluoroalkylated oxiranes and aziridines by using Ru- or Ir-photocatalysts under visible light irradiation. The mild conditions tolerate various functional groups.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1004**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficiencies of bulk-heterojunction polymer solar cells based on phenanthrothiadiazole

심주영 송수희 박혜지 진영읍[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

Recently, polymers solar cells(PSCs) have attracted much attention in the field of renewable energy technologies due to their potential for low cost, lightweight, and good compatibility with the roll-to-roll process for making flexible large area devices. we reported novel conjugated donor/acceptor conjugated polymers containing phenanthro[9,10-*c*][1,2,5]thiadiazole. The polymerization to generate PCPDTPT, PCPDTDTPT and PCDTPT were performed by using Stille polymerization with Pd catalysis. All of polymers have good solubility in common organic solvents . PCPDTDTPT has the lowest band gap of these polymers. Optical and electrochemical characterizations reveal that polymers have proper energy diagram. The power conversion efficiencies of these polymers show 0.77 ~ 1.24 %.

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장소: 부산BEXCO

발표코드: **ORGN.P-1005**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One pot reaction of alcohol oxidation, aldol condensation and [1,4] addition by Ru(OH)x/ZrO_2 catalyst

박성준 조홍준 이윤식

서울대 화학생물공학부

Macromolecular C-C coupling by aldol condensation and Michael-addition is one of the challenging tasks in organic syntheses. In addition, with the oxidation of the alcohol substrates employed prior to these reactions, the challenge becomes even greater. In this study, we synthesized 1-5 diketones by the reaction of acetophenone with alcohol substrates. Using ruthenium hydroxide catalyst prepared on ZrO_2 support (Ru(OH)x/ZrO_2) as a heterogeneous catalyst, alcohol was effectively oxidized to aldehyde with molecular oxygen. After oxidation, 1-5 diketones were obtained by aldol reaction and [1,4] Michael-addition in a consecutive manner. The retrieved catalyst after the reaction was capable of being reused keeping its high catalytic performance.

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발표코드: **ORGN.P-1006**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Unsymmetrical Formacetals and Alkyl/aryloxymethyl Carboxylate from1-Alkyl/aryloxymethyl-3-methyl-1H-1,2,3-triazol-3-ium Triflate

조우진 박찬수 지대윤

서강대 화학과

Powerful leaving groups expedite to form formacetal linkage (ROCH2OR'). A new reaction of unsymmetrical formacetal formation was developed by utilizing 1-alky/aryloxymethyl-3-methyl-1H-1,2,3-triazol-3-ium triflate. This novel leaving group can be applied to both aliphatic and aromatic alcohols effectively. This mechanism can be extended to protect alcohols and carboxylic acids.

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발표코드: **ORGN.P-1007**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Poly(N-Heterocyclic Carbene)s from Histidine: A Recyclable Organocatalyst

서의령 정영근

서울대 화학부

Vinylimidazoliums have been synthesized in three steps from commercially available L-histidine. The vinylimidazoliums were polymerized via radical polymerization using AIBN to give water-soluble poly(imidazolium)s. The corresponding poly(NHC)s display catalytic activities in a benzoin condensation reaction that were superior to those displayed by monomeric analogues. Moreover, the new catalyst was successfully recovered and reused.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표코드: **ORGN.P-1008**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Characteristics and Synthesis of Conjugated Polymers Based on Phenanthrothiadiazole and Cyclopentadithiophene Moiety

심주영 송수희 박혜지 진영읍[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

Last few years, all solutions processed polymer solar cells (PSCs) have attracted scientific and industrial interests. To realize needs for low-cost manufacturing, lightweight, large-area and flexible photovoltaic devices, p-type photoactive conjugated polymer materials have important role on boosting high efficiency of PSCs. These donor-acceptor conjugated polymers, PCPDTPTp and PCPDTPTm, were synthesized by Stille polymerization of cyclopenta[2,1-*b*:3,4-*b*']dithiophene and phenanthro[9,10-*c*][1,2,5]thiadiazole. The spectra of the solid films show absorption bands with maximum peaks at 450, 550 nm, respectively. Under white light illumination (AM1.5G, 100 mW/cm^2), polymer:PCBM layers showed PCE of 1.80, 1.00%, respectively.

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발표코드: **ORGN.P-1009**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photovoltaic Performance of Conjugated Copolymers Utilizing Dimethyl-benzimidazole for Solar Cells

심주영 송수희 박혜지 진영읍[1] 서홍석

부산대 화학과 [1]부경대 공업화학과

Polymer solar cells (PSCs) are the most suitable for roll-to-roll and flexible cells because organic-based photoactive materials can be coated or printed on lightweight plastic foil to achieve good conformal flexibility. Successful approaches to leading low bandgap (LBG) polymers include the incorporation of electron-rich donor and electron-deficient acceptor segments along the conjugated polymer backbone. Planarization of polyaromatic system facilitates the π -electron delocalization and extends the effective conjugation length, providing another effective way to decrease the optical bandgap. Organic photovoltaics (OPVs) device utilizing a new type of acceptor, 2,2-dimethyl-2*H*-benzimidazole, show the absorption range with the wider extention of the solar spectrum, these donor-acceptor conjugated polymers were synthesized by the Stille coupling reaction. The solid films of PCPPDTMBIs show absorption bands with two maximum peaks at about 408 ~ 417 and 613 ~ 640 nm. The PCPPBBTMBIs show two maximum peaks at about 440 ~ 444 and 627 ~ 650 nm which are red-shifted about 5 ~ 30 nm as compared to PCPPDTMBIs caused by the introduction of bithiophene units. The bulk heterojunction photovoltaic device using PCPPBBTMBIs as the p-type material delivered a promising efficiency of 0.21 ~ 0.46% with an enhanced a V_{oc} value of 0.82 V, J_{sc} value of 1.42 ~ 2.12 mA/cm^2, and a *FF* of 0.26 ~ 0.34.

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발표코드: **ORGN.P-1010**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Water-soluble Imidazolium Salts and Their Use in Palladium-Catalyzed Oxidation of Alcohols in Water

조범신 정영근[1] 한진욱[2]

서울대 화학과 [1]서울대 화학부 [2]한양대 화학과

Imidazolium salts having a quaternary ammonium salt were synthesized. They formed vesicles in water. The size of vesicles could be controlled by the chain length of alkyl substituents at the 1,3-positions on the imidazolium salt. The effect of a vesicle size in a catalytic activity of a palladium-catalyzed oxidation of alcohols in water was examined

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장소: 부산BEXCO

발표코드: **ORGN.P-1011**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of New Heteroleptic Blue Phosphorescent Iridium (III) Complexes Using Benzimidazole Carboxylate Derivatives as Ancillary ligands

박혜정 김지나 유현지 윤웅찬

부산대 화학과

유기 발광 다이오드(Organic Light Emiiting Diode)는 빛을 내는 발광 층을 포함하는 여러 유기화합물들의 얇은 막으로 이루어진 디바이스로 구동전압이 낮고, 유연하여 구부릴 수 있으며(flexible), 색 재현성이 뛰어나 차세대 발광 디바이스로 각광받고 있다. 이 유기 발광 다이오드에 전압을 걸어주면 발광 층의 물질의 들뜬 상태인 엑시톤이 생성되고 이 엑시톤 중 일중항 상태의 엑시톤이 25% 삼중항 상태의 엑시톤이 75%의 분율로 생성되며, 이때 주된 분율로 생성되는 삼중항 엑시톤은 긴 수명시간을 가지며 인광 발광이 효율적으로 일어나지 못하고 열 에너지로 소비된다. 전기에너지가 삼중항 엑시톤을 거쳐 열 에너지로 소비되는 에너지를 효율적으로 빛 발광으로 수확하기 위해 첨가되어 사용되는 도판트 물질인 이리디움 착화합물 개발에 대한 연구가 진행 되어 왔으며 특히 청색 도판트 물질인 청색 인광 이리디움 물질 개발에 많은 관심이 집중되고 있다. 본 연구에서는 벤즈이미다졸카르복실레이트 유도체 3 종을 새로운 보조리간드(ancillary ligand)로 그리고 2-(2,4-다이플루오로페닐)-4-메틸-피리딘 및 2-(2,4-다이플루오로-3-트리플루오로메틸-페닐)-4-메틸-피리딘을 주리간드 (main ligand)로 사용하여 새로운 청색 인발광의 이리디움 화합물 6 종을 합성하고 이들 합성된 이리디움 착화합물들의 흡수스펙트라, 인발광스펙트라, 인발광 양자효율을 측정하여 기존의 착화합물과 비교하여 새로운 청색 인광물질로 개발하고자 하였다. 이들 이리디움 화합물들은 365nm~373nm 과 441nm~449nm 에서 각각 최대 흡수 파장을 가지며 456nm~467nm 에서 최대 발광 파장을 나타내고 0.12~0.28 의 비교적 높은 인발광 광자효율을 가짐을 보여주고 있다.

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장소: 부산BEXCO

발표코드: **ORGN.P-1012**

발표분야: 유기화학

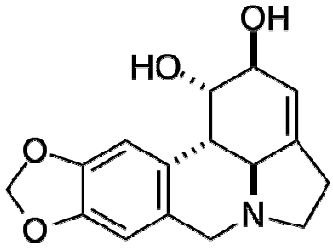
발표종류: 포스터, 발표일시: 수 16:00~19:00

Unified approach toward the total syntheses of (±)-lycorine, (±)-α-lycorane and (±)-1-deoxylycorine

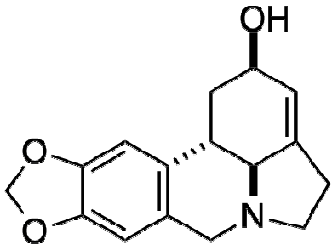
정용근 이상철 조천규

한양대 화학과

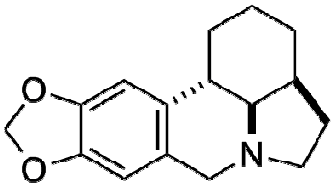
Lycorine 1 is a toxic crystalline alkaloid present in various Amaryllidaceae plant species that include Lycoris, Pancratium, Narcissus, Galanthus, Zephyranthes and Haemanthus. Arising from norbelladine in its biosynthesis, lycorine has the pyrrolo[de]phenanthridine framework that is common to many other congeneric natural compounds (Figure 1). It has a wide variety of important biological activities range from the inhibition of ascorbic acid biosynthesis, the prevention of cyanide-insensitive respiration to the inhibition of growth and cell division in higher plants. Similar to other Amaryllidaceae small molecule constituents, such as pancratistatin and trans-dihydronarciclasin, it has attracted much attention for its highly potent antitumor effects, both in vitro and in vivo, as well as in cancer cells that display resistance to proapoptotic stimuli. Such biological importance together with challenging chemistry of lycorine and related alkaloids have induced many synthetic studies and the generation of many structural analogs. As a part of our ongoing study exploring the utility of 3,5-dibromo-2-pyrone in target-oriented synthesis, we have envisioned the pyrrolo[de]phenanthridine skeleton of lycorine and related natural alkaloids could be rapidly constructed from the cycloadduct of 3,5-dibromo-2-pyrone with a styrene type dienophile. Present herein would be our path-finding effort that affords the eventual synthesis of (±)-lycorine and (±)-α-lycorane



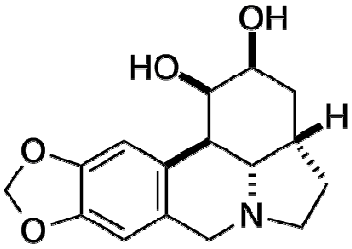
1: lycorine



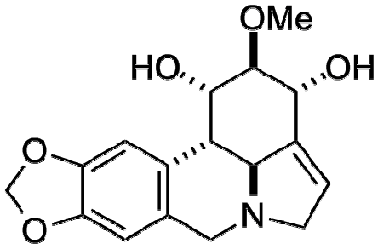
2: 1-deoxylycorine



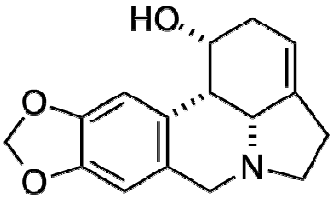
3: α-lycorane



4: trianthine



5: giminorine



6: fortucine

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1013**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Phototriggered Mass Migrations Leading to Aggregation Induced Fluorescence Patterning in Discotic Cyanostilbene Thin Films

박진욱 박수영[1]

서울대 재료공학과 [1]서울대 재료공학부

Fluorescent contrast with high quantum yield in the fluorescence patterned films is a significant performance parameter of optical information storage due to the high sensitivity, selectivity of fluorecence spectroscopy. To achieve such patterns, several patterning techniques have been proposed like scanning-beam lithography, photolithography and nanoskiving. However, these methods require multiple steps and stringent conditions such as cleanroom condition and high process/maintenance cost. To solve this problem, recently, simple and single-step fabrication method has been reported to combine photoinduced mass migration (PMM) with fluorescence functionality. Commonly, the key to PMM behavior is known to the repeatable trans-cis isomerization cycles of azobenzene chromophore on irradiation with an appropriate wavelength light. However, azobenzene derivatives exhibit no or low fluorescent efficiency in solid state. To provide fluorescence functionality, the stringent requirements are demanded such as complex synthesis and spectral separation. Now, many researchers have studied to develop the material which shows PMM behiavror with their own photolumnisecence (PL) porperty with high quantum yield in condensed state for the amplification of fluorescent contrast ratio.In this presentation, we report a novel hexacatenar cyanostilbene derivative, (Z)-2,3-bis(3,4,5-tris(dodecyloxy)phenyl)acrylonitrile, [GCS] which shows discotic liquid crystal (LC) property at room temperature and forms photo-responsive crystalline film. We successfully demonstrate a novel facile method to provide highly fluorescent micro-patterns by combining aggregation induced enhanced emission (AIEE) with PMM behavior by using GCS material.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1014**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Substituent Effects on Hydride Transfer Reactions of Acridinium Ion with Benzimidazoline Derivatives

한인숙

강원대 과학교육학부

The kinetics of hydride transfer reactions of 10-methylacridinium ion (Ac+) with a series of 5-X-1,3-dimethyl-2-(Y-phenyl)benzimidazoline (X-BIH) (X: CH3, H, F, Cl; Y: p-CH3, H, p-F, p-Cl, m-F, m-Cl, m,m'-Cl2) Cl2) have been measured spectrophotometrically in 2-propanol-H2O (4 : 1, v/v) at 25 ? 0.1 oC in order to explore the substituent effect at the 5-position of benzimidazole ring. The reactivity is decreased when the electrowithdrawing group is added in the benzimidazole ring as we expected. However inductive effect is more significant than the resonance effect. The rate constants for the reactions of Ac+ with a series of X-BIH are linearly correlated with the Hammett parameters with the slopes of -1.596, -1.620, -1.666 and -1.678. The reactivity-selectivity principle can be applied to the present system with the reaction constants. This result will be discussed in terms of mechanism and compared with those of other hydride transfer reactions with NADH analogues.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1015**

발표분야: 유기화학

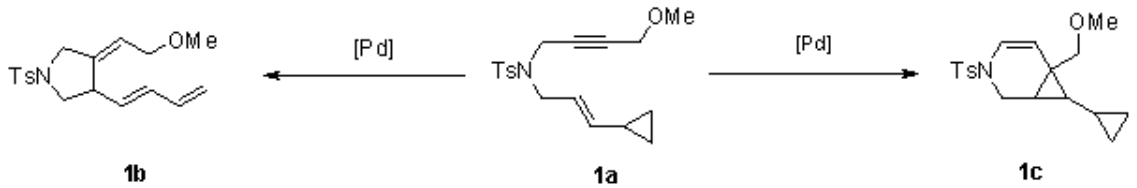
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Cycloisomerization of Enynes to Bicyclo[4.1.0]hept-2-enes.

오혜미 정영근

서울대 화학부

Transition metal-catalyzed cycloisomerization of enynes has been reported. The cycloisomerization of 1,6-enynes gives various cyclic compounds. Among them, the formation of bicyclo[4.1.0]heptenes has been known for Pt, Au, Ir, and Rh-catalyzed cycloisomerization of 1,6-enynes. Recently, we found that a cycloisomerization of 1,6-enynes in the presence of palladium catalyst led to a formation of bicyclo[4.1.0]heptenes. This is the first observation of the catalytic use of palladium compounds in the synthesis of bicyclo[4.1.0]heptenes from 1,6-enynes. 1a in the presence of Pd with PPh3 forms an monocyclic triene compound (1b). However, 1a in the presence of Pd with some ligand forms bicyclo[4.1.0]heptanes.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1016**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemical Elucidation of Lucentamycin A

윤지혜 이지연[1] 이원구 심태보[2]

서강대 화학과 [1]KIST 화학키노믹스센터 [2]KIST 생체과학연구본부

A synthesis of the E-isomer of the proposed structure of the novel tripeptide, lucentamycin A, was performed in an attempt to define the correct stereochemistry of this natural product. The route developed employs a stereoselective Rh-catalyzed reductive cyclization process to generate the key pyrrolidine residue in the target and a stereospecific inversion of the Z-olefin geometry to form desired E-isomer. Subsequent amide coupling reactions afforded the desired E-isomer of putative lucentamycin A. The results of spectroscopic studies on the synthesized substance show that olefin geometry is not the source of the mis-assignment of the lucentamycin A structure.

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장소: 부산BEXCO

발표코드: **ORGN.P-1017**

발표분야: 유기화학

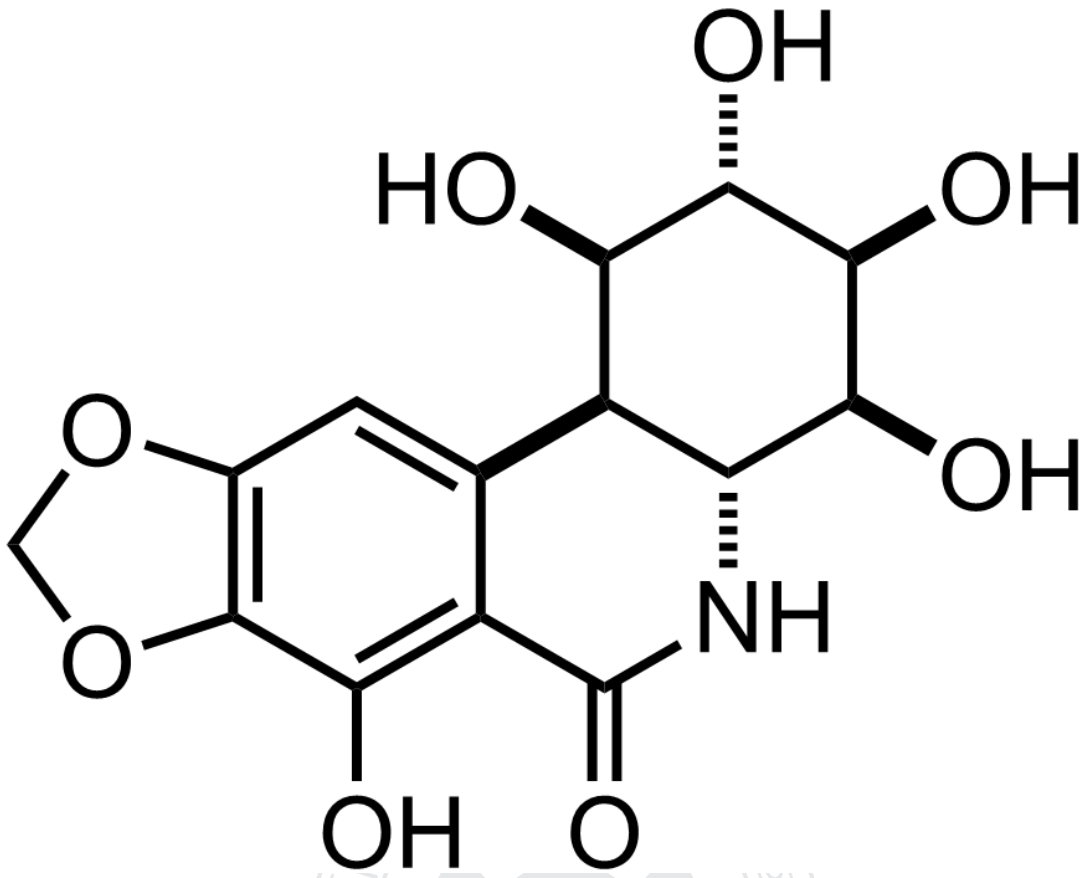
발표종류: 포스터, 발표일시: 수 16:00~19:00

Use of β-boronyl styrene in the cycloaddition reaction with 3,5-dibromo-2-pyrone for the total synthesis of (±)-pancratistatin

조현규 조천규

한양대 화학과

Pancratistatin is a natural compound that was initially extracted from Spider Lily a Hawaiian native plant that belongs to the family of Amaryllidaceae. It has been shown to have potent anti-cancer activities and selectively induce apoptosis in several human cancer cell lines. The promising biological activity and natural paucity has made pancratistatin an interesting target for total synthesis. Ever since the first total synthesis reported by Danishefsky and coworkers in 1989, many research groups around the world have presented novel strategies and routes to this natural compound. A few years ago, we have reported the first total synthesis of trans-dihydronarciclasine, very close congenor of pancratistatin, by utilizing Diels-Alder reaction of 3,5-dibromo-2-pyrone. Recently, we have successfully executed the total synthesis of pancratistatin by utilizing the same strategy. During the synthesis, we have learned b-boronyl stryrene can undergo cycloadditiion reaction with 3,5-dibromo-2-pyrone and the boronate group of the cycloadduct can be readily converted into hydroxy group. Herein, we report the successful realization of our concept which allowed more efficient total synthesis of (±)-pancratistatin.



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1018**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

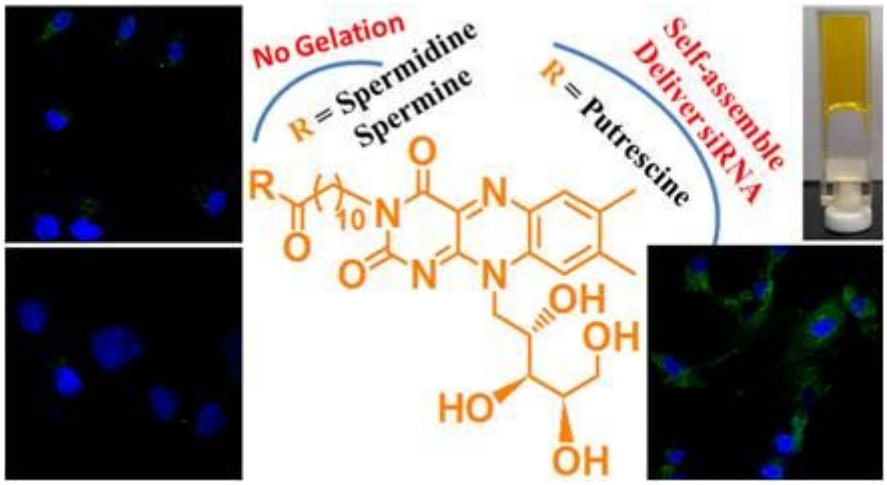
Low-molecular-weight supramolecular hydrogel of riboflavin for VEGF-siRNA delivery

Patil Sachin Prakash 김병현[1]

포항공과대 chemistry [1]포항공과대 화학과

The use of an efficient carrier for siRNA delivery is one of determining factors for successful siRNA therapy. Current approaches for the delivery of siRNA in vivo include the preparation of siRNA-bioconjugates and the incorporation of siRNA into multifunctional polymeric or lipidic nanodevices. Most of these techniques involve the formation of nanoscale siRNA composites, which are likely to disperse rapidly. Sustained intracellular release of siRNA might be useful approach towards maintaining the cytosolic siRNA concentration above the critical threshold for longer period of time. Recently, several polymeric hydrogels have been developed for the intracellular sustained release of siRNA. Hydrogels are typically biocompatible, making them suitable for a wide range of applications. Low-molecular-weight hydrogels (LMWGs) can be employed as substitutes for polymeric gels in many applications, even though they possess unique properties.Main interest is the design of biomaterials for delivery of drugs, bioactive agents including siRNA.1?2 Herein, we will present the first LMWG-based biomaterial, derived from riboflavin an essential biomolecule, which mediates the siRNA delivery into cells with nearly equal proportion to that of the lipofectamine2000 at higher concentration. Most notably, the siRNA delivery was affected by the hydrogelation properties of the compound. The LMWG delivers siRNA specifically into the cytosol of the cell by endocytosis pathway, where the siRNA is uniformly diffused, and functionalized through the RNAi mechanism. We observed the siRNA activity occurring specifically from VEGF-siRNA released from the hydrogel; however, no gene downregulation was occurred from the scrambled sequence. The biocompatible and temperature sensitive fluorescent hydrogel from vitamin B2 forms an entangled fibers similar to extracellular matrices, have potential to be used for several biological applications such as tissue engineering, bio-sensing, and effective delivery with controlled release of

drugs including siRNA.References: 1. S. P. Patil, H. S. Jeong, and B. H. Kim, Chem. Commun. 2012, 48, 8901. 2. S. P. Patil, J. W. Yi, E. K. Bang, E. M. Jeon and B. H. Kim, MedChemCommun. 2011, 2, 505.



대한화학회
THE KOREAN CHEMICAL SOCIETY

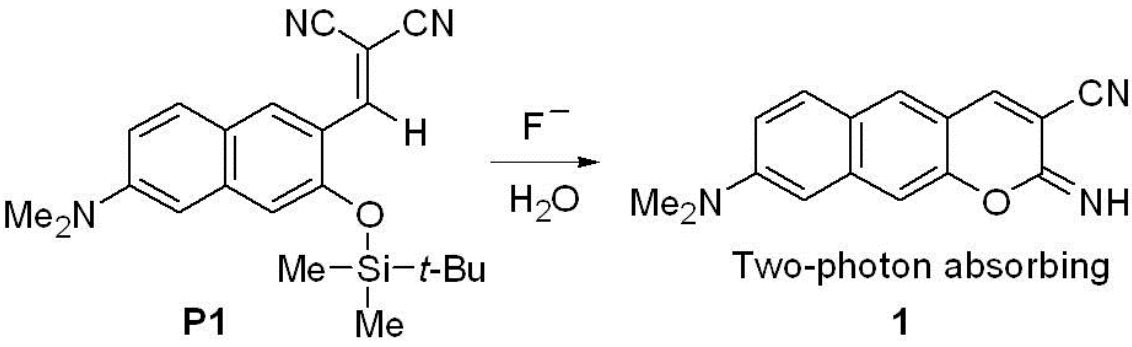
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1019**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

In vivo Two-photon Fluorescent Imaging of Fluoride with a Desilylation-based Reactive Probe

김도경 안교한

포항공과대 화학과

Fluoride is added to drinking water to promote dental health in some countries. Fluoride is also found in many common household products, including toothpaste and dietary supplements. Other uses of fluoride are as glass-etching and chrome-cleaning agents, and insecticides and rodenticides. An acute intake of fluoride can cause gastric and kidney disorders, skeletal fluorosis, and urolithiasis in humans. Therefore, tools that allow us to detect fluoride in our environment as well as to monitor fluoride in living species are indispensable. The fluorescent analysis method has received continuing attention owing to its highly sensitive and handy features as well as its versatility for bioimaging purpose. Accordingly, various fluorescent probes for fluoride have been developed in recent years based on novel sensing strategies. The fluoride mediated desilylation approach, originally devised by Swager and co-workers, can alleviate these problems and thus has received growing interest recently.Herein, we report such a probe that shows high sensitivity and selectivity toward fluoride ion, and, furthermore, that allows two-photon fluorescent imaging in living species for the first time.



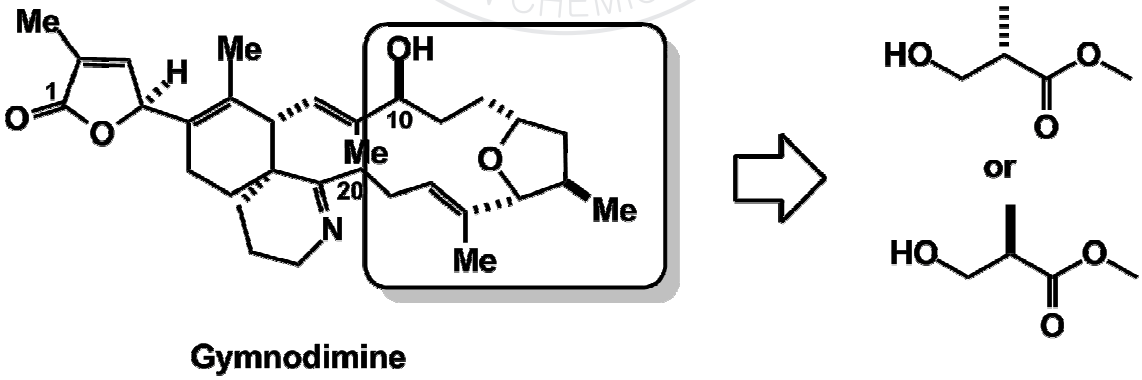
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1020**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of the Tetrahydrofuranyl Subunit of Gymnodimine

GAOYAQIONG 이효원

충북대 화학과

A macrocyclic marine toxin gymnodimine was isolated oysters in 1994. This macrocyclic imine phycotoxin was produced from dinoflagellate such as *Karenia selliformis* and *Gymnodinium cf. mikimotoi.* Gymnodimine includes a spirocyclic imine ring system and a trisubstituted tetrahydrofuran embedded within a 16-membered macrocycle. The toxtic effects of gymnodimine arise from the binding to nicotinic acetylcholine receptorsThe C10?C20 fragment of gymnodimine is composed of a tetrahydrofuranyl moiety. The synthesis of the tetrahydrofuran ring is based on a stereocontrolled cyclization by using either 5-*exo* opening reaction on an epoxide or the Michael reaction. Disclosure of further details will be followed.



Gymnodimine

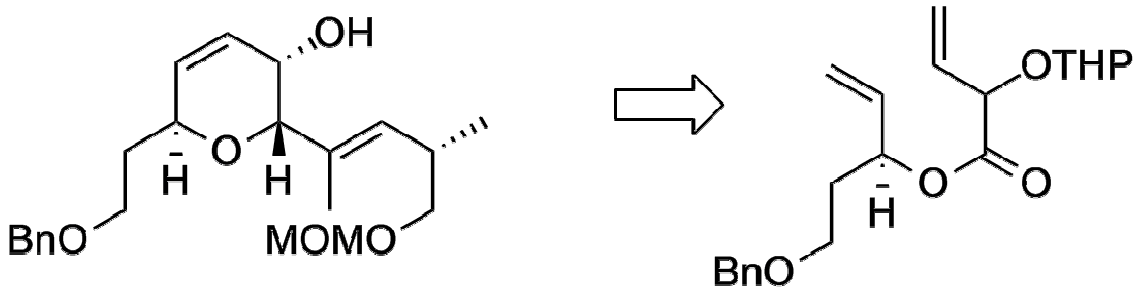
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1021**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of the C1-C15 Fragment of Sorangicin A by Using Cross-Coupling Reactions

한선영 최일영[1] 이효원

충북대 화학과 [1]한국화학연구원 의약화학연구센터

Antibiotic macrolide (+)-sorangicin A was isolated from *Sorangium cellulosum* in 1985. Its extraordinary antibiotic activity demonstrated against a broad panel of both Gram-positive and Gram-negative bacteria. A key synthetic strategy for the (*E*)-double bond at C7-C8 of sorangicin A was the metal-catalyzed cross-coupling reactions such as the Suzuki-Miyaura cross-coupling reaction.Herein, we report the synthetic efforts towards the key fragments of sorangicin by utilization of several reactions such as ring-closing metathesis (RCM) for the preparation of (*Z*)-double bond (C11-C12), the Suzuki-Miyaura cross-coupling reaction for the (*E*)-double bond (C7-C8), and the Evans aldol reaction. Details of the synthesis will be described.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1022**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of highly thermal conductive Liquid crystalline epoxy polymers.

김지연

명지대 화학과

Recently the metal electric and electronic devices have been replaced by plastic for to reduce the weight. But thermal conductivity of plastic is very poor compared to metal. So those devices particularly requiring heat dissipation are not suitable for plastic. Epoxy resin containing liquid crystal substituents have high thermal conductivity so these problems can be solved easily.In this study, we synthesize various form of high thermal conductivity epoxy resin through substituential and structural change. And then we make Liquid Crystalline epoxy polymers through curing process and check the physical and thermal properties.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1023**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-Density Assembly of Gold Nanoparticles with Zwitterionic Carbon Nanotubes and Metal-free Electrocatalytic Activity of Ionic Carbon Nanotubes for Oxygen Reduction Reaction

신주연 김연수[1] 차아름[2] 이종목[3] 이상기

이화여대 화학/나노과학과 [1]이화여대 화학나노과학과 [2]이화여대 나노화학과 [3]이화여대 화학과

Gold nanoparticles (AuNPs) were assembled with high density onto multi-walled carbon nanotubes, which were functionalized with zwitterionic poly(imidazoliumsulfonate). The AuNP/zwitterionic CNT hybrids exhibited excellent electrocatalytic activity in oxygen reduction reaction (ORR). In order to elucidate the origin of positive effects of imidazolium salt on electrocatalytic activity, the metal-free electrocatalytic activities of the imidazolium salt-functionalized ionic multi-walled carbon nanotubes (IM-f-MWCNTs) in the oxygen reduction reaction (ORR) have been investigated. The zwitterionic poly(imidazoliumsulfonate)-functionalized MWCNTs exhbited remarkable electrocatalytic activity, which can be attributed to the induced-polarization of the pi-electrons of CNT surfaces accelerating interfacial electron transfer. The IM-f-MWCNTs showed better fuel selectivity than the commercial Pt/C electrocatalyst.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1024**

발표분야: 유기화학

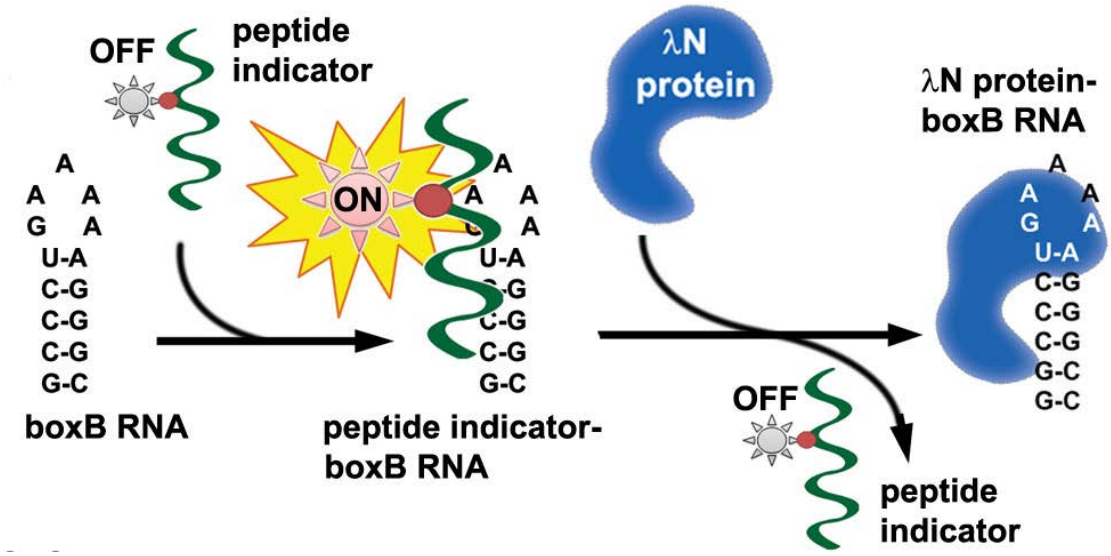
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Peptide Indicator Displacement Assay for Monitoring of RNA-RNA Binding Protein Interactions

정현석 김병현

포항공과대 화학과

RNA plays diverse biological roles as RNA-protein complex forms in cellular gene regulations, for examples, RNA transcription, mRNA translations, mRNA splicing, and post-transcriptional RNA regulation. These regulations are mainly controlled by specific type of proteins called RNA binding proteins (RBPs). They modulate RNA diverse function through specific interactions with RNAs through RNA recognition motifs, forming stable RNA-RBP complexes. Thus, monitoring of RNA-RBP interactions by fluorescence can contribute the real-time identification of RNA-RBP in diverse assay and the new types of sensors for RNA-RBP interactions in vivo. However, there are no reports of non-covalent labeling or immobilization for fluorescent monitoring RNA-RBP interactions. Here we describe a new type of fluorescent indicator displacement assay that monitor RNA-RBP interactions based on a fluorescent peptide indicator. The developed pyrene fluorophore labeled fluorescent peptide indicators recognize target RNAs with minimal RNA binding motifs and they are displaced with corresponding RBPs that recognize the target RNAs. This sensitive and non-destructive type of assay can monitor specific RNA-RBP interactions that mediate diverse RNA processing and this assay helps us to open new possibilities for studying meaningful RNA-RBP interactions.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1025**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

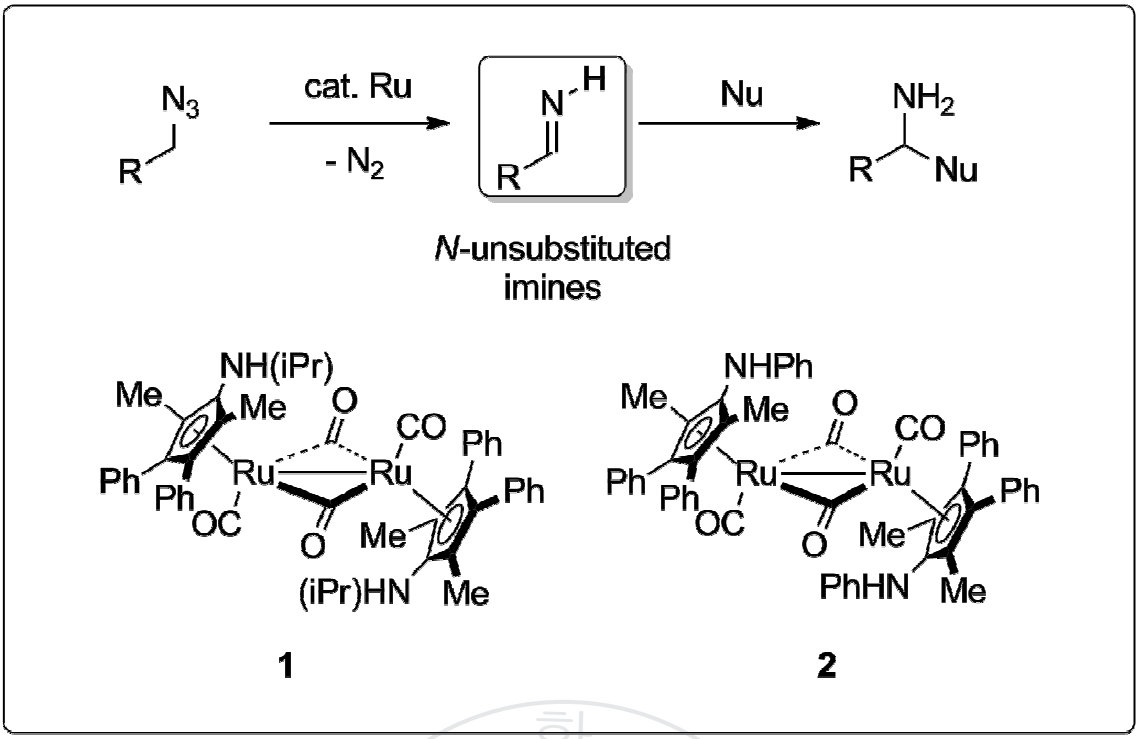
N-unsubstituted Imines: Ru-catalyzed Synthesis from Alkyl Azides, Characterization, and the Utility

한정훈 이영호 박재욱

포항공과대 화학과

Imines have been recognized as pivotal intermediates in organic synthesis, particularly for the preparation of nitrogen-containing bioactive natural products and derivatives. Unlike *N*-substituted imines, however, the synthetic scope of*N*-unsubstituted imines is still very limited. *N*-unsubstituted imines are known to be much less stable than the *N*-substituted analogs. This feature can be easily addressed by the fact that only few free *N*-unsubstituted imines have been successfully isolated or characterized.

Herein, we report that *N*-unsubstituted imines can be efficiently generated using1 and structurally related Ru complex 2 from alkyl azide. Remarkably, the mild conditions used in this transformation even allowed the observation of cis/trans isomers of *N*-unsubstituted imines on the basis of the NMR spectroscopy taken at room temperature. Moreover, this new protocol enabled various chemoselective transformations of *N*-unsubstituted imines such as one-pot imine formation-asymmetric allylation.



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THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1026**

발표분야: 유기화학

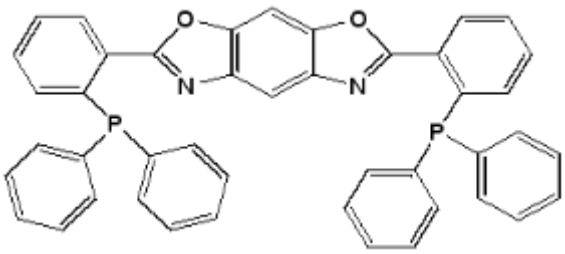
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Blue-Emitting Material of Bis[2-(2-(diphenylphosphino)phenyl)]benzo[d]oxazole (BPB)

임영훈 김익환 **TRINH DAC HOANH** 이범종[1]

인제대 화학과 [1]인제대 의생명화학과

Organic light emitting diodes (OLEDs) have a lot of advantages to compare with other display technologies such as thinner, brighter, low power consumption, etc. However, the lifetime, luminance efficiency and other OLED propertiesshould be still improved, especially the lifetime of blue emitting materials. In this work, we synthesized a new organic compound, bis[2-(2-(diphenylphosphino)phenyl)]benzo[d]oxazole (BPB), which based on the phosphino-benzoxazole structure. The structure of BPB was determined by ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-Vis and elemental analysis. This compound shows a blue emission under excitation by UV lamp of 365 nm. The photoluminescence (PL) property will be discussed.



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1027**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Tandem Catalytic One-Pot Synthesis of Caprolactam from Phenol with Multi-Function Pd/Sc(OTf)$_3$/Ionic Liquid Catalyst

신주연 정다정[1] 이상기

이화여대 화학/나노과학과 [1]이화여대 화학나노과학과

We developed a novel multi-function catalyst, consisting of Pd/Sc(OTf)$_3$/ionic liquid (IL), for the tandem one-pot conversion of phenol to caprolactam, a precursor of nylon-6, which is one of the world's largest commercial scale products. Synthesis of caprolactam generally involves a four-step procedure: two-step synthesis of cyclohexanone from phenol, i.e., hydrogenation of phenol to cyclohexanol, which is oxidized to cyclohexanone, cyclohexanone oxime formation, and Beckmann rearrangement of cyclohexanone oxime to caprolactam. Therefore, the development of a multi-function catalytic system for the tandem one-pot synthesis of caprolactam from phenol is highly challenging. Important finding is that Pd and Sc(OTf)$_3$selectively cooperated to catalyze the hydrogenation of phenol to cyclohexanone under extremely mild conditions (1 atm of H_2 pressure at room temperature) with excellent conversion (>99.9 %) and selectivity (>99.9%) within 2 h. Whereas, Sc(OTf)$_3$ and [bmim][PF_6] cooperated to catalyze the tandem transformation of the resulting cyclohexanone to cyclohexanone oxime and Beckmann rearrangement, affording caprolactam. The results will pave the way to the development of environmentally friendly production of the industrially important caprolactam, and will be useful for the future design of multi-function catalysts.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1028**

발표분야: 유기화학

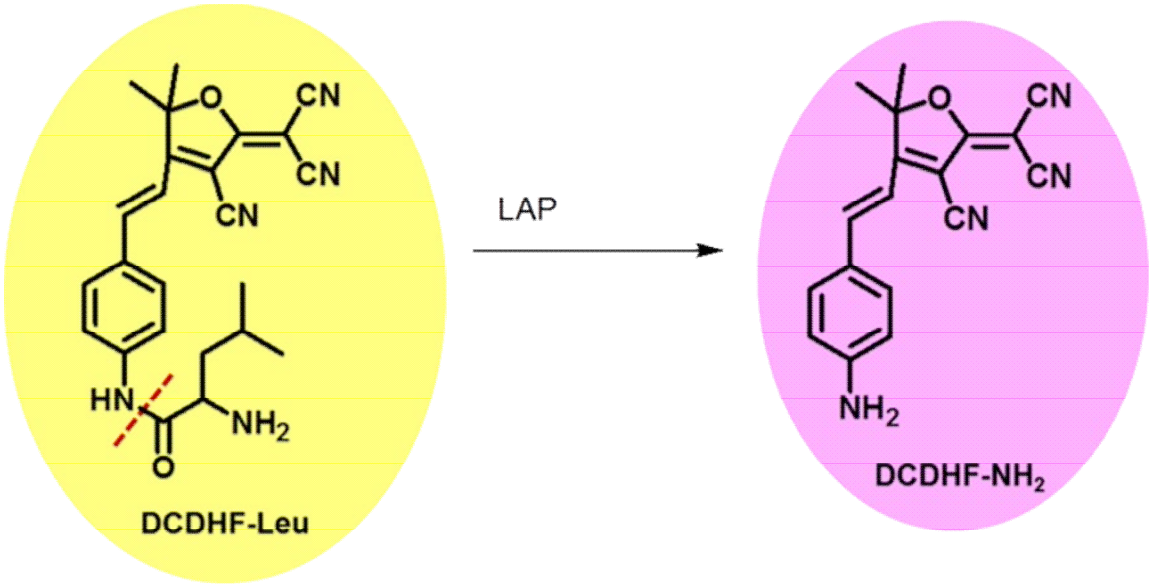
발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of Leucine aminopeptidase activity through DCDHF probe showing dual signals

윤혜영

서울대 화학부

l-Leucine aminopeptidases (LAPs) are metallopeptidases which cleave leucine residues at N-terminal amino acid from peptides or protein substrates. They are widely distributed in organisms from bacteria to humans and play crucial roles in cell maintenance and cell growth. Thus, assays for leucine aminopeptidase are necessary for measuring its activity and inhibitor potency. Recently, we developed a new small molecule probe which exhibits colorimetric and fluorogenic changes according to LAP activity. This probe is comprised of 2-dicyanomethylene-3-cyano-2,5-dihydrofuran fluorophore (DCDHF) and the capped aniline functionality which enabled quenching the emission at 603 nm of the probe. Uncapping of the probe by LAP shows about 10-fold fluorescence enhancement in time-dependent manner. In addition, this enzyme activity can be observed via the naked eye. Collectively, the DCDHF-based probe is successfully applied to LAP activity assay and has the utility for the high through-put screening of inhibitors.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1029**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic dye based on squaraine and benzothiadiazole for efficient dye-sensitized solar cells.

성지연 전용준 홍종인

서울대 화학부

Since the first report in 1991 by Michael Gr?tzel et al., dye-sensitized solar cells (DSSCs) have received much attention because of their low production cost and relatively high energy conversion efficiency. Conventional DSSCs typically consist of a nanocrystalline titanium oxide, a sensitizer, and an electrolyte. Among these three parts, a suitable photosensitizer is essential in realizing highly efficient DSSCs. The general configuration of most reported organic dyes is a D-π-A structure because of its effective photoinduced intramolecular charge transfer (ICT) properties. The photo physical and electrochemical properties of such dyes can easily be tuned by incorporating a variety of donor, spacer, and acceptor moieties. Herein, in an effort to realize panchromatic dyes, we combined an additional 400-550 nm light harvesting dye with the donor moiety to extend the absorption range from Uv-vis to the near-IR region.

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발표코드: **ORGN.P-1030**

발표분야: 유기화학

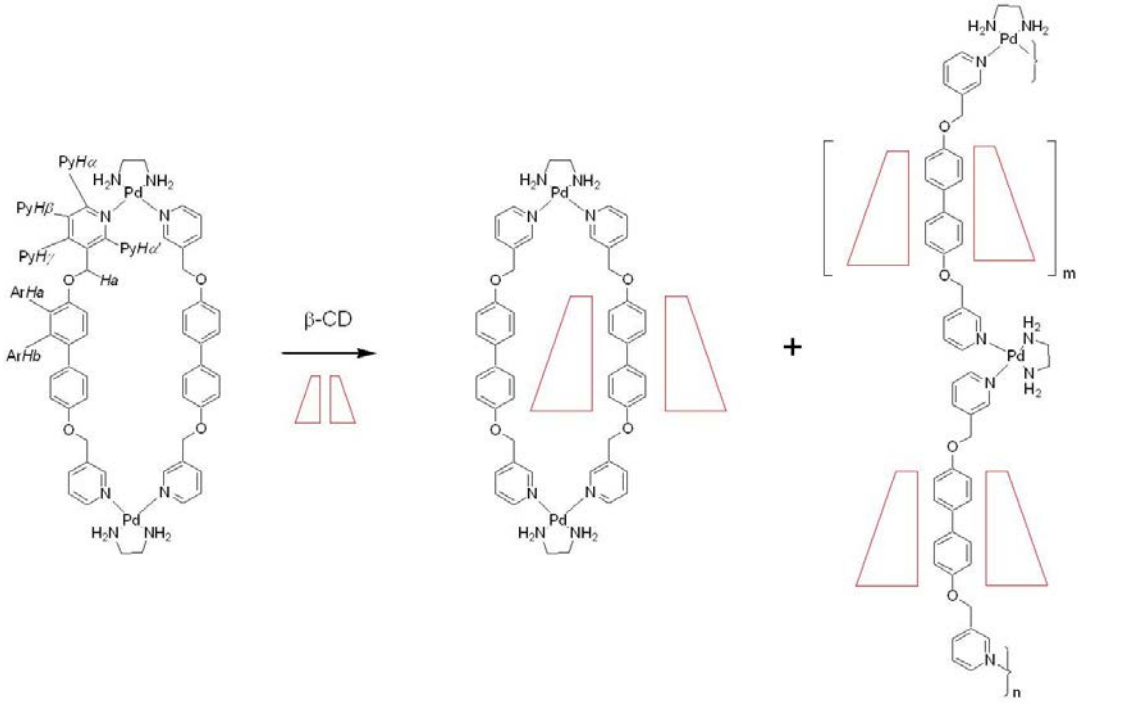
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stability Study of Self assembled Macrocycle between Pd(II) metal and Isomeric Pyridyl Ligand Molecules

임춘우 김태우 Le Thi Hoa 김성현[1] 김동환[2]

경희대 동서의학대학원 [1]경희대 정보전자신소재공학과 [2]경희대 동서의과학과

The formation of macrocycle between Pd(II) metal and isomeric pyridyl molecules was investigated using NMR spectroscopy. Dynamic [2]catenation of Pd(II) metal self assembled macrocycle with beta cyclodextrin formed through hydrophobic attractions in water and the interaction of relatively unstable isomeric macrocycle with beta cyclodextrin leads to poly-catenane or rotaxane formation. The existence of a self assembled polymeric structure with high molecular weight was identified through 2D NMR spectroscopy(DOSY). Activation energy barrier of dynamic self assembly was studied through 2 dimensional exchange NMR spectroscopy (EXSY).



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1031**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent sensing of gold species through a gold promoted intramolecular nucleophilic addition to o-ethynylphenyl moiety

전미은 안교한

포항공과대 화학과

Gold-mediated organic transformations have attracted much attention in recent years for their unique reactivity. An accompanying concern in using the gold species in the synthesis of drug intermediates is that a residual amount of gold often persists in the product can cause a health hazard. Moreover, gold ions can bind to proteins, DNA or other bio-molecules and thereby may disturb a variety of cellular processes.[1] Therefore, easy detection of gold species becomes an important issue. Gold species have been widely used in nucleophilic addition reactions as they strongly activate the carbon-carbon triple bond.[2] Recently, we developed a *N*-propargyl rhodamine derivative as a fluorescent probe for gold species based on this alkynophilicity of gold species.[3] Herein, we describe a new fluorescent probe for gold species, which utilizes a rhodamine ring opening process through the gold mediated intramolecular nucleophilic addition to *o*-ethynylphenyl moiety. The ring opening process accompanies a vivid color change from colorless to pink and also a turn-on fluorescent change. Our newly designed probe for gold species generates only single reaction product in contrast to the previous rhodamine based sensing system that provide several side products.[4] The present sensing system is expected to be readily developed into the corresponding fluorescence resonance energy transfer system. The work demonstrate again the versatility of the reaction-based approach to molecular probes.[5]

References

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5.Jun, M. E.; Roy, B.; Ahn, K. H. *Chem. Commun*. 2011, *47*, 7583.

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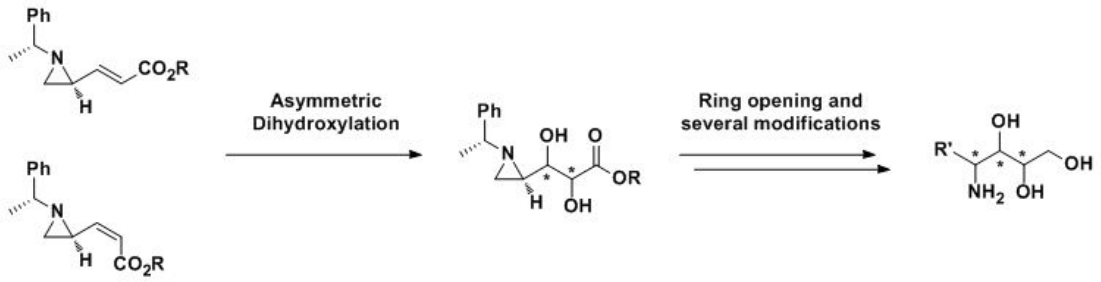
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1032**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Dihydroxylation of Aziridine-Enoate : Expedient synthetic route for Polyhydroxylated amine natural product

윤호종 강보람[1] 심태보[2]

KIST 화학키노믹스연구센터 [1]KIST 키노믹스센터 [2]KIST 생체과학연구본부

Asymmetric dihydroxylation of (E) or (Z)- Aziridine-Enoate using AD-mix α & β was successfully performed with high yield and diastereomeric selectivity. We developed this methodology that can generate various dihydroxylated isomers. This expedient and efficient methodology could be applied to stereoselective synthesis of polyhydroxylated amine natural product because the chirality of three stereogenic centers on 3-amino-1,2-diol system could be readily controlled.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1033**

발표분야: 유기화학

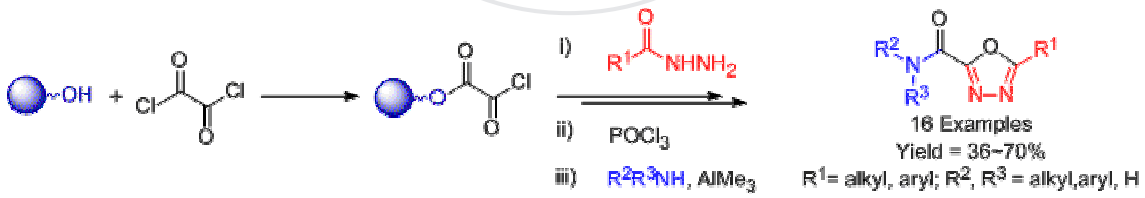
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid-Phase Approach for the Synthesis of 2-Amido-1,3,4-oxadiazoles

이상협 BALAJI[1]

대구가톨릭대 생명화학과 [1]대구가톨릭대 화학과

A new solid-phase approach for the synthesis of 2-amido-1,3,4-oxadiazoles has been developed. In this synthesis, hydroxypentyl JandaJel polymer support was treated with excess of oxalyl chloride to give resin-bound 2-chloro-2-oxoacetate and this intermediate was then coupled with different hydrazides to give resin-bound 2-(N'-acylhydrazinyl)-2-oxoacetate. Intra-molecular dehydrative cyclization of resulting resin-bound linear precursor followed by direct amidation using aluminum amide reagent provided 5-substituted 1,3,4-oxadiazoles as 2-carboxamides. To explore the scope of this reaction sequence, we synthesized a small set of library using a combination of hydrazides and amines and the desired products were obtained in good to excellent yields.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1034**

발표분야: 유기화학

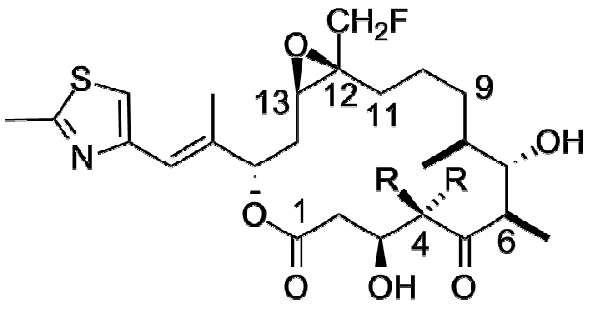
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Studies on Deuterium and Fluorine Substituted Epothilone

이재호 백윤기[1] 최일영[2] 이효원

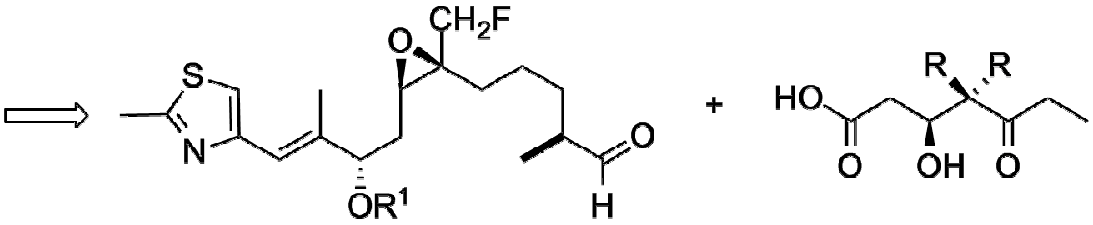
충북대 화학과 [1]한국기초과학지원연구원 대구센터 [2]한국화학연구원 의약화학연구센터

Epotilones were isolated from Myxobacterium *Soransium cellulosum (myxococcales) strain So ce90* and S. *cellulosum* SMP44. These antimiotic agents exert their cytotoxicity through the interruption of cancer cells. The structural feature of epothilones includes a 16-membered macrolide ring, a side chain with a thiazole, a *cis*-epoxide at C12-C13, a *gem*-dimethyl group at C4, and a spacer region at C9-C11.Epothilone with deuterium and fluorine substituents is of our objective for solid NMR study on its conformation in the biological system. Our synthetic plan towards this derivative from epothilone B was composed of the northern fragment of C7-C21 with a fluoromethyl group and the southern fragment C1-C6 with two germinal trideuteromethyl groups. The aldol reaction and the following lactonization would lead to the required product. The detail will be disclosed.



Epothilone B

R=CD_3



R^1=TBS

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1035**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Turn on detection of Hg(II) and Pb(II) ions in aqueous solution with Pyrene labeled Tryptophan

Neupane Lok Nath

인하대 화학과

Chemosensors that monitored metal ions are of great interest because a variety of natural and environmental contaminations of heavy and transition metal (HTM) ions causes serious global problems for human health and ecology. Recently, amino acid based sensors are frequently used to detect the heavy metal ions because the amino acid based sensors are highly water soluble and shows sensitive response to speci?c metal ions. Herein, we designed and synthesized a fluorescent sensor (PW) derived from pyrene sulfonic chloride and tryptophan. The sensor shows selective detection of Hg(II) and Pb(II) among other metal ions with turn-on response . The sensitivity, detection limit, stoichiometry, binding mode and reversibility of selective metal ions were also studied.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1036**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidation/reduction-mediated controlled release systems by conjugation peptide sequences on mesoporous silica nanoparticles.

한송이

인하대 화학과

Peptide is coated on mesoporous silica through the facile solide phase synthesis method.The anchored peptide can works as gatekeeper to control the release of entrapped guest molecules from mesoporous silica.When peptide is oxidize, release of entrapped guest molecles from mesoporous silica is close.On the contrary, when peptide is reduct, guest molecles is release from silica nanoparticles once more.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1037**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric and Fluorescent Sensing of heavy metal ion by chemosensor based on amino acid with an intramolecular charge transfer fluorophore

박주영

인하대 화학과

Colormetric and Fluorescent Sensors (NBD-H, NBD-C) based on amino acid was synthesized in solid phase. The compound is purified by HPLC. The sensor shows sensitive response in mixed aqueous organic solvent system.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1038**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design of fluorescent chemosensors based on dipeptide containing His for monitoring heavy metal ions in aqueous media

박주헌

인하대 화학과

The detection and quantification of heavy metal ions are important in many applications, including environmental monitoring, waste management, developmental biology, and clinical toxicology. As amino acid and peptides are water-soluble and biologically and environmentally compatible, a new chemosensor based on dipeptides are a promising route of development for monitoring heavy metal ions in aqueous system. We designed and synthesized some dipeptides containing pyrene fluorophore monitoring the metal ions. The sensor shows ratiometric detection of selective heavy metal ions in aqueous media

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1039**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Two-Photon Fluorescent Probe for Nitric Oxide in Live Tissue

서은원 허철호 신재호[1] 조봉래[2] 김환명

아주대 에너지시스템학부 [1]광운대 화학과 [2]고려대 화학과

Nitric oxide (NO) is a ubiquitous signaling molecule that modulates a variety of physiological and pathological processes in living organisms. NO plays a key role in synaptic activity in the brain and defends immune systems. On the other hand, misregulation of NO production can cause various diseases, such as cancer and neurodegenerative disorders. In order to understand its roles in biology, it is crucial to monitor NO in intact tissues with two-photon microscopy (TPM). TPM, which employs two near-infrared photons as the excitation source, offers a number of advantages over one-photon microscopy, including increased depth of penetration (> 500 μm), localized excitation, and prolonged observation times.We have therefore developed a small-molecule TP turn-on probe (ANO1) that shows a rapid and specific NO response, pH insensitivity in the biologically relevant range, strong TPEF enhancement in response to NO, and a maximum TP-action cross-section of 170 GM upon reaction with excess NO. This probe can be easily loaded into cells and can real-time monitor the NO in living tissues at 100-180 μm depth for a long period of time with minimum interference from other biologically relevant species through the use of two-photon microscopy.

일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ORGN.P-1040**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective and sensitive ratiometric detection of Hg(II) in aqueous solution and live cells by fluorescense sensor using cation-π interaction

김다혜

인하대 화학과

Pyrene-Tyrosine (P-Tyr) is synthesized in solid phase synthesis. P-Tyr shows highly sensitive and selective response to Hg(II) ions among various metal ions. The sensor detects Hg(II) ions ratiometrically in aqueous dimethylformamide solution. In DMF percentages 1.5, this sensor exhibits strong and selective dual fluorescence responses of monomer and excimer to Hg(II) by cation-π interaction. The sensor penetrates live HeLa cells and detects intracellular Hg(II) by ratriometric response.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design of Two-Photon Fluorescent Probe for Ratiometric Detection of Hydrogen Peroxide

박미연 김형중 허철호 김환명

아주대 에너지시스템학부

Hydrogen peroxide (H_2O_2) is a prominent member of the ROS family and plays crucial roles in physiology, aging, and disease in living organisms. While controlled bursts of H_2O_2 are utilized for cell signaling, abnormal production or accumulation of H_2O_2 within the cell has been linked to severe disorders such as cancer, and neurodegenerative diseases. To understand the biological roles of H_2O_2 in living systems, it is crucial to quantitative monitor H_2O_2 in the intact tissues with two-photon microscopy (TPM), which has the advantages of increased penetration depth (> 500 μm), localized excitation, and prolonged observation times. We have developed two-photon fluorescent ratiometric probes for imaging of intracellular H_2O_2 in mitochondria and cytosol, respectively, in live cells and tissues by TPM. These probes show a significant TP action cross-section, a marked blue-to-yellow emission color change in response to H_2O_2, good cytosolic H_2O_2 selectivity, and insensitivity to pH in the biologically relevant pH range.

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장소: 부산BEXCO
발표코드: **ORGN.P-1042**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Two-Photon Probe for Amyloid-β Plaques in Living Mouse

허철호 김형중 김환명

아주대 에너지시스템학부

Alzheimer's disease (AD) is an age related neurodegenerative disorder with cognitive impairment and chronic dementia. The pathogenesis of AD is associated with beta amyloid (Aβ) containing amyloid plaques and neurofibrillary tangles in specific brain region. Direct detection of Aβ plaques is emerging as a key challenge for elucidating fundamental aspects and early diagnosis of AD. Recently, available methods for in vivo imaging for AD patients include positron emission tomography (PET), single photon emission computed tomography, magnetic resonance imaging, and fluorescent imaging. PET and fluorescent imaging have been widely applied for in vivo imaging of Aβ plaques. PET imaging, however, is limited by short-term data acquisition process and relatively low spatial resolution.An attractive method for the in vivo imaging of Aβ plaques is the use of two-photon microscopy (TPM). However, to the best our knowledge, there has been no report on the rational design and evaluation of two-photon (TP) fluorescent probe that is applicable for in vivo imaging for Aβ plaques by TPM. Herein, we have developed a new Aβ plaque-specific TP probe (SAD1) that shows a significant TP action cross section (170 GM), binds to Aβ plaque specifically, and readily enters the brain through the blood brain barrier (BBB). Unlike the previously available probes, SAD1 can direct three dimensions (3D) monitor the individual Aβ plaque in living transgenic mice brains at more than 250 μm depths with minimum background emission and photo-bleaching artifacts. We expected that this probe may be useful in biomedical research for AD through the use of TPM.

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장소: 부산BEXCO

발표코드: **ORGN.P-1043**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ratiometric Detection of Mitochondrial Hydrogen Sulfide with a Two-Photon Fluorescent Probe

배성근 허철호 김환명

아주대 에너지시스템학부

Hydrogen sulfide (H_2S) has attracted substantial interest as an endogenous gaseous transmitter and physiological mediator. Studies in animals and humans have shown H_2S to be involved in diverse physiological processes, such as learning and memory, neurodegeneration, regulation of inflammation and blood pressure, and metabolism. However, research in this field is hindered by the lack of specific analytical and physiological tools for living specimens.An attractive approach to the detection of H_2S deep inside live specimens is two-photon microscopy.Therefore, we have developed a novel ratiometric and mitochondrial specific two-photon fluorescent probe, which shows a significant TP action cross-section, a marked blue-to-yellow emission color change in response to H_2S, good mitochondrial H_2S selectivity. This new probe enables visualization of the changes in mitochondrial H_2S levels in live cells, as well as in living tissues at more than 100 μm depth without interference from other biologically relevant reactive oxygen, nitrogen and sulfide species.

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장소: 부산BEXCO

발표코드: **ORGN.P-1044**

발표분야: 유기화학

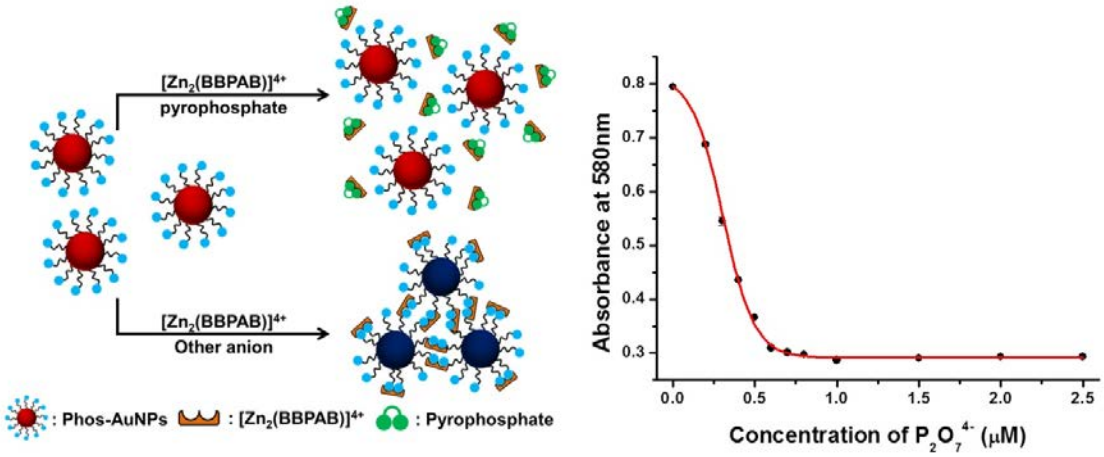
발표종류: 포스터, 발표일시: 수 16:00~19:00

A highly sensitive gold nanoparticle-based colorimetric probe for pyrophosphate using a competition assay approach

김수덕 엄민식 한민수

중앙대 화학과

We report a competitive-assay-based colorimetric sensing system for pyrophosphate which uses a combination of $[Zn_2(1,3\text{-bis[bis(2-pyridylmethyl)aminomethyl]benzene})]^{4+}$ as the receptor unit for pyrophosphate and 11-mercaptoundecylphosphoric acid functionalized gold nanoparticles as the reporter unit. This sensing system can easily detect pyrophosphate at less than ~200 nM with the naked eye and has selectivity for pyrophosphate over various common anions, including ADP and ATP. This approach might be applicable in improving the sensitivity of other colorimetric sensing systems.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1045**

발표분야: 유기화학

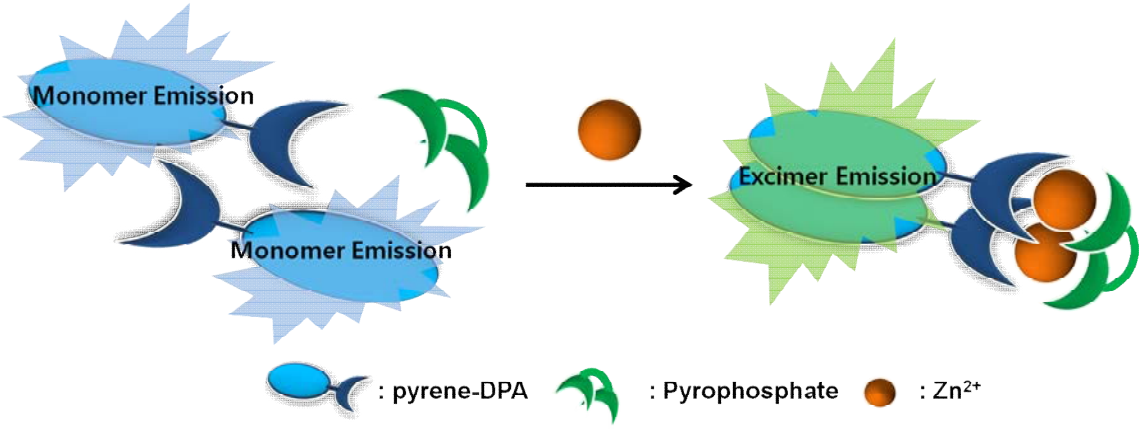
발표종류: 포스터, 발표일시: 수 16:00~19:00

A efficient excimer-formation of pyrene-bis(2-pyridylmethyl)amine using pyrophosphate as a bridging substrate and its application of ratiometric fluorescent probe the Zn^{2+} ion

백경규 엄민식 한민수

중앙대 화학과

Many efficient Zn^{2+} sensors have been developed based upon several strategies including metal-ligand interaction. because Zinc, an second most abundant transition metal ion found in the body, is plays an essential role in many cellular processes, such as gene expression, apoptosis, enzyme regulation, and neurotransmissions.Most these chemosensor detected Zn^{2+} ions using single emission spectrum. Although these chemosensor detected Zn^{2+} ions with high sensitivity and selectivity, have several problem in detecting analyte, which is to need internal standard. Excimer based-chemosensors have been developed to solve the problem because this ratiometric chemosensors have a dual emission system that can minimize the measurement errors induced by the factors such as phototransformation, receptor concentrations, and environmental effects. In general, these system have intra-conformational change in the presence of analyte and that result in fluorescent changes.We designed another type exciemr probe for Zn^{2+} ion with mixture of pyrene-bis(2-pyridylmethyl)amine (DPA) derivatives and pyrophosphate. Pyrophosphate, an additional bridging substrate, affect to make excimer of pyrene-DPA-Zn which has 2:1 ratio of pyrene-DPA derivatives and pyrophosphate(scheme 1).



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1046**

발표분야: 유기화학

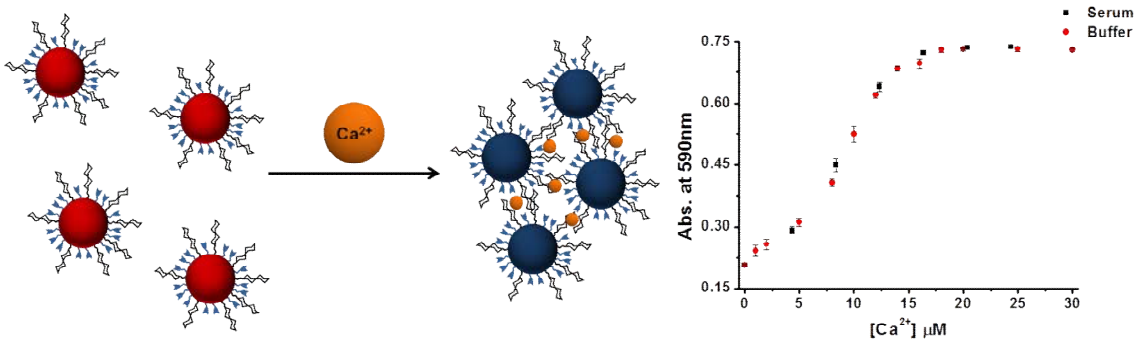
발표종류: 포스터, 발표일시: 수 16:00~19:00

bi-ligand co-functionalized gold nanoparticles-based calcium ion probe and its application to the detection of calcium ions in serum

엄민식 장우정[1] 권용억[1] 한민수

중앙대 화학과 [1]이화여대 화학.나노과학과

Oligosaccharides are well-known to chelate Ca<sup)2+ ions and the interaction enhances the oligosaccharide?oligosaccharide interaction. This property has been used to develop gold nanoparticles(AuNP)-based colorimetric probes to detect Ca<sup)2+. However, these probes exhibited interference from the presence of Mg<sup)2+ ions and low sensitivity in mM ranges. We speculated that these problems can be solved by introducing a combination of carboxylic acid and oligosaccharide groups into AuNPs. The carboxylic acid group can relax the steric constraints of the recognition moiety in saccharides and provide additional cooperative binding sites. Although saccharides and carboxylic acids have weak binding affinities for Ca<sup)2+ ions, self-assembly of the two ligands on the AuNP surface can provide a cooperative effect for Ca2+ recognition. AuNPs were functinalized with various rations of 1-thiohexyl carboxylic acid(A) and 1-thiohexyl β-D-lactopyranoside(S) and AuNPs functinalized with a 2 : 1 ratio of A and S. We selected as a effective Ca<sup)2+ probe. This probe was highly selective for Ca<sup)2+ ions over other metal ions relevant to blood serum and it allowed assay of the Ca<sup)2+ ions up to 1.9 μM. Moreover, the probe determined Ca<sup)2+ concentrations in various serum samples and the results correlated well with those obtained by using ICP-AES.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1047**

발표분야: 유기화학

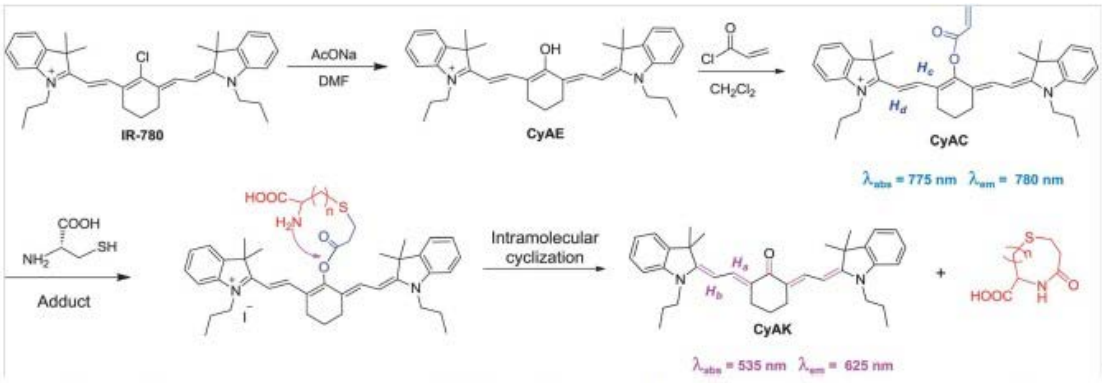
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cyanine-based NIR Fluorescent Probes for Zinc Ions and Cysteine in Vivo

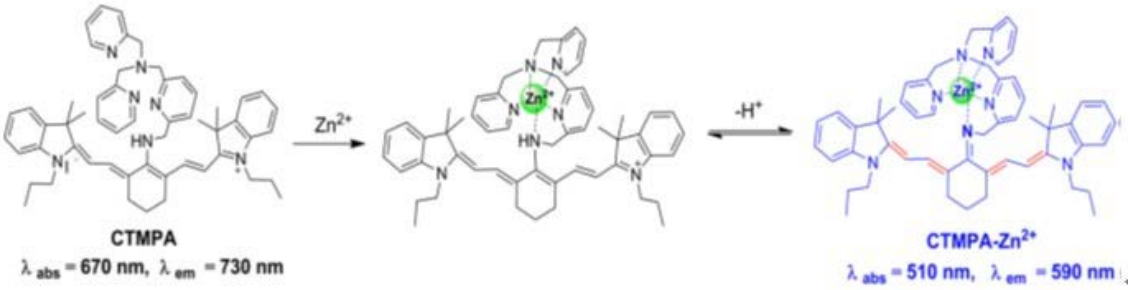
Hu Ying 김건희[1] 신인재[1] 윤주영[2]

이화여대 나노과학과 [1]연세대 화학과 [2]이화여대 화학-나노과학과

Selective detection of zinc and cysteine in vivo are important, because they are essential components in a variety of biological processes. Herein, we developed highly selective ratiometric near-infrared cyanine-based Zn2+ probe CTMPA[2]. The strategy we have devised, which relies on the modulation of the conjugation length of the p-electron system of the cyanine chromophore/fluorophore by metal ion coordination, should be applicable to the generation of a highly sensitive and selective, ratiometric cyanine-based metal ion sensor. Also, we have developed a highly selective ratiometric NIR cyanine-based probe for discrimination of Cys[3] from other structurally and functionally similar amino acids and thiols. The remarkable shift (over 200 nm) of CyAC with Cys was implemented by modulation of the conjugated p-electron system of cyanine dyes. This ratiometric NIR fluorescent sensor was successfully applied for bioimaging Cys in breast cancer cells. More broadly, the strategy of reversibly modulating the polymethine p-electron system by conjugation and removal of the specific trigger moiety is employed for the generation cyanine-based NIR sensors.



Scheme 1 Synthetic route for CyAC and proposed mechanism for detection of Cys.



Scheme 2 The proposed binding mode of CTMPA to Zn^{2+}

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1048**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Binap 유도체인 ARCA의 촉매작용에 의한 아미노산 유도체의 가수분해 반응과 입체구조 전환에 대한 연구

최문실 이민경 최용준 전근호[1]

숭실대 화학과 [1]숭실대 화학

ARCA(Alanine Racemase Chiral Analogue)는 binap 구조를 갖는 비대칭 합성 촉매로서 pyridoxal phosphate(PLP)기를 조효소로 갖는 아미노산을 라세믹화 하는 라세메이즈 효소의 모방체이다. 다양한 구조의 ARCA 들이 알려져 있으며 이를 이용하여 L-아미노산을 D-형태로 바꿔주는 반응이 발표 되었다. 최근 아미노로직스(주)는 이 촉매와 shuttle 공법이라는 신공법을 결합하여 D-아미노산을 대량 생산하는 공정을 개발하여 발표 하였다. 본 연구실에서는 지난 1 년간 ARCA 의 일종인 (S)-2-Hydroxy-2'-(4-toluenyl-benzyl)-1,1'-binaphthyl-3-carboxaldehyde (HTBS)를 이용하여 라세믹화 반응 외에 아미노산 유도체 합성에 적용 할 수 있는 새로운 반응을 찾는 연구를 수행하여 왔다. 라세메이즈 모방체로서 HTBS 는 분자내에 아미노산이 이민 형성으로 결합 할 수 있는 알데히드 작용기와 부착된 아미노산의 3 차원적 배열을 고정시키기 위한 분자내 수소 결합 부위인 유레아기를 가지고 있다. 그러나 HTBS 에 아미노산 대신 아미노산 에스터나 아마이드를 부착시켜 반응시킨 결과 D-아미노산으로의 전환 외에 에스터 나 아마이드의 가수분해 반응이 빠르게 일어남을 발견하였으며, 사용된 에스터나 아마이드의 종류에 따라 D-아미노산으로 전환 되는 정도도 민감하게 달라짐을 관찰 하였다. 이 경우에는 분자내 유레아기가 수소결합 주게가 아닌 일반 염기 또는 친핵성 촉매 작용기로 작용하기 때문으로 생각되며 염기성 조건에서 비교적 가수분해가 어려운 t-부틸 에스터도 쉽게 가수분해 되는 것으로 보아 매우 효과적인 분자내 촉매작용을 하는 것으로 추측된다. 본 발표에서는 다양한 아미노산 유도체들의 ARCA 에 의한 가수분해 반응과 D-아미노산으로의 전환 결과를 소개하며 protease 모방체로서의 ARCA 의 반응 메커니즘도 제시하고자 한다.

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발표코드: **ORGN.P-1049**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure Determination of Self-assembled Peptides by Powder Diffraction Analysis

공진택 전아람 조성준[1] 이희승

KAIST 화학과 [1]전남대 응용화학공학부

Powder diffraction analysis has been used for structural determination of various crystalline materials, especially in the cases that the single crystal X-ray diffraction data of material are not available[1]. To the best of our knowledge, however, the analytical technique has rarely been employed to analyze the molecular packing mode of self-assembled peptides.Recently we have developed a PXRD analysis technique for elucidating molecular structures of β-peptide self-assembled foldamers[2]. Herein we present the analysis results and the strategy of structure determination of peptide self-assembled structure which was obtained by the controlled self-assembly in aqueous solution.

Reference

[1] David, W. I. F., Shankland, K., McCusker, L. B. & Baerlocher, Ch. Structure Determination from Powder Diffraction Data, Oxford University Press, (2002) . pp. 1-11

[2] S. Kwon, H.S. Shin, J. Gong, J.-H. Eom, A. Jeon, S.H. Yoo, I.S. Chung, S.J. Cho, H.-S. Lee, J. Am. Chem. Soc., 133 (2011), pp. 17618?17621

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장소: 부산BEXCO

발표코드: **ORGN.P-1050**

발표분야: 유기화학

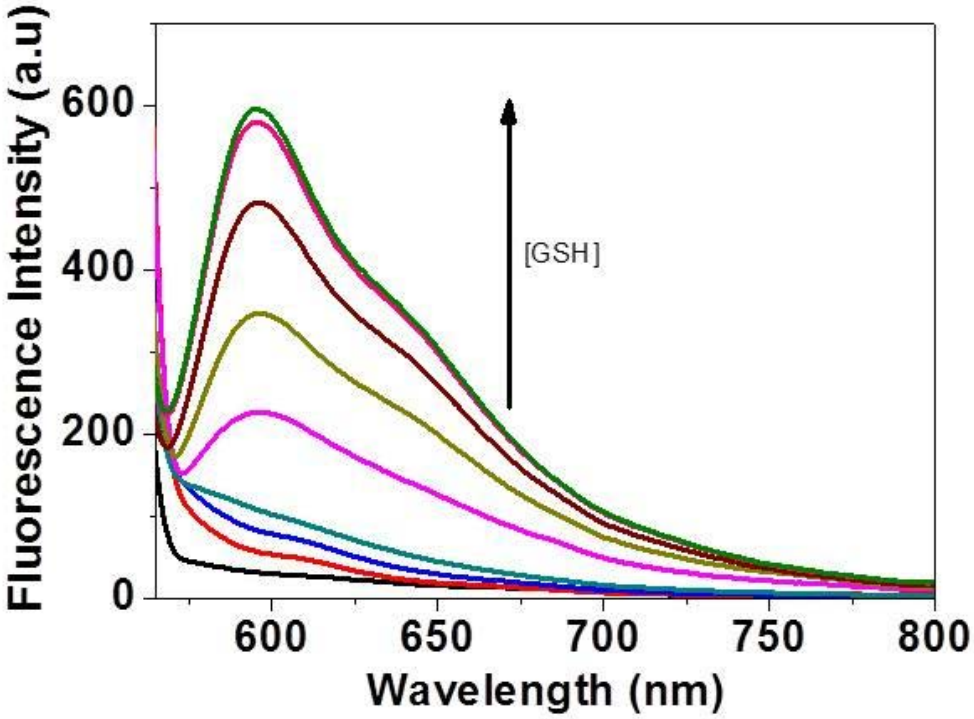
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Fluorescence Tune-on Probe Based on Cu (II)-BODIPY Complex for Detection of Thiol Group

김지영 김영미

단국대 화학과

Intracellular thiols such as glutathione (GSH), cysteine (Cys), and homocysteine (Hcy) play important roles in biological systems. Generally, the level of cellular thiols has been linked to many diseases such as liver damage, cancer, and AIDS. Therefore, the selective and sensitive detection of thiols can be used as various disease-associated biomarkers. We present the detection of thiols by probe 1-Cu(II) and probe 1-Pb(II) complex, respectively. The fluorescence intensity of probe 1 decreases upon addition of Cu(II) or Pb(II), but its fluorescence intensity recovered when thiol compounds were added to the solution of 1-Cu(II) or 1-Pb(II) complex.



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1051**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-substituted 4-phenylquinoline derivatives under microwave irradiation

이수지 이용균 이언진 이도훈 정대일 한정태[1]

동아대 화학과 [1]영동대 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 assiste-d 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 synthesis of 2-substituted 4-phenylquinoline derivatives by using halogen substituted 2-amino benzophenones and aromatics having acetyl group for 5 minutes under microwave irradiation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1052**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Synthetic method for Rosuvastatin

이정선 강용한

한양대 응용화학과

Rosuvastatin is a competitive inhibitor of the enzyme, HMG-CoA reductase, and has a mechanism similar to that of other statins. Rosuvastatin is a cholesterol-lowering medication that blocks production of cholesterol (a type of fat) in the body. It works by reducing the levels of "bad" cholesterol (low-density lipoprotein, or LDL) and triglycerides in the blood, while increasing the levels of "good" cholesterol (high-density lipoprotein, or HDL). An efficient method for the preparation of Rosuvastatin has been developed by the coupling reaction of {4-(4-fluorophenyl)-6-isopropyl-2-[(N-methyl-N-methylsulfonyl)amino]-pyrimidin-5-ylmethyl}- phosphonium derivative with tert-butyl-2-[(4R,6S)-6-formyl-2,2-dimethyl-1,3-dioxane-4-yl)]acetate.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1053**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-substituted 2,3-Dihydro-4(1H)-Quinazolinones with Cyanuric Chloride

양정우 정대일 김윤영 한정태[1]

동아대 화학과 [1]영동대 뷰티케어과

2-substituted-2,3-dihydro-4(1H)-quinazolinones are class of heterocycles which exhibit biological and pharmaceutical activity as antitumor, diuretic, and herbicidal agents. Recently, the synthesis of 2-substituted-2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids such as SmI_2, $Sc(OTf)_3$, NH_4Cl, and $H_3PW_{12}O_{40}$ as catalysts has been described and their catalyst-free synthesis in ionic liquids or 2,2,2-trifluoroethanol has also been reported. We now report our reactions of anthranilamide and aldehydes in acetonitrile with cyanuric chloride(or 1,3-acetonedicaboxylic acid) as a catalyst.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1054**

발표분야: 유기화학

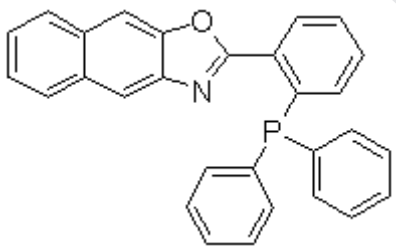
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 2-(2-(Diphenylphosphino)phenyl)]naphto[d]oxazole (PPN) as Blue-Emitting OLED Material

김익환 임영훈 TRINH DAC HOANH 이범종[1]

인제대 화학과 [1]인제대 의생명화학과

In the course of investigation for finding new light-emitting materials based on the phosphino-oxazole structure, we have employed 3-amino-2-naphthol and 2-(diphenylphosphino)benzoic acid as starting materials for synthesizing 2-(2-(diphenylphosphino)phenyl)]naphto[d]oxazole (PPN) in this work. The chemical structure of PPN was determined by ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-Vis and XPS. PPN shows a strong-blue emission by excitation by UV-lamp of 365 nm. The photoluminescence (PL) and electroluminescence (EL) properties of PPN will be discussed.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1055**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of Bis(triazinylamino)stilbenes as the Fluorescent Whitening Agents

고덕환 이정선 강용한

한양대 응용화학과

Disodium 4,4’-bis(triaznylamino)stilbene-2,2’-disulfonate derivatives are most widely used as fluorescent brighteners for the whitening of both cotton and wool. A typical fluorescent brightener absorbs light in ultraviolet ray (330~380nm) and emits of the visible blue lights (400~450nm). A series of non-symmetrically substituted di(triazinylamino)stilbene derivatives were synthesized. For the synthesis of asymmetric stilbene fluorescent brighteners, the key intermediate, 4,4'-bis(2,6- dichloro-1,3,5-triazinyl)diaminostilbene-2,2’-disulfonate (1), was prepared by reacting 4,4'-diamino- stilbene-2,2’-disulfonate with cyanuric chloride (CNC). Without isolating the intermediate 1, two remaining chloro groups of the compound 1 were substituted with two kinds of amines. From this reaction, three types of stilbenes were produced. The yield rate of each compound was compared to see how they change depending on the pKa value of amines and reaction temperature.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1056**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of new Quinoxalines by using 2,3-butanedionemonoxime and aromatic vicinal diamines

이상곤 이용균 송주현 이도훈 한정태[1]

동아대 화학과 [1]영동대 뷰티케어과

Micro-assisted heating under controlled condition has been proven as an invaluable technology for organic synthesis and their application in several cases has lead to acceleration of reaction, improvement of yield and selectivities. Especially, Quinoxaline is very important structure in antibiotics like echinomycin, levomycin and actinoleutin. Moreover, it is basic structure in organic semiconductor, anion receptor, and DNA cleavage reagent. Generally, we have known combination of 1,2-diamines and α-diketones and 1,4-addition of 1,2-diamines and diazenylbutenes for synthetic method of Quinoxalines. We now report our reactions of 2,3-bu-tanedionemonoxime instead of using α-diketone with various of aromatic vicinal diamines under Microwave irradiation.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1057**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 8-Azabicyclo[3.2.1]octan-8-ylphosphonate and 1H-pyrrol-1-ylphosphonate

김아영 정대일 최순규 송주현 이도훈 한정태[1]

동아대 화학과 [1]영동대 뷰티케어과

As a part of a research program related to the synthetic study of pharmacologically interesting tropane compounds and heterocycles containing nitrogen atom, we now report a convenient one-pot synthesis of 8-azabicyclo[3,2,1]octan-8-ylphosphonate and heteroaromatic compounds like pyrroles in the reaction of phosphinicamide (or phosphoramiate) with 2,5-dime-thoxytetrahydrofuran and acetone equivalents at room temperature. Synthesized products are as follow : Diethyl 1H-pyrrol-1-ylphosphonate, Diethyl 1H-indol-1-ylphosphonate, Diethyl 3-oxo-8-azabicyclo[3.2.1]octan-8-ylphosphonate, 1-(Diphenylphosphoryl)-1H-pyrrole and (1H-Indol-1-yl)diphenylphosphine oxide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1058**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 7-Dialkylaminocoumarin Derivatives as Fluorescent Agents

김주영 이은영 강용한

한양대 응용화학과

Because of industrial development, the fuel oil industry has grown into one of the largest markets in the world. Petroleum companies have invested a colossal sum to develop high quality petroleum products and to stay competitive with the products in the oil market. Coumarin derivatives, which are usually used as fluorescent whitening agents, were developed to be used as fluorescent markers for petroleum products. Various 7-dialkylaminocoumarin derivatives were synthesized from the reaction of 3-dialkylaminophenols with ethyl phenylformylacetate and ethyl acetoacetate by Pechmann reaction. Chemical structures of 7-dialkylaminocoumarins were analyzed by proton NMR spectrum and their physical properties were characterized by the measurements from UV/VIS and photoluminescence spectrum.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1059**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence Ratiometric Probes for Detection of Singlet Oxygen

송다영 유영민[1] 남원우[2]

이화여대 바이오융합과학과 [1]KIST 의공학연구소 [2]이화여대 화학과

Biological singlet oxygen ($^1O_2$), a highly reactive oxygen species (hROS), is linked to various pathological and physiological processes in the human body. However, molecular mechanisms underlying the $^1O_2$-mediated processes remain unestablished. We created a series of fluorescence ratiometric $^1O_2$ probes by attaching various fluorogenic aryl groups to the 1 position of isobenzofuran that undergoes the [2+4] pericyclic reaction with $^1O_2$. The $^1O_2$ probes displayed fluorescence ratiometric responses with excellent $^1O_2$ selectivity over other ROSs, including hydrogen peroxide, hydroxyl radical, alkylhydroperoxide, and superoxide. The $^1O_2$ response rate increased in proportional to the conjugation length of the aryl substituent of isobenzofuran. Fluorescence ratiometric $^1O_2$ detection ability was conserved in the aqueous nanosuspension state of the probe. Finally, we successfully visualized intracellular $^1O_2$ production by PMA (phorbol 12-myristate 13-acetate) stimulation of RAW 264.7 macrophage cells.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1060**

발표분야: 유기화학

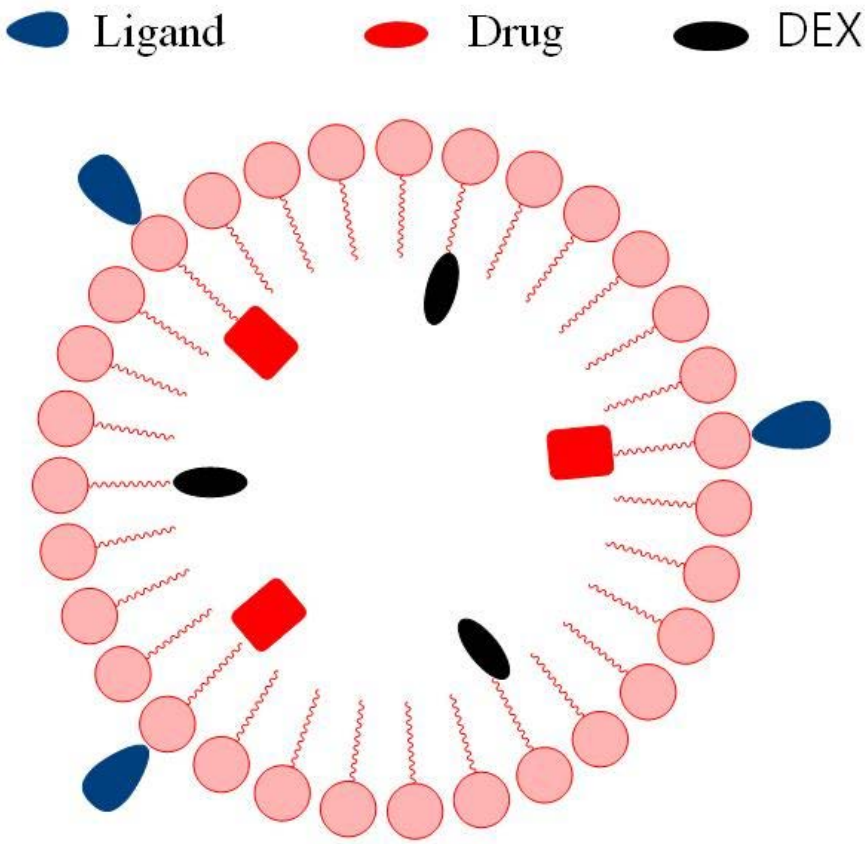
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stimuli-Responsive Supramolecular Nanocapsules based on the Amphiphic Perylene dye Assembly

이연옥 이재홍 이윤학 정단비 김종승

고려대 화학과

Water-soluble, self assembled nanocapsules composed of a functional membrane can provide smart way for drug delivery system. Owing to remarkable optical properties, perylene bisimide chromophores are interesting building blocks for a functional membrane in water environment. Here, we report a liposome composed of the three kinds of amphiphilic perylene bisimide derivatives. Low pH of extracellular environment in cancer tissue not only triggers a rapid release of dexamethasone (DEX) but also results in the quarternization of amine groups. This leads to the collapse of the vesicles with concomitant release of the constituent molecule, which is conjugated with the camptothecin (CPT) and the biothine. These separated molecules are penetrated into cell, and undergo cleavage -S-S- bond by stimuli of glutathione (GSH).



Vesicular perylene dye nanocapsules

1) Nanocarriers for drug delivery
2) GSH-responsive bond for the drug release
3) Fluorescent chromophores for cell imaging
4) Detectors for real time–monitoring of cell uptake

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1061**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Introduction of a novel reactive moiety for the reaction based fluorescent sensing system for gold species

서혜원 전미은 안교한

포항공과대 화학과

Recently gold complexes have drawn intense research interest because of their unique reactivity towards carbon-carbon multiple bonds. Gold complexes are used for rheumatoid arthritis treatments, and also show anticancer activity. However, gold(III) ions have neurotoxicity, complicating some patients during the gold therapy. Recently, we initiated the reaction based approach[1] that utilizes the alkynophilicity of gold species to develop a fluorescent probe for gold species. Thus, we developed an N-propargyl-lactam derivative of rhodamine as a turn-on fluorescent probe for Au(I) and Au(III) species.[2] Concurrently, others also pursued related approaches by utilizing the alkynophilicity of gold complexes.[3] Our previous probe, however, provides several side reaction products along with a fluorescent compound.[4,5] Formation of the non-fluorescent side reactions would undermine the gold sensing system. Therefore, we investigated a new approach that could alleviate the side reactions observed in the original system. Our idea is to separate the reactive moiety from the fluorescence dye, thereby the reaction product(s) from the sensing process can be detached from the signaling unit. As a proof-of-concept model, we have devised (2-ethynyl)benzoate as the reactive moiety. One of the fluorescein benzoates showed selective turn-on type fluorescence change upon interaction with gold species as the gold species promoted hydrolysis of the ester moiety.5 This new sensing scheme is promising for the development of efficient gold probes.References1. J.-Nu´n?ez, E.; Echavarren, A. M. Chem. Commun. 2007, 333?346.2. Egorova, O.; Seo, H.; Chatterjee, A.; Ahn, K. H. Org. Lett. 2010, 12, 401.3. (a) Jou, M. J.; Chen, X.; Swamy, K. M. K.; Kim, H. N.; Kim, H. J.; Lee, S.-g.; Yoon, J. Chem. Commun. 2009, 7218?7220. (b) Yang, Y. K.; Lee, S.; Tae, J. Org. Lett. 2009, 11, 5610?5613. . (c) Do, J. H.; Kim, H. N.; Yoon, J.; Kim, J. S.; Kim, H. J. Org. Lett., 2010, 12, 932?934.4. Egorova, O.; Seo, H.; Ahn, K. H. Angew. Chem. Int. Ed. 2011, 50, 114465. Seo, H.; Jun, M. E.; Egorova, O.; Lee, K.-Ha.; Kim, K.-T.; Ahn, K. H. Org. Lett. in press.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1062**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Sodium terephthalate를 이용한 소듐 이온 배터리의 유기 음극 물질 합성 및 특성

신동선 홍성유

울산과학기술대 나노생명화학공학부

최근 유기 전극 물질은 무기 전극 물질에 비해 유연하고 재상 가능성과 에너지 소비가 적다는 점에서 미래 전극 물질 후보 중 하나라고 평가받고 있다. 그 중 소듐 이온 배터리는 리튬에 비해 자원적으로 풍부하고 독성이 없어 최근 각광 받고 있다. 본 연구는 Terephthalic acid 와 Sodium hydroxide 를 합성하여 얻은 염인 Disodium terephthalate 와 amino group 등이 붙은 derevative 들을 합성하였다. 또한 FT-IR, TGA 와 DTA, XRD 분석을 이용해 구조 및 물리/화학적 특성을 조사하였으며, capacity 와 cycle number 를 포함하는 전기적 특성을 확인하였다.

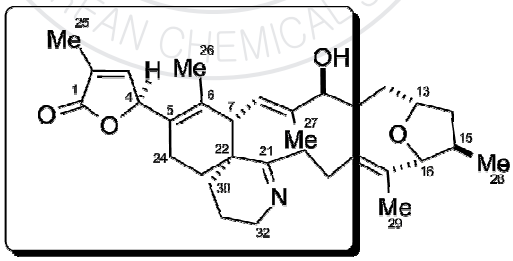
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1063**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective Synthesis of Spiroimine System of (-)-Gymnodimine A Containing a Butenolide

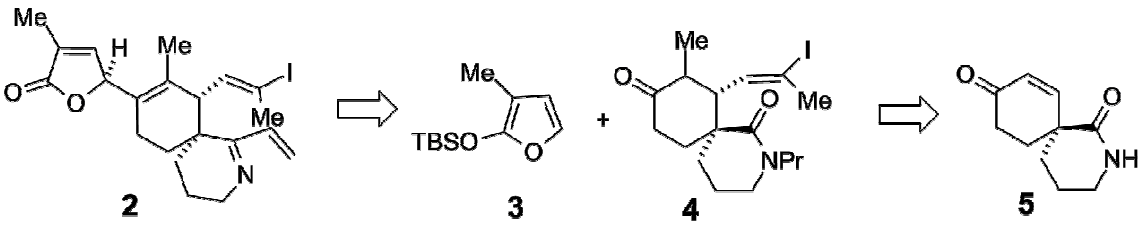
최소영 최일영[1] 이효원

충북대 화학과 [1]한국화학연구원 의약화학연구센터

Gymnodimine A (1) is a growing family of spirocylic imine phycotoxin produced by the dinoflagelate *Karenia selliformis*. Spirocylic system of Gymnodimine A was shown to bind and block different subset of muscle and neuronal nicotinic acetylcholine receptors (nAChRs). For the purpose of preparing a highly enantioselective spiroimine system, we conducted aldol condensation to compound 5 using some organic catalysts. Further elaboration such as the Michael reaction and introduction of a betenolide unit on this spiro ring will be described.



(-)-Gymnodimine A (1)



일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1064**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Polydiacetylene-Based Zn(Ⅱ)-Cyclen Liposome Micro-array Chip System for ATP.

마동희 안교한

포항공과대 화학과

Conjugated polymer, Poly(diacetylene) (PDA) is well known for its ability to color change from blue-to red color as well as fluorescence change in response to environmental perturbations (heat, organic solvents, mechanical stress, and ligand-receptor interaction). In addition, PDA vesicles can be readily immobilized on solid substrates. By using this PDA properties, we developed new Zn^{II}(cyclen)-functionalized PDA liposomes for the selective sensing of nucleotides. Zn^{II}(cyclen), Lewis-acidic metal complex, can coordinate with Lewis-basic analyte such as phosphate containing anions. In this study, we focused on the sensing behavior of Zn^{II}(cyclen) liposome toward various nucleotides. Nucleotides are key components of life, but the selective sensing of nucleotides remains a challenging task because they have rather common functional groups: nucleobase, sugar, and phosphate groups.In solution assay, the blue liposome solution became red-purple upon interaction with ATP, ADP, CTP and GTP. A microarray chip system fabricated with the liposomes, however, show red fluorescence only in the presence of ATP down to 1 pM level. In addition, red fluorescence spot images were clearly observable in the presence of ATP from ?M level to 1 pM range. Such a selectivity behavior manifests again that the recognition behavior can be modulated by changing the receptor environment, from solution to the solid state.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1065**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New EML Materials for Solution Process

이선미

가톨릭대 화학과

OLEDs(Organic light-emitting diodes)를 기반으로 한 디스플레이는 저전압구동, 높은 발광 효율, 넓은 시야각, 그리고 빠른 응답속도 등의 장점을 가지고 있어서 고화질의 동영상을 표현할 수 있는 차세대 평판 디스플레이 기술 중의 하나로서 현재 제품화를 위한 기술개발이 활발하게 진행되고 있다. 일반적으로 저분자는 thermal vacuum evaporation 에 의해서 제작이 되는데, thermal vacuum evaporation 은 높은 효율과 multi layer 를 만들 수 있지만, 제작비용이 비싸고 대면적의 디스플레이를 만들기 어려운 단점을 갖고 있다. 반면에 solution process 는 device 제작비용이 thermal vacuum evaporation 보다 싸고, 대면적 디스플레이에 적용될 수 있는 장점을 가지고 있다. 따라서 Anthracene 유도체에 bulky side 를 도입하여 solution process 에 사용할 새로운 EML 층 물질을 개발하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1066**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on N-1 -> N-7 isomerization of pyrrolo[2,3-d]pyrimidine nucleoside

김영종 권순호 김병문

서울대 화학부

BMK-Y101 is new pyrrolopyrimidine-based inhibitor, which has strong inhibition activity of CDK7 and CDK9. Inhibition of CDK7 and CDK9 exert consequent negative effects on RNA synthesis, strongly promotes apoptosis. It has N-1 structure unlike previous nucleoside analogs based on pyrrolo[2,3-d]pyrimidine which has N-7 sturucture. N-1 nucleosides appeared rarely in the literature, as well as, had been considered as by-product of glycosylation.The stability of N-1 and N-7 nucleosides, difference in glycosylation and isomerization condition, efficiency of isomerization reaction were tested.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1067**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Efficient Blue Emitting Materials Based on Pyrene Derivatives

이하윤

가톨릭대 화학과

새로운 평판 디스플레이 중 하나인 유기발광다이오드(Organic Light Emitting Diodes :OLEDs)디스플레이는 저전압구동, 자기 발광, 경량박형, 광시야각, 그리고 빠른 응답속도 등의 장점이 있어 이에 대한 연구가 전 세계적으로 활발히 진행되고 있다. 그러나 청색발광 재료의 경우 색순도 및 효율, 소자의 안정성 등의 문제로 충분한 수명을 확보하지 못하여 실제 상용 제품에 사용되는 재료들은 극히 제한적이어서 아직도 많은 연구 개발을 필요로 하는 분야이다. 본 연구에서는 blue materials 로 잘 알려져 있는 Pyrene 을 이용해 유도체들을 합성하고, 합성물질이 blue material 로써 사용할 수 있는지 그 특성을 알아보았다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1068**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Functionalized 3D Organic Molecular Architecture by the Self-assembly of β-Peptide Foldamer

유성현 윤은영 정윤철 이희승

KAIST 화학과

By defined arrangement of building blocks and spontaneous synthetic methodology, molecular self-assembly has been used to fabricate intelligent nano- and micro materials. Especially, plenty of peptide self-assembly was reported in the past decades because of its attractive natures for biological and non-biological applications. However, morphologies of peptide self-assemblages' were limited to simple shape like sphere, tube and wire. Recently, we have reported that helical β-peptide foldamer, an artificial peptide, could self-assemble into unprecedented 3D molecular architecture, called foldecture, in a controlled manner. Here, we report functionalized foldectures by self-assembly of helical β-peptide foldamer with carboxylic acid or alcohol groups at C-terminal. Parallelogram shaped foldectures were obtained by SEM and molecular arrangement of the foldecture was proposed by Powder X-ray diffraction analysis. Function was characterized by attachment of Pt nanoparticles on specific facets of the foldecture.

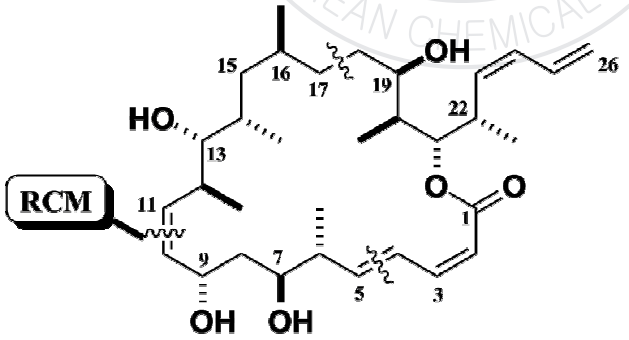
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1069**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Studies towards C5-C26 Subunits of (-)-Dictyostatin

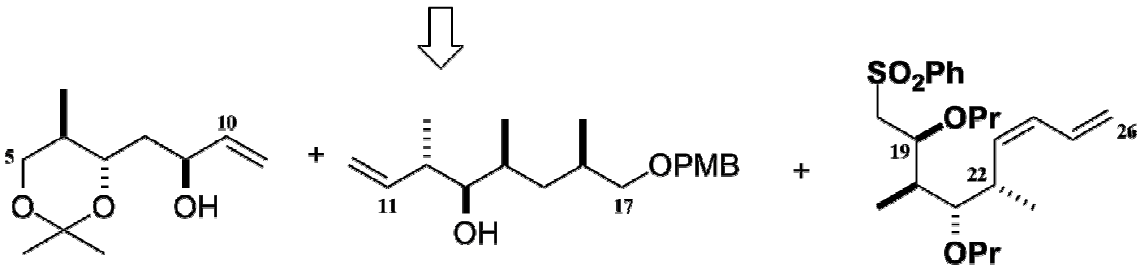
곽달용 이효원

충북대 화학과

Antimiotic macrolide (-)-dictyostatin was isolated from the marine sponge *Spongia sp*. by in 1994. It is structurally related to discodermolide. Dictyostatin inhibits the growth of cancer cells by binding to tubulins.We carried out the asymmetric synthesis of C5-C17 fragment of (-)-dictyostatin. This structural unit was prepared using key chemical manipulations such as silicon-tethered ring-closing metathesis (RCM). The other C18-C26 fragment was prepared using key chemical manipulations such as the Roush asymmetric allylation and the Evans aldol reaction. The details including coupling reaction will be disclosed.



(-)-Dictyostatin



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1070**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic approach toward Resiniferatoxin and Kirkinine Core Structure

Ahmed H. E. Hassan 이재균[1] 민선준[2] 조용서[3]

과학기술연합대학원대 화학과 [1]KIST 케모인포매틱스연구단 [2]KIST 뇌의약연구단 [3]KIST 생체과학연구본부

Resiniferatoxin and Kirkinine belong to daphnane orthoesters group of molecules. They consist of tricyclic core structure having tetradecahydrobenzo[e]azulene ring system. Binding of resiniferatoxin (RTX) to the transient receptor potential cation channel subfamily V member 1 (TRPV1) stimulates and then inactivates heat and vanilloid-responsive nerve endings involved in heat and inflammatory pain signaling. RTX causes to become permeable to cations, most particularly the calcium cation; this evokes a powerful irritant effect followed by desensitization and analgesia. Kirkinine has a remarkable neurotrophic activity. It demonstrates nerve growth factor (NGF) like activity at nanomolar concentrations. It effectively promotes neuronal survival against serum deprivation in nanomolar concentrations. As a result, kirkinine and its analogs present very promising therapeutic opportunities against neurodegenerative diseases such as Alzheimer's.In an attempt to develop a diverted total synthesis program for synthesis of the core structure of resiniferatoxin and kirkinine, we suggest possible synthetic strategies based on [3+4] cycloaddition reactions. Herein, we will report our current progress toward synthesis of the core tricyclic structure of the title compounds.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1071**

발표분야: 유기화학

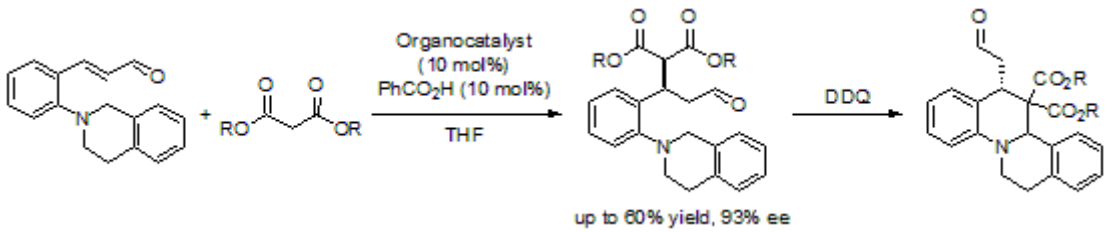
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of Ring-Fused Tetrahydroquinolines Using Organocatalytic Enantioselective Conjugate Addition and Cross-Dehydrogenative Coupling

김성곤 권성혁[1]

경기대 화학과 [1]경기대 자연과학대학 화학과

Enantioenriched ring-fused tetrahydroquinolines were synthesized by a facile and straightforward process involving the organocatalytic enantioselective conjugate addition reaction of malonates with o-N-tetrahydroisoquinolinyl-substituted cinnamaldehyde followed by intramolecular cross-dehydrogenative coupling. Diphenylprolinol TMS ether was used as an organocatalyst in the asymmetric catalytic conjugate addition reaction and 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ) was used as an oxidant in the cross-dehydrogenative coupling (CDC) reaction. The desired ring-fused tetrahydroquinolines were obtained in moderate yields with high enantioselectivities (up to 97% ee).



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1072**

발표분야: 유기화학

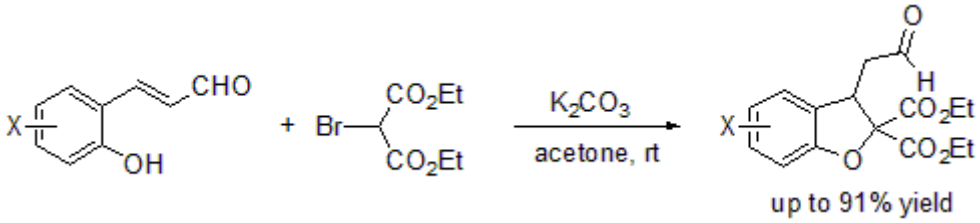
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Cascade Michael?Cyclization Reactions of o-Hydroxycinnamaldehydes: Synthesis of Functionalized 2,3-Dihydrobenzofuranes

김성곤 서승우

경기대 화학과

We describe the cascade Michael?cyclization reaction of o-hydroxycinnamaldehydes with diethyl α-bromomalonate promoted by potassium carbonate. The reactions provide functionalized 2,3-dihydrobenzofurans in good yields for a variety of o-hydroxyaromatic α,β-unsaturated aldehydes.



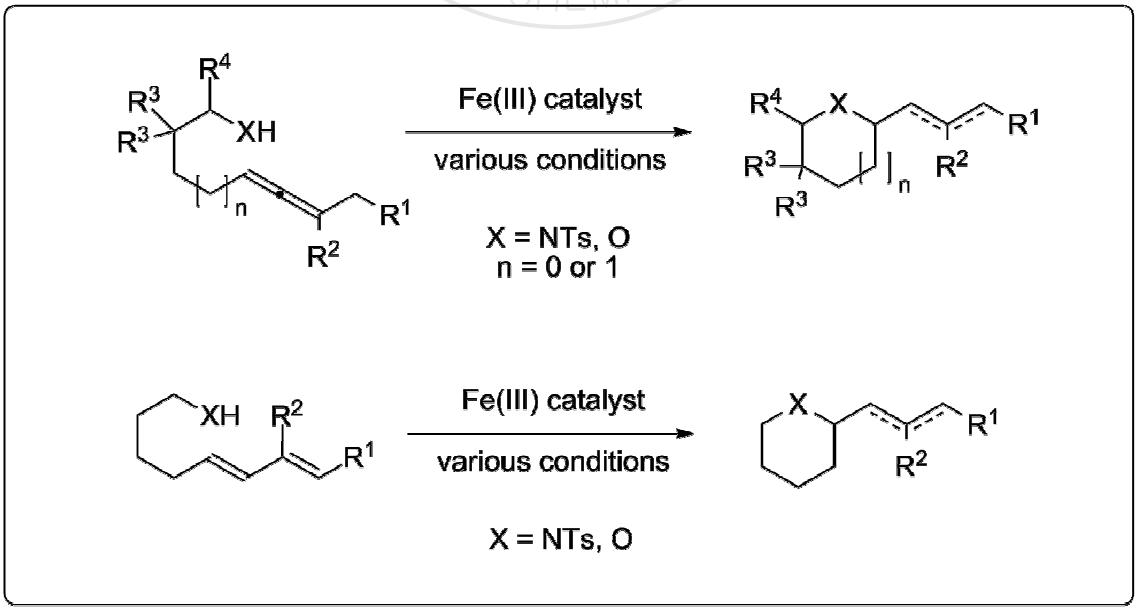
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1073**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on the different reactivities of C-C multiple bonds towards Fe(III) catalyzed hydrofunctionalization reactions

정민석 신예호 진하정 강은주[1]

경희대 응용화학과 [1]경희대 화학과

In chemistry, C-C multiple bonds have been widely used to produce various kinds of products via addition, cross coupling, or reduction reactions. Especially, transition metal catalyzed hydrofunctionalization is one of the most convenient ways to induce new C-O or C-N bond. In our research aiming to investigate the different reactivities of various C-C multiple bonds and control the chemoselectivity and regioselectivity, the hydrofunctionalization reactions of alkynes, allenes and dienes having nucleophilic heteroatoms, were carried out using Fe(III) catalysts to afford the corresponding heterocyclic compounds.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1074**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly efficient yellow and white phosphorescent organic light-emitting diodes using a benzothiazole-liganded new iridium complex

김희운 FEI XU[1] 김지훈 황도훈[1]

부산대 [1]부산대 화학과

We designed and synthesized a novel yellow-emitting iridium complex, bis[2-(9-ethyl-9H-carbazol-3-yl)-benzothiazole]iridium(III)acetoacetonate [(Btc)2Ir(acac)], for use in phosphorescent organic lightemitting diodes. The synthesized compound was characterized by 1H NMR and 13C NMR. Photophysical and electrochemical studies revealed photoluminescence emission at 555 nm (in solution) with a band gap energy of 2.37 eV. The phosphorescent organic light-emitting diodes based on ITO/PEDOT:PSS/α-NPD/TCTA/CBP:(Btc)2Ir(acac)(8%)/BCP/Alq3/LiF/Al exhibited a yellow emission at 562 nm with a high luminous ef?ciency of 35.4 cd/A, a maximum external quantum ef?ciency of 12.9% at 7.4V, and a very outstanding luminance of 100,048 cd/m2. Because of its high electroluminescent performance, ef?cient white phosphorescent organic light-emitting devices using this new iridium complex in the structure of ITO/TAPC/DCzPPy(x%):FIrpic(14%):(Btc)2Ir(acac)(y%)/Bphen/LiF/Al were fabricated. The device, with a new iridium(III) complex doping concentration of 0.15%, exhibited a maximum luminous ef?ciency as high as 41.6 cd/A at 5V, CIE coordinates of (0.34, 0.46), a maximum luminance of 25,010 cd/m2, and a maximum power ef?ciency of 28.9 lm/W, respectively.

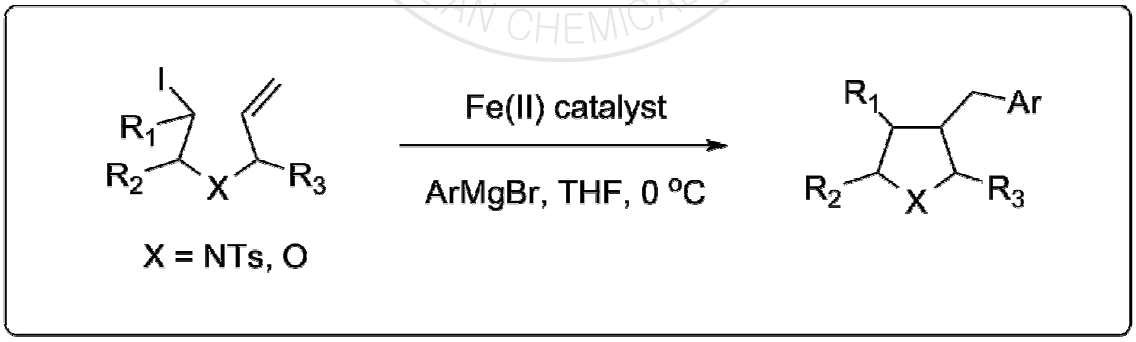
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1075**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

FeCl2-Catalyzed Sequential Radical Cyclization and Cross-coupling Reactions of 6-Halo-1-hexene Derivatives

김재곤 정시현[1] 강은주[1]

경희대 화학과 [1]경희대 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: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1076**

발표분야: 유기화학

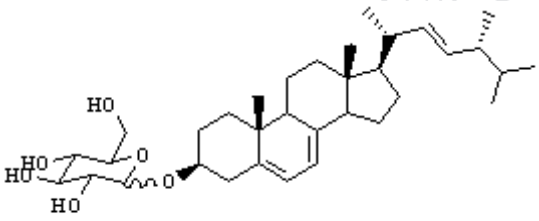
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the stereoselective glycosylation of ergosterol and 5,6-dihydroergosterol with glycosyl trichloroacetimidate

박훈규 김보정 오세한[1] 김학원[1]

경희대 화학과 [1]경희대 응용화학과

Several glycosyl steroids, such as glucosyl spinasterol and glucosyl ergosterol, have shown very interesting biological activities (anti-photoaging activity and anti-inflammatory activity). Especially, glucosyl spinasterol is known powerful anti-inflammatory activity. The efficient synthetic methods of various glycosyl steroids have been reported, for example Lewis acid-catalyzed trichloroacetimidate glycosylation. Therefore,we have investigated the glycosylation of some sterols, such as ergosterol and 5,6-dihydroergosterol, with glycosyl trichloacetimidates in the presence of the Lewis acid.



alpha, beta anomer

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1077**

발표분야: 유기화학

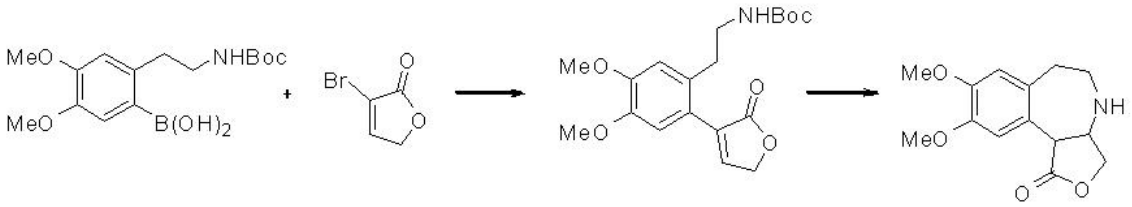
발표종류: 포스터, 발표일시: 수 16:00~19:00

Sythesis Study of 3-benzazepine structure using Suzuki reaction and intramolecular Michael type addition.

김희동 김건철

충남대 화학과

The Suzuki reaction and intramolecular Michael type 1,4-addition producing seven-membered rings for the synthesis of benzazepine derivatives are reported. The 3-benzazepine framwork is widespread among biologically active and natural compounds. Several efforts have been made towards the synthesis of alkaloids such as lennoxamine, aphanorphine due to their challenging chemical structures and interesting biological activities. The seven membered ring synthesis of the different 3-benzazepine is reported through Pd-catalyed Suzuki reaction and intramolecular Michael type addition.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1078**

발표분야: 유기화학

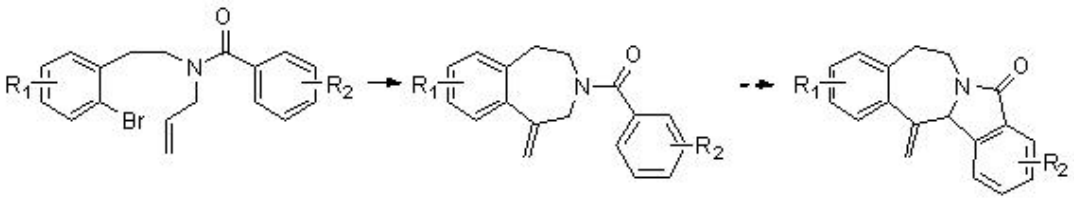
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Study of Lennoxamine

송경헌 김건철

충남대 화학과

Isoindolobenzazepine akaloid, lennoxamine and chilenine, was isolated from the plants of the Chilean Berberis species. Their unique structure feature, five- and seven-membered rings fused with aromatic moiety has drawn the synthetic interest of many group. We have studied the synthesis by intramolecular Heck reaction and the following oxidation for cyclization.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1079**

발표분야: 유기화학

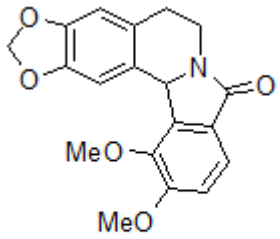
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Nuevamine

민지영 김건철

충남대 화학과

Nuevamine is the first known isoindolo[1,2-a]isoquinolinone alkaloid. Regioselective reduction, intramolecular dehydrative cyclization, aryne-mediatid cyclization are already known methods of synthesizing Nuevamine. In this study Nuevamine has been synthesized by the acid-catalyzed cyclization and rearrangement. Using this method, it would be possible to synthesis various types of isoquinoline alkaloids.



Nuevamine

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1080**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of iFRET acceptor fluorescence molecules to detect target proteins.

김주환 강효진[1] 정상전[1]

과학기술연합대학원대 나노바이오공학과 [1]한국생명공학연구원 바이오나노연구센터

Fluorescence technology has afforded the most robust biological detection tools due to its stability in biological environment. Among many fluorescence detection methods, FRET has represented a real-time imaging of target proteins. One of the drawbacks of FRET is that requires a labeling process of target proteins. Since “Intrinsic F?rster Resonance Energy Transfer (iFRET)” utilizes intrinsic fluorescence of the target proteins as a FRET donor and probe as a FRET acceptor, respectively, it does not require the labeling process. Tryptophan (Ex/Em = 280/350 nm) represent intrinsic fluorescence source in proteins. IFRET probe consists of two structural parts, target-specific ligand and FRET acceptor for tryptophan. Previously, two research groups have reported iFRET acceptor molecules for tryptophan and applied for developing iFRET probes, resulting in successful detection of the target proteins without a labeling process. Although the iFRET acceptors already developed could detect the purified target proteins, they may not be able to detect the target proteins in cells or cell lysate due to their short emission wavelength (< 340 nm) or low quantum yield. In this study we have screened many fluorescence molecules for iFRET acceptors with improved iFRET property and discovered three fluorescence molecules with high quantum yield and longer emission wavelength. The selected molecules were conjugated with biotin to prepare iFRET probe specific to streptavidin. iFRET probes thus prepared were tested for detecting streptavidin and characterized their fluorescence properties, FRET efficiency (0.14?0.36), R0 (1.6?2.2 nm). Currently, the detection of the target proteins in cellular environment is underway. In this conference, the details of iFRET acceptors will be presented.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1081**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Regioselective synthesis of N-1 nucleoside based on pyrrolo[2,3-d]pyrimidine

김영종 권순호 김병문

서울대 화학부

BMK-Y101 is new pyrrolopyrimidine-based inhibitor, which has strong inhibition activity of CDK7 and CDK9. Inhibition of CDK7 and CDK9 exert consequent negative effects on RNA synthesis, strongly promotes apoptosis. It has N-1 structure unlike previous nucleoside analogs based on pyrrolo[2,3-d]pyrimidine which has N-9 sturucture. N-1 nucleosides appeared rarely in the literature, as well as, had been considered as by-product of glycosylation.In the course of synthesis of N-1 nucleoside, some reagent was changed for easy of synthesis and higher yield. Then it showed drastic change, which means very high yield of N-1 nucleoside without N-7 isomer. N-1 structure was identified by X-ray diffraction spectrometry.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1082**

발표분야: 유기화학

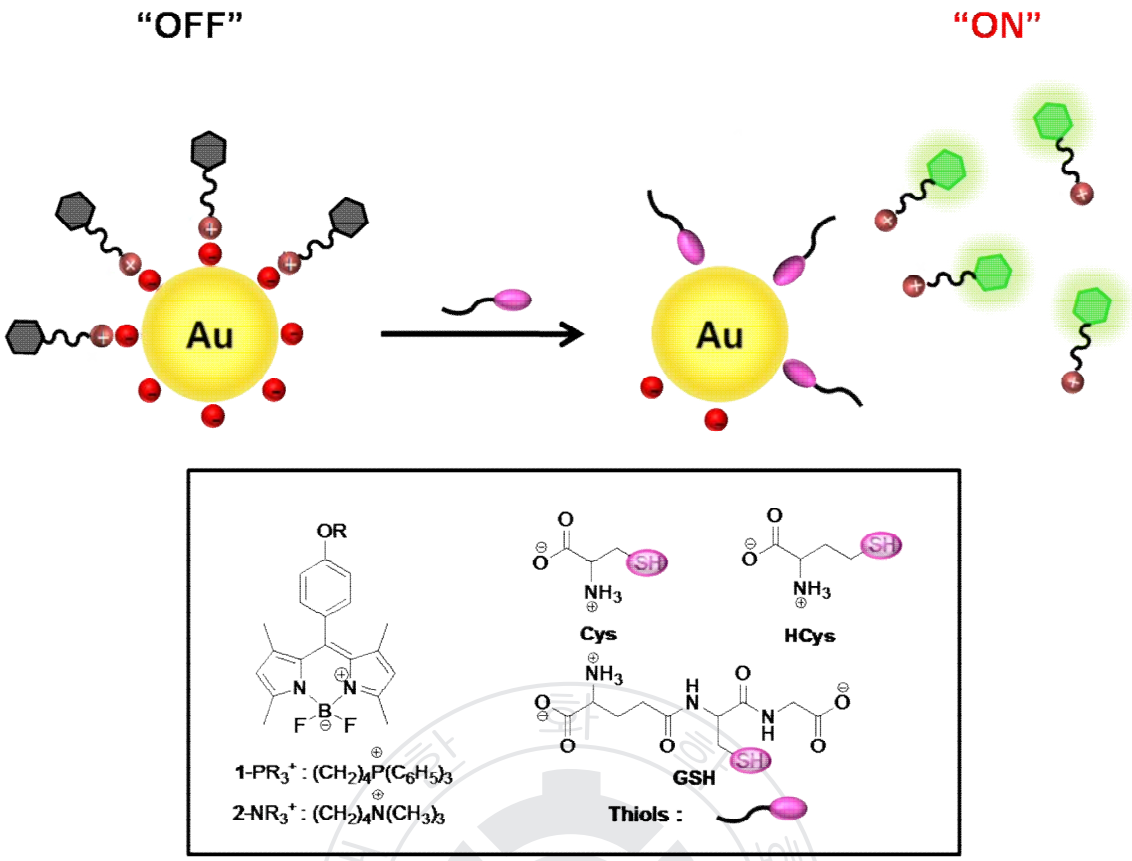
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Fluorescence Turn-on Probe Based on AuNPs/1-PR_3^+ Adsorbate for the Detection of Intracellular Thiols in Living Cells

최소희 김영미

단국대 화학과

Intracellular thiols such as cysteine (Cys), homocysteine (HCys), and glutathione (GSH) play crucial roles in numerous biological processes, including redox homeostasis, detoxification, and cellular metabolism. Abnormal levels of certain thiols such as HCys are linked to a number of disease, including cancer, Alzheimer's disease, and cardiovascular disease. Therefore, the detection of thiols is important. Herein, we report a new fluorescent probe based on the AuNPs/1-PR_3^+ and AuNPs/1-NR_3^+ adsorbates respectively, which induces high fluorescence turn-on response upon reaction with thiols in aqueous buffer solution. The AuNPs/1-PR_3^+ adsorbate was applied successfully to the imaging of thiols in living cells, suggesting its great potential as a direct tool for the detection and visualization of thiols in vitro and in cellular environments.



THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1083**

발표분야: 유기화학

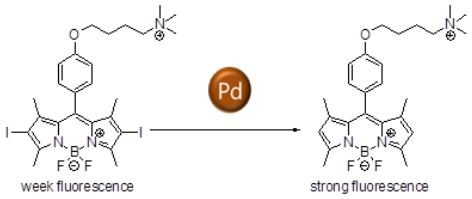
발표종류: 포스터, 발표일시: 수 16:00~19:00

A BODIPY-Based Probe for Detection of Palladium Species by C-I Bond Cleavage

금동호 김영미

단국대 화학과

Palladium species plays a key role as a catalyst in the synthesis of various molecules including drugs. In our body, palladium ions can bind to thiol-containing amino acids, proteins, DNA or other macromolecules and thereby may disturb a variety of biological processes. Therefore, easy detection of palladium species is an important issue.Herein, we present a sensitive and selective fluorescent probe based on C-I bond cleavage reaction under mild conditions by palladium species.



THE KOREAN CHEMICAL SOCIETY

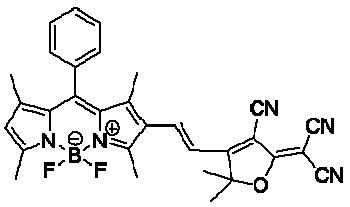
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1084**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Fluorescence Turn-on Probe for the Detection of Hypochlorous Acid

박지숙 김영미

단국대 화학과

Reactive oxygen species (ROS) are essential for a wide range of biological and pathological events. Among ROS, hypochlorous acid (HOCl/OCl$^-$) plays significant roles in the human immune-defense system. However, abnormal levels of HOCl in living organism are implicated in many human health and disease, such as cancer, cardiovascular diseases, rheumatoid arthritis, Alzheimer's disease. Therefore, the detection of HOCl is of great importance. We present a new BODIPY- based probe 1, which induces high ratiometric fluorescent turn-on response upon oxidation cleavage reaction with HOCl. In addition, the probe 1 showed a fluorescent response rapidly to hypochlorous acid with high sensitivity and selectivity. A new probe 1 advances the molecular toolkit of HOCl detection in physiological conditions.



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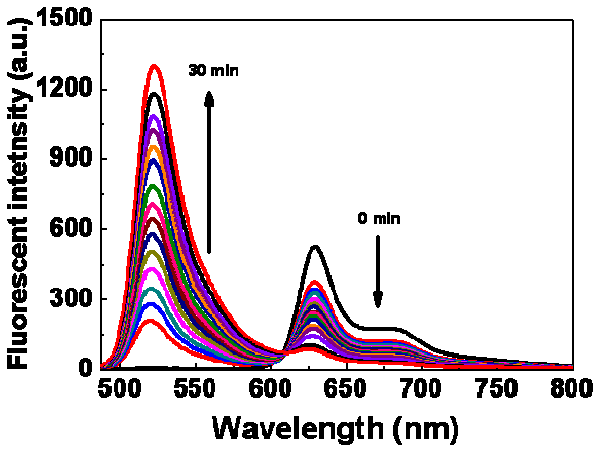

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1085**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A simple and efficient synthetic method of alkynyl ketones from acid chlorides

지윤진 임소희 신원규 안덕근

강원대 화학과

Alkynyl ketones are valuable intermediates widely used in organic synthesis. α,β-Acetylenic carbonyl compounds can, for example, undergo sequential nucleophilic additions and cyclizations, leading to various heterocyclic derivatives. They can also serve as intermediates for the synthesis of natural products, heterocyclic ligands, or precursors for materials with interesting properties. Most known methods for the preparation of the alkynyl ketones proceed via couplings of terminal acetylenic derivatives with acid chlorides using palladium and/or copper-catalyzed. Recently, we carried out experiences to find simple and effective method for partial acetylation of acid chlorides under convenient reaction conditions, as the result, we have found the new one-pot synthetic method of alkynyl ketones from acid chlorides in very good yields using new methodology.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1086**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Lithium diisobutylmorpholinoaluminum hydride (LDBMOA) as an effective partial reducing agent for tertiary amides and nitriles

김유리 안재성 안덕근

강원대 화학과

The direct synthetic method of aldehydes from carboxylic acid derivatives without oxidation step is important and valuable tool in organic synthesis. Many synthetic methods have been reported for preparation of aldehydes from carboxylic acid derivatives such as acid chlorides, esters, amides, and nitriles. Recently, we developed that LDBMOA as new partial reducing agents simply prepared by reacting commercially available DIBALH with lithium morpholide. Furthermore, we established a convenient method for the conversion of tertiary amides and aromatic nitriles to corresponding aldehydes in very good yield using the LDBMOA. Also, we found that this reagent did not reduce aliphatic nitriles, thus allowing chemoselective partial reduction of tertiary amides or aromatic nitriles in the presence of aliphatic nitriles. Therefore, LDBMOA is believed to be an alternative new reagent for reducing tertiary amides and aromatic nitriles to the corresponding aldehydes without affecting aliphatic nitriles.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1087**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new and useful one-pot synthetic method of alkynyl ketones from esters

김유리 이동진 안덕근

강원대 화학과

Alkynyl ketones are useful precursors and intermediates in the synthetic organic chemistry. In the case of esters, the preparation of the alkynyl ketones proceeds via addition reaction using metal acetylides such as alkynyl lithium, alkynyl lithium with $BF_3.OEt_2$ or alkynyl lithium with lithium morpholinide and $BF_3.OEt_2$. This addition reaction could be one of convenient ways to synthesize alkynyl ketones. However, these methods gave great problems in that the use of esters was limited to aliphatic or aromatic esters. Herein, we wish to report a new and use synthetic method for synthesizing aromatic and aliphatic alkynyl ketones both of them which is based on partial acetylation of esters by using morpholine and alkynyl lithiums without any Lewis acid.

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장소: 부산BEXCO

발표코드: **ORGN.P-1088**

발표분야: 유기화학

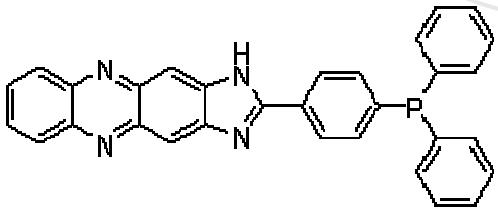
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photoluminescence of 2-(4-(Diphenylphosphino)phenyl)-1H-Imidazo[4,5-b]phenazine

TRINH DAC HOANH 임영훈 이범종[1]

인제대 화학과 [1]인제대 의생명화학과

The finding new materials for OLED application still have interests to the scientists due to the challenge toward diverse-structured materials. In this work, we synthesized 2-(4-(diphenylphosphino)phenyl)-1H-imidazo[4,5-b]phenazine (DPP) and investigated the photoluminescence properties of the compound for OLED application. Here DPP have phophino-, imidazo-, and phenazine groups within the compound structure. The structure of DPP was determined by ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-Vis, and elemental analysis. DPP shows a green emission under excitation by UV lamp of 365 nm. The photoluminescence properties of DPP will be discussed.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1089**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Aqueous-Phase Heterogeneous Catalyst Based on Pd-NP Imbedded Inside Silica Nanotube

이상희 박기남[1] 이우승 **VUTHANHCONG**[2]

경원대 바이오나노학과 [1]한양대 자연과학대학 [2]경원대 Bionano

Sanghee Lee[2], Ginam Park[1,2] , Wooseung Lee[2], Thanh Cong[2], Sang Jun Son[2], Seunghoon Shin[1,*1]Department of Chemistry, Hanyang University, Seoul 133-791, South Korea[2]Department of Chemistry, Gachon University, Gyeonggi 461-701, South KoreaWe prepared a novel Pd nanoparticle (Pd NP) nanocatalyst by forming Pd-NPs onto the inner surface of silica nanotbe (SNT). SNT has two independent surfaces, inner and outer, which can be differentially functionalized. Using thermal reduction, we prepared Pd-NP electively at the N-(3-Trimethoxysilylpropyl)dimethylenetriamine(DETA)-modified inner surface without ligand or stabilizer which are known to reduce the efficiency of Pd catalyst by limiting accessibility of substrates. We successfully applied this catalytic system in Suzuki coupling as well as direct arylation of thiazoles in water. Low catalyst loading (0.5 mol % Pd) and mild reaction conditions (60-80 ^{o}C) indicated the high catalytic activity of the current system. We confirmed that there is no catalyst leaching during the reaction, confirming that the reaction proceeds inside of SNT. Furthermore, after the reaction, Pd@SNT could be precipitated and a simple decantation allows separation of the catalyst.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1090**

발표분야: 유기화학

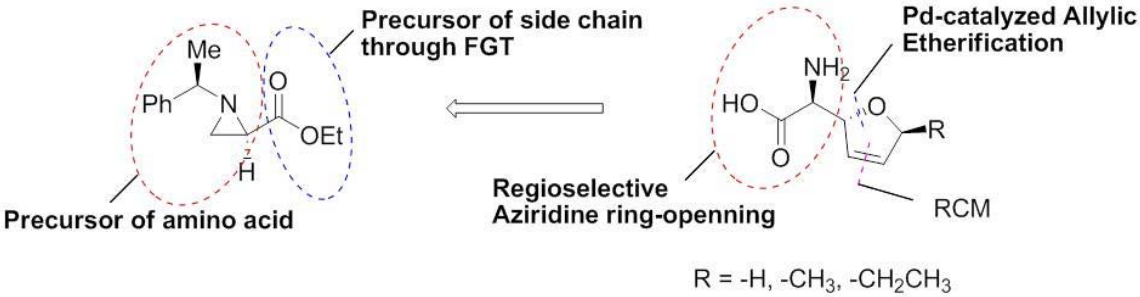
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Furanomycin and it's analogues from aziridin-2-carboxylate

윤두하 하현준 이원구[1]

한국외국어대 화학과 [1]서강대 화학과

The antibiotic natural product furanomycin isolated from the fungus Streptomyces threomyceticus is an ?-amino acid with 4-methyl-2,4-dihydrofurayl ring. The synthesis of furanomycin and its analogs bearing ethyl and hydrogen instead of methyl at 2,4-dihydrofurayl ring for furanomycin was prepared from aziridin-2-carboxylate. The key steps of this synthesis starting from aziridin-2-carboxylate include alkynylation, stereoselective reduction of aziridin-2-yl propynyl ketone, allylic etherification and RCM of diallyl ether with Grubbs' catalyst to elaborate 2,4-dihydrofurayl ring. The part of amino acid was achieved from the regioselective ring opening of aziridine by the hydroxy nucleophile followed by oxidation.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1091**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and conformational analysis of cyclic amino acids that promote interesting helical folding

이우형

연세대 화학과

The study of oligomers that contain alternative α- and β-amino acid residues is a fascinationg topic to explore synthetic foldamers that adopt helical secondary structure. What is more, the conformationally restricted β-amino acid residues give the ability to maintain conformational stability with hydrogen bonding interaction. In this work, we synthesized several α/β peptides in a 1:1 alternating pattern by using [2+2] cycloaddition and peptide coupling strategies. Furthermore, we studyed structural information of our foldamers.

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장소: 부산BEXCO

발표코드: **ORGN.P-1092**

발표분야: 유기화학

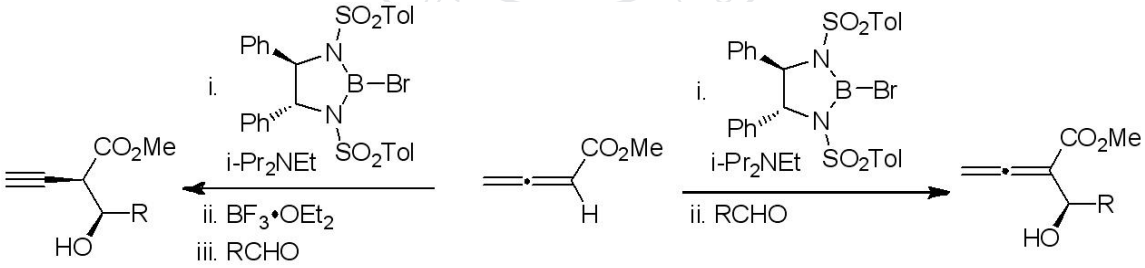
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Stereoselective Aldol Reaction of Allenoates with Aldehydes for the Synthesis of Alkynyl Aldol Adduct

유찬모 김지현 김현아 최미라

성균관대 화학과

Recently, we have developed a new adol method of the allenoate process in forming 2-hydroxy allenolate in high levels of enantioselectivity. In light of this result, we turned our attention to achieve alkynyl addut without isomerization to allenyl ester. After conversion of alleneoate with i-Pr2NEt in the presence of chiral bromoborane complex to borone enolate, 1 equivalent of trifluoroborane etherate 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, and its applications.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1093**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

1,8-Naphthalimide appended DTTA Derivative is a Zinc ion triggered Bimodal Contrast Agent.

장주희 양정호 김종승

고려대 화학과

Magnetic resonance imaging (MRI) is an important imaging in diagnostic medicine. It provides high-quality three-dimensional images of tissue and anatomical resolution without use of injurious ionizing radiation. Gadolinium-based chelates are the most commonly used MRI contrast agents because the chelated Gd^{3+} metal ion enhanced MR signal by decreasing the longitudinal relaxation time (T1). As a result, T1-weighted MR image is brighter. We developed metal ions induced MR/Fluorescence signal enhanced bimodal imaging agent by taking of 1,8-naphthalimide framework with appended DTTA as Gd^{3+} chelating site. MR signal was enhanced in presence of biologically relevant target metal ions and fluorescence signal also altered. This dual modulated CA can be used as cationic sensor which is a new biocompatible detector for biologically relevant metal ions to detect them in a noninvasive manner.

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장소: 부산BEXCO

발표코드: **ORGN.P-1094**

발표분야: 유기화학

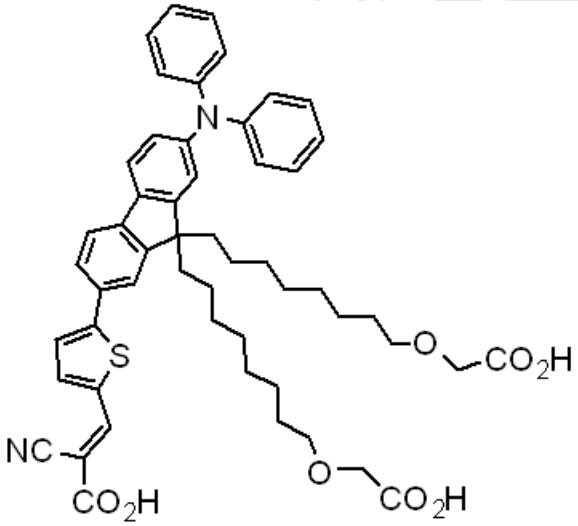
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of long alkyl anchoring group on photovoltaic performance in DSSC

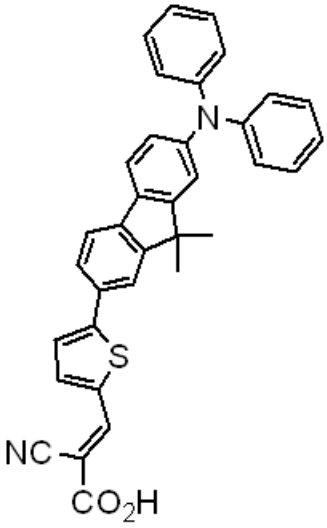
이상희 유수창 김동희 한승훈 최규석

군산대 화학과

Tripodal dye KS-12 was synthesized for dye sensitized solar cell. KS-12 has two extra anchoring groups as well as long alkyl groups. By comparison of KS-12 to KS-13, effect of two long alkyl and carboxyl group on photovoltaic performance will be described.



KS-12



KS-13

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1095**

발표분야: 유기화학

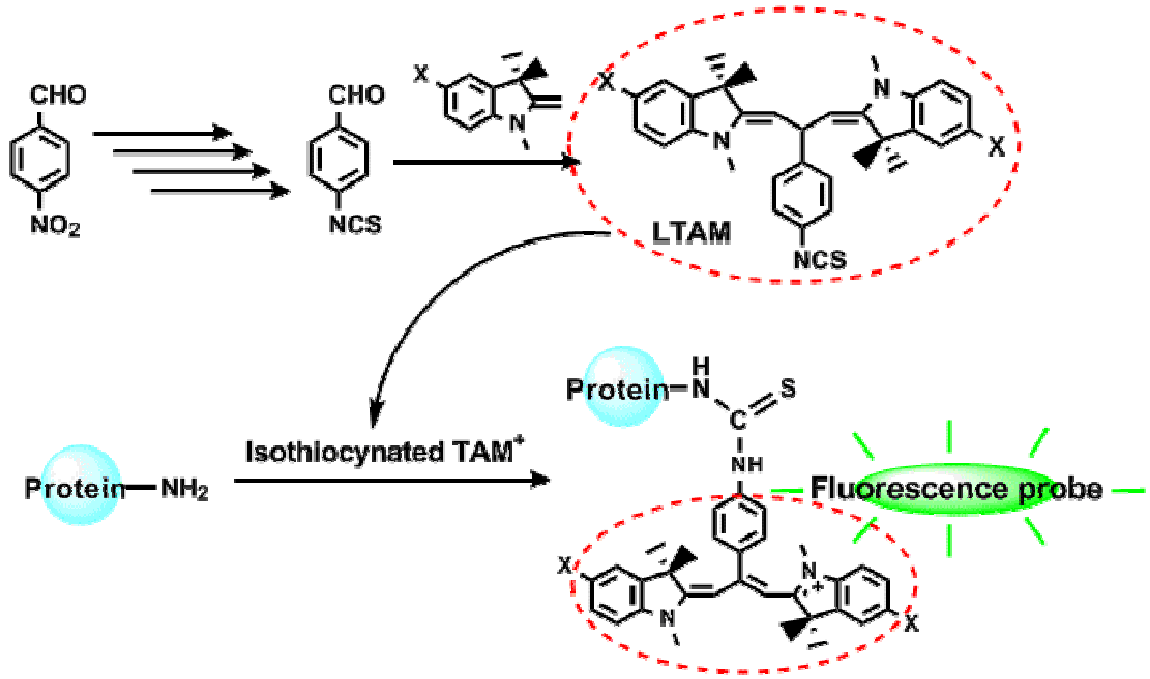
발표종류: 포스터, 발표일시: 수 16:00~19:00

NIR Fluorescence Dyes LTAM/TAM^{+} for Optical Imaging: Synthesis and Spectroscopic Characterization

마소영 금삼록[1]

고려대 소재화학과 [1]고려대 소재화학과

One of optical imaging techniques is NIR fluorescence-based (650-900nm) high-resolution imaging. The Fischer's base (FB)-analog of leuco-TAM (LMG)/TAM+ dyes, developed by our group, are expected to be the most possible candidate for the fluorophore probes. The potent NIR Fluorescence LTAM Dyes, (2E,2'Z)-2,2'-(2-(4-isothiocyanatophenyl)propane-1,3-diylidene)bis(1,3,3-trimethylindoline) derivatives were prepared from the reaction of excess Fischer's base(FB) with 4-isothiocyanatobenzaldehyde, which was obtained from the 4-nitrobenzaldehyde. The prepared molecules were characterized by 1H, 13C-NMR, COSY, HETCOR, IR, UV-VIS spectroscopy.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1096**

발표분야: 유기화학

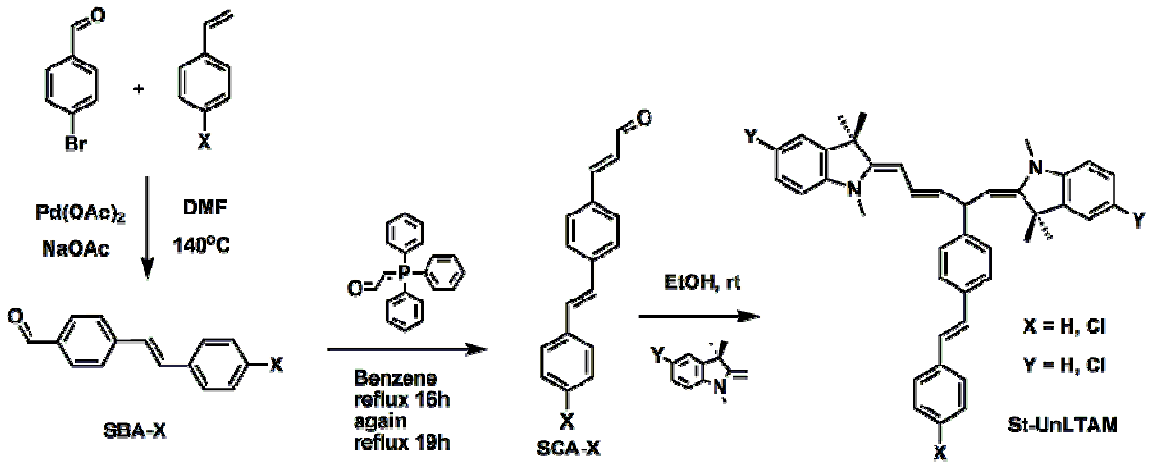
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of unsymmetric stilbene-based leuco-TAM Fischer's base analogs

한태휘 금삼록

고려대 소재화학과

Novel unsymmetric stilbene-based LTAM molecules, (2E)-1,3,3-trimethyl-2-((3E,5Z)-5-(1,3,3-trimethylindolin-2-ylidene)-2-(4-styrylphenyl)pent-3-enylidene)indoline St-UnLTAM were prepared from the reaction of excess 5-substituted Fischer base (FB) with (E)-3-(4-styrylphenyl)acrylaldehyde SCA and excess Fischer's base in EtOH at rt. From the reaction of 4-bromobenzaldehyde and the correspondingly substituted styrene, 4-styrylbenzaldehyde SBA derivatives was formed. The (E)-3-(4-styrylphenyl)acrylaldehyde SCA were then obtained from the reaction of (triphenylphosphoranylidene)acetaldehyde with SBA.The prepared St-UnLTAM molecules were characterized by 1D and 2D NMR experiments including DEPT, COSY, HETCOR and NOESY. The St-UnTAM$^+$ dyes were confirmed by UV-Vis spectroscopy.



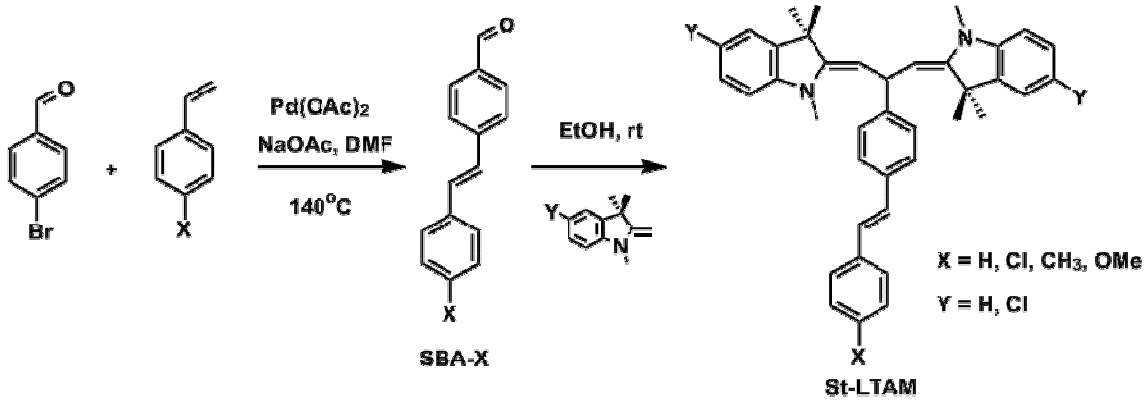
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **ORGN.P-1097**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of novel stilbene-based leuco-TAM Fischer's base analogs

임현우 금삼록

고려대 소재화학과

Novel stilbene-based leuco-TAM molecules, (2E,2'Z)-2,2'-(2-(4-styrylphenyl)propane-1,3-diylidene)bis(1,3,3-trimethylindoline) derivatives was prepared from the reaction of excess 5-substituted Fischer base (FB) with (E)-4-styrylbenzaldehyde (SBA). The SBA molecule was obtained from the reaction of 4-bromobenzaldehyde with 4-substituted styrene by the Heck reaction using palladium catalyst. The St-TAM$^+$ dyes are expected to have an π-extended chromorpore from the nitrogen of FB ring to the central stilbene-ring. The prepared St-LTAM molecules were characterized by 1D and 2D NMR experiments including DEPT, COSY, HETCOR and NOESY. The St-TAM$^+$ dyes were confirmed by UV-Vis spectroscopy.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1098**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Transition metal-free carboxylation of acetylene with carbon dioxide

Wang Xi

아주대 에너지시스템학부

The use of carbon dioxide (CO2) as a C1 building block for chemical synthesis has recently attracted much interest because of its abundance, low cost, nontoxicity, and high potential as a renewable source. However, activation of this thermodynamically and kinetically stable molecule usually requires organometallic reagents or large amount of inorganic bases in the previous work. Here, for the first time, carboxylation of acetylene, phenyl acetylene and other alkynes by environmentally friendly bases has been reported.

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장소: 부산BEXCO

발표코드: **ORGN.P-1099**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Tandem Michael addition/oxyamination of aldehydes under organophotocatalytic conditions.

이화정

아주대 응용화학과

By using a chiral amine organocatalyst along with N719/TiO2 under visible light, asymmetric iminium catalysis was combined with photo-catalysis. Because the photocatalytic oxidation under visible light has advantage such as environmentally friendly nature, cost-effective and no use of chemical oxidants. So, Ru complex-based reusable photocatalysts and visible-activated organic dye-bound photocatalysts are synthesized. A variety of photocatalysts were employed for the stereoselective synthesis of α, β-disubstitued aldehydes, showing good yield and high levels of enantio- and diastereoselectivity.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1100**

발표분야: 유기화학

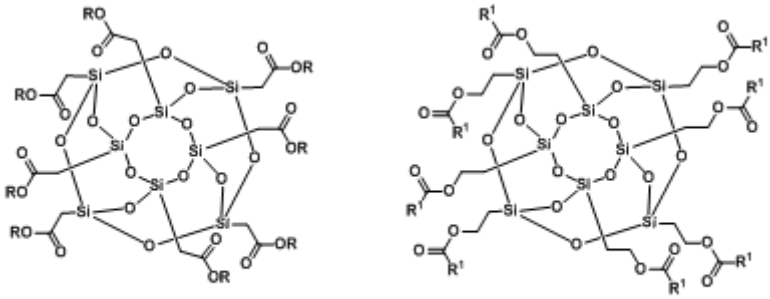
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of POSS derived inorganic/organic hybrid insulating oils

Vijay kumar S.J. Hashavardhan 신동수

창원대 화학과

Biodegradables oils show the importance of biodegradability and nontoxicity. Polyhedral oligomeric silsesquioxanes (POSS), having 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.



R = Alkyl group

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1101**

발표분야: 유기화학

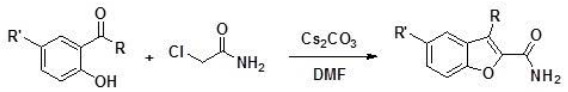
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot synthesis of benzofuran-2-carboxamides

xieyongsheng 장희재[1] 문기철[1] 신동수

창원대 화학과 [1]창원과학고 화학연구실

A convenient one-pot synthesis of benzofuran-2-carboxamide derivatives from substituted salicylaldehydes with 2-chloroacetamide using cesium carbonate as a base in dimethyl formamide solvent has been developed in moderate to good yields



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1102**

발표분야: 유기화학

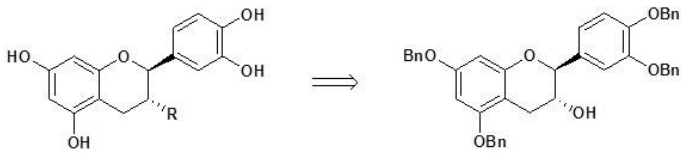
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and synthesis of (-)-Catechin analogues for its biological activity

Vijay kumar kumar deepak 신동수

창원대 화학과

(-)-Catachin found to possess a wide range of biological activities via anti-oxidant, anti-proliferative, anti-HIV etc. (-)-Catechin have emerged as promising chemopreventive agents because of their observed efficacy in various animal models. We have initiated a program for the synthesis of (-)-Catachin and its analogs for its biological activity.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1103**

발표분야: 유기화학

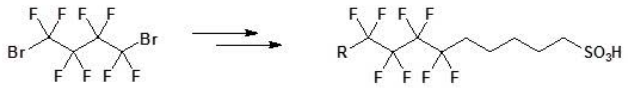
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic approach to PFOS alternatives in ionic liquid

Vijay kumar B.Prem kumar S.J. Hashavardhan 신동수

창원대 화학과

Synthesis of a new surfactant and their derivatives with less number of fluorine atoms to overcome some draw backs of the well-known fluorosurfactant perfluorooctanesulfonic acid (PFOS), has been achieved by using a conjugate radical addition of partially perfluoroalkyl halides to phenylvinylsulfonate in ionic liquid (IL).



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1104**

발표분야: 유기화학

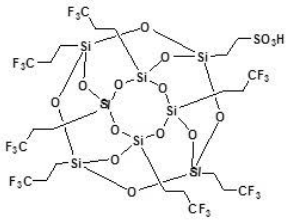
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of fluoro-POSS-sulfonic acid

B.Prem kumar Vijay kumar S.J. Hashavardhan 신동수

창원대 화학과

Organo-composites of polyhedral oligomeric silsesquioxanes (POSS) in the form of sulfonic acid derivatives and various alkyl groups can be synthesized by POSS triol with 3- chloropropyltrichlorosilane to form POSS cage monochloride. And this chloride was converted to sulfonicacid by sodium dithionate.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1105**

발표분야: 유기화학

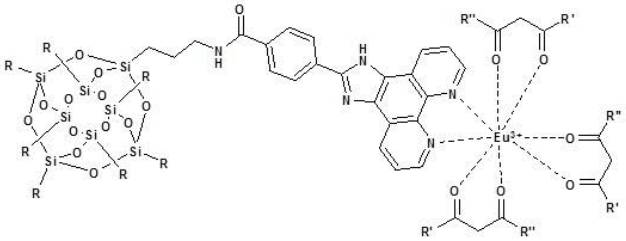
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of POSS-based hybrid fluorescent

B.Prem kumar 장희재[1] 문기철[1] 신동수

창원대 화학과 [1]창원과학고 화학연구실

A new kind of fluorescent organic-inorganic hybrid material consisting of europium, diketone ligands (1,3-diketones) 1,10-phenanthroline complexes covalently attached to a polyhedral oligomeric silsesquioxane (POSS). Modified 1,10-phenanthroline grafted to POSS -amine was used as one of the precursors for the preparation of an organic-inorganic hybrid materials.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1106**

발표분야: 유기화학

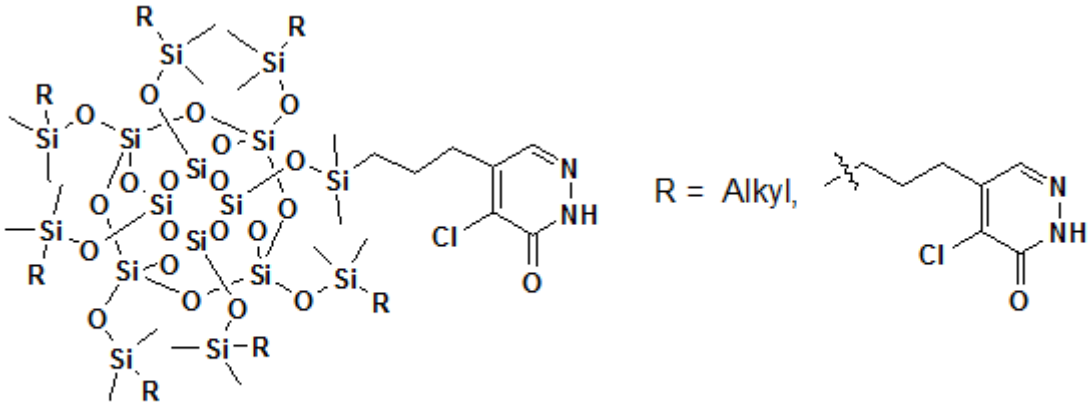
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and application of POSS-Pyridazin-3(2H)-ones

dongwenliang B.Prem kumar 윤용진[1] 신동수

창원대 화학과 [1]경상대 화학과

POSS-Pyridazinones were synthesized by hydrosilylation of POSS hydrides and allyl substituted pyridazinones which were used in esterifiction and acylation. Our main aim to recover the POSS-Pyridazinone after the reaction by different method and to reuse.



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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1107**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Biological properties and synthesis of 1,3,5-triazines containing o-carborane and water-soluble functional groups as potential BNCT agents

이채호 이종대[1] 강상욱[2] 박관희[3] 조석준[3]

원광대 생명나노화학부 [1]조선대 화학과 [2]고려대 소재화학과 [3]원광대 화학과

Carboranes are stable, lipophilic structures which resemble benzene in term of reactivity and bulkiness. Therefore it is not surprising that carborane-based biomolecules which an aromatic group is replaced by the boron cage have been prepared. Since carboranes whi-ch linked a biomolecule contain ten boron atoms, they theoretically may help deliver m-uch higher concentrations of 10B atoms in cancer cells for boron neutron capture therapy (BNCT). We here in report on the synthesis of carboranyl-1,3,5-triazine containing water-soluble functional groups as potential BNCT agents.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1108**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Transition metal-free, NaO^{t}Bu-O_2-mediated one-pot cascade oxidation of allylic alcohols to α,β-unsaturated carboxylic acids

김선민 김영석 김동완 양정운

성균관대 에너지과학과

We developed a protocol for the transition metal-free, direct oxidation of allylic alcohols using the simple base NaO^{t}Bu under oxygen atmosphere. The NaO^{t}Bu-O_2 system exhibited unprecedented activity and selectivity in this oxidation reaction. In particular, a competing epoxidation reaction was suppressed under these conditions.

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1109**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of novel molecular frameworks containing two distinct heterocyclic cores in a single molecule with enhanced 3-dimensional shape diversity

임동현 박승범[1]

서울대 생물물리 및 화학생물학과 [1]서울대 화학부

The synthesis of fused-triazole scaffolds that are connected with prymidine, pyrazole, or pyrazolopyrimidine through carbohydrate-derived stereodivergent linkers is reported here. Prymidine, pyrazole, or pyrazolopyrimidine-based carbohybrid was constructed through the condensation of the key intermediate, 2-C-formyl glycals, with various dinucleophiles. Fused-triazole scaffolds were constructed through the intramolecular 1,3-dipolar cycloaddition after functionalization of the hydroxyl groups of the carbohybrid with azide and alkyne functionality using SN2-type alkylation or Mitsnobu reaction. Overall, the synthetic method described here afforded two distinct privileged structures in a single molecule, conserving the stereogenic centers of the carbohydrates. In addition, the stereodivergent diol functionality at the linker position was modified to obtain chemical collections with maximized 3-dimensional shape diversity.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1110**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

젬-다이나이트로 에스터형의 에너지화 가소제 합성

김승희 김진석[1]

국방과학연구소 4본부2부 [1]국방과학연구소 4본부 2부

젬-다이나이트로를 에너지기로 도입하고 반대편에는 비극성 화합물인 선형 혹은 가지친 알킬기를 도입하여 기존의 에너지화 가소제의 극성을 낮추는 것을 연구의 목적으로 한다. 위 화합물의 합성은 상업적으로 구할 수 있는 원료인 1,1-dinitroethane 을 출발물질로 하고 butyl, hexyl, heptyl, 2-ehtylhexyl 등의 아크릴 화합물과 Micheal addition 반응으로 얻는다.본 화합물을 복합화약에 적용할 경우, 기존의 에너지화 가소제보다 극성을 낮추어 분자화약의 형상변형을 예방할 수 있으며, 비활성 가소제보다는 성능이 높아 둔감성과 성능을 동시에 향상시킬 수 있을 것으로 판단된다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1111**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Heteroaromatic Moieties in the Sphingosine Backbone of α-Galactosylceramides for Noncovalent Interactions with CD1d

송희범 김용주[1] 김종훈[2] 박승범[1]

서울대 자연과학대학 화학부 [1]서울대 화학부 [2]서울대 화학과

Natural killer T (NKT) cells are a subset of T cells and play a central role in regulating immune responses. The potent immunostimulatory lipid antigens such as KRN7000 have led to activation of NKT cell when presented by CD1d proteins expressed on antigen-presenting cells. In vitro and in vivo studies with NKT cells indicate that the stimulation of NKT cells initiates a cascade of events leading to the release of different Th1- or Th2-type cytokines including proinflammatory (e.g., INF-r, TNF-α) or immuno-modulatory response (e.g., IL-4, IL-10), respectively. Disruption of the balance betweenTh1 and Th2 cytokines is involved in a broad range of diseases such as infections, cancer, multiple sclerosis, lupus, rheumatoid arthritis and type-1 diabetes. Although several studies of KRN7000 and its derivatives have been reported to confirm structure-activity relationship, almost studies use the similar sphingoid backbone of KRN7000 containing just changes in sphingoid base lengths and in acyl chain. Here, we desrcribe synthesis of a new α-galactosylcereamides containing new ceramide skeleton as KRN7000 analogues.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1112**

발표분야: 유기화학

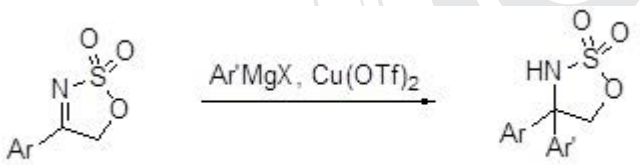
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cu-Catalyzed aryl Grignard additions to cyclic sulfamidate imines

김미리 A.PITCHAIAH[1] 이선아[2] 황인택[3] 이기인[2]

과학기술연합대학원대 청정화학 및 생물학 [1]한국화학연구원 바이오리파이너리 [2]한국화학연구원 그린화학연구단 [3]한국화학연구원 바이오리파이너리연구센터

Cu-Catalyzed addition of aryl Grignard reagents to cyclic sulfamidate imines has been described. This method tolerates a variety of aryl groups and is effective in the synthesis of quaternized aminoethanols and ethylenediamines by way of ring-opening with an appropriate nucleophile.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1113**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of privileged tetra-substituted ?5-2-oxopiperazine mimicked β-turn sturcuture via reductive alkylation and construction of compound library embedded tetra-substituted ?5-2-oxopiperazine

이정애 김종훈[1] 박승범[2]

서울대 생물물리및화학생물학부 [1]서울대 화학과 [2]서울대 화학부

Oxopiperazine moiety is important pharmacophore which is used as peptidomimetics, specially mimicked β-turn and γ-turn structure, which is one of the three main secondary structural motifs found in proteins and peptides. We constructed ?5-2-oxopiperazine compound library via iminium ion cyclization and rearrangement under mild acidic condition. For synthetic efficiency, we applied fluorous tag-based solution phase parallel synthesis strategy. The library scaffold has four diversity points of substitution so we introduced diverse scaffold through reductive amination with Grignard reagent and simple amide coupling concisely. The fluorous tag was facilitated utilizing synthetic strategy optimized in solution phase without fluorous tag. we utilized diverse substrates as 4 diversiting points such as 4 grignard reagent, 6 amino acids and 5 amines that can be induced after cyclization step. Through this novel strategy, a 144-membered drug like oxopiperazine library has been constructed efficiently.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1114**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aerobic Oxidative Cleavage of Triple Bond in the Gold-Catalyzed Cyclization of 1,6-Enynes Derived from Propiolamide

박현섭 구재영 신승훈

한양대 화학과

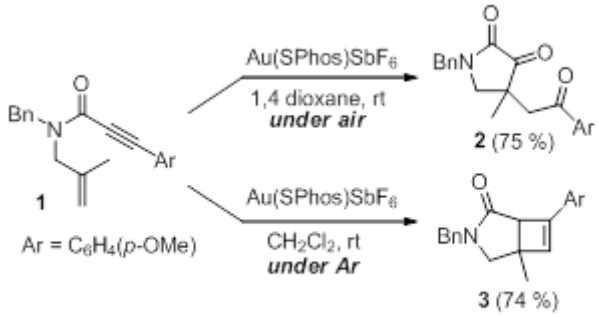
The metal-catalyzed cleavage of a carbon-carbon triple bond has stimulated new conceptual strategies in organic synthesis.[1] The use of oxygen to cleave a carbon-carbon bond catalytically is economically and environmentally important. Use of dioxygen has recently received a great deal of attention as an ideal end-oxidant in various oxidative transformations, because it is non-toxic and do not generate stoichiometric waste.

Since a pioneering work of Y. Liu in 2006 on the gold catalyzed oxidative cleavage of triple bond in the cyclization of (Z)-enynol,[2a] several reports followed that report aerobic triple bond cleavage in gold catalysis.[2b-d] In the course of our study on the gold catalyzed cyclization of 1,6-enynes derived from propiolamides, we observed an efficient formation of tricarbonyl compound 2 under an aerobic condition whose structure was identified by X-ray crystallography. This oxidative cleavage occurs even under ambient air (P_{O2} = 0.2 atm) and at room temperature. In contrast, the reaction of 1 in chlorinated solvents under Ar led to a fused cyclobutene 3.[3] For the mechanism of this solvent-dependent divergence, the following experimental evidences have been obtained; (1) the fused cyclobutene 3 is not a viable intermediate *en route* to 2. (2) in the presence of radical inhibitors (BHT, TEMPO), production of 2 is completely inhibited. These suggest that 2 is not obtained by oxidation of 3, but a gold-bound radical species is formed and undergoes reaction with O_2 prior to the formation of 3.

Acknowledgement.This work was financially supported by National Research Foundation of Korea (NRF-2011-0023686 & NRF-2012-015662).

References1. (a) Morris, M. J. In Metal Clusters in Chemistry; Braunstein, P., Oro, L.A., Raithby, P. R.,

Eds.; Wiley-VCH: Weinheim, Germany, 1999; Vol.1; pp 221-235. (b) Chamberlin, R. L. M.; Rosenfeld, D. C.; Wolczanski, P. T.; Lobkovsky, E. B. Organometallics 2002, 21, 2724 and the references therein.2. (a) Y. Liu, F. Song, S. Guo, J. Am. Chem. Soc., 2006, 128, 11332. (b) Egorova, O. A.; Seo, H.; Kim, Y.; Moon, D., Rhee, Y. M.; Ahn, K. H. Angew. Chem. Int. Ed. 2011, 50, 11446. (c) Hashmi, A. S. K.; Jaimes, M. C. B.; Schuster, A. M.; Rominger, F. J. Org. Chem. 2012, 77, 6394. (d) Das, A.; Chaudhuri, R.; Liu, R. S. Chem. Commun. 2009, 4046.3. Y. T. Lee, Y. K. Kang, Y. K. Chung, J. Org. Chem. 2009, 74, 7922.



대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1115**

발표분야: 유기화학

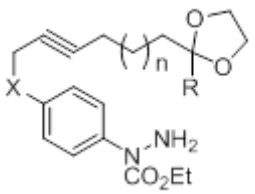
발표종류: 포스터, 발표일시: 수 16:00~19:00

Linear combination of intramolecular Fischer indolization and orthro-Claisen rearrangement toward the synthesis of multi-cyclic chromeno-indole

박준 김지은 임병윤 조천규

한양대 화학과

We have previously demonstrated that aryl hydrazides are effective surrogates of aryl hydrazines, undergoing the Fischer indolization reaction to afford the corresponding indoles, when treated with enolizable aldehydes and ketones in the presence of an acid. Unlike aryl hydrazines, the aryl hydrazides are readily accessed from aryl halides via the Pd(0) or Cu(I)-catalyzed coupling reaction with N-Boc hydrazine. We have also reported that N-Cbz-aryl hydrazide can proceed in a Fischer indolization reaction to give N-Cbz-indole without the elimination of N-Cbz group. Prompted by our recent interest on the synthesis of ergot alkaloids, we set out to study the intramolecular Fischer indolization reaction of the aryl hydrazide that are linked to carbonyl functions by various tether groups as a new synthetic means to the construction of tricyclic indole system. We found that aryl hydrazide with carbonyl function tethered at the C(4) position of the aromatic ring undergoes intramolecular Fischer indolization to afford novel indolophanes. A strategic insertion of a double bond in the tether allowed for an aromatic Claisen rearrangement to proceed in a tandem fashion, providing tricyclic benzo[cd]indole system. A similar system with alkyne tether also undergoes the above reaction sequence, but in a bit different manner.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ORGN.P-1116**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Naphthalene-based fluorescent receptor for selective recognition of Aluminum (III)

김보연 Jadhav Jyoti 김홍석

경북대 응용화학과

Aluminum is the third abundant element in the lithosphere and its compounds are widely dispersed and used in the environment around us in modern society: in water treatment, in food additives, in medicine, as the production of light alloy etc. Aluminum toxicity causes bone and joint diseases neuronal disorder leading to dementia myopathy and Alzheimer's disease. Development of fluorescent chemosensors has currently attracted significant interest because of their potential application in medicinal and environmental research. Among several methods for the detection of Al3+ in the literature, spectrofluorimetry is widely used for its high sensitivity, selectivity and easy operation procedure. Herein we synthesized and characterized compound 1 obtained by condensing 2-hydroxynapthaldehyde with 3-(1-aminopropyl)imidazole. Compound 1 is used as an efficient fluorescent probe for the detection of Al3+ in EtOH and 5% water in EtOH.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1117**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Quinolinylphenylamide Derivatives and Their Antiproliferative Activities against Melanoma Cell Line

고은정 이상기 유경호[1]

이화여대 화학/나노과학과 [1]KIST 화학키노믹스연구센터

The signal transduction pathway in which Raf kinase operates has long been implicated in oncogenesis and is critical for proliferation, survival, and angiogenesis in various cancer models. Recently, activating somatic mutations in b-Raf have been reported in 70% of melanomas. These mutations are also present in premalignant atypical or dysplastic nevi and may thereby implicate b-Raf activation as an initiating event in tumorigenesis. The purpose of this study is to develop b-Raf serine/threonine kinase inhibitors for the treatment of malignant melanoma. Small molecule-based quinazolinylphenylamide derivatives with a novel scaffold were designed and synthesized. As a result of cell-based assay, several compounds exhibited excellent antiproliferative activities against A375 human melanoma cell line.

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장소: 부산BEXCO

발표코드: **MEDI.P-1118**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-inflammatory Effect of Sulforaphane Derivatives by the Inhibition of Nitric Oxide Production

강남규 최정훈 유경호[1]

한양대 화학과 [1]KIST 화학키노믹스연구센터

Parkinson's disease (PD) is a degenerative disorder of the central nervous system.The motor symtoms of PD result from the death of dopamine-generating cells in the substantia nigra, a region of the midbrain; the cause of this cell death is unknown. Investigations on neuroprotection are at the forefront of PD reasearch. Several molecules have been proposed as potential treatments. However, none of them have been conclusively demonstrated to reduce degeneration.It has been suggested that inflammation is involved in the development of Parkinson's disease.Based on a core structure of sulforaphane with potent nitric oxide inhibitory activity, new scaffolds were designed and synthesized. Anti-inflammatory activities by the inhibition of nitric oxide production of these compounds were evaluated.

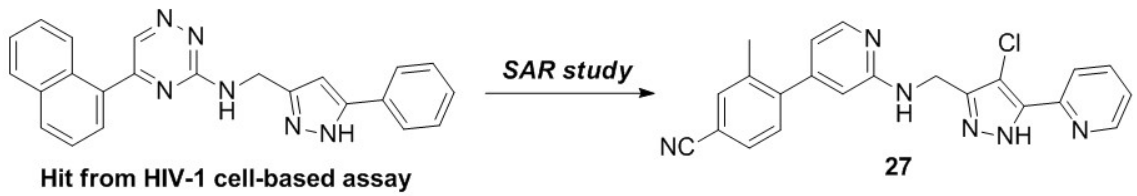
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1119**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of Phenylaminopyridine Derivatives as Novel HIV-1 Nonnucleoside Reverse Transcriptase Inhibitors

김준원 권정진 조수연 공선주 박동식 최지현 김영미 황종연 고윤애 최인희 박은정 노재성 이진화[1]

한국파스퇴르연구소 의약화학 [1]한국파스퇴르연구소 late discovery program(LDP)

We identified a novel class of aryl-substituted triazine compounds as potent non-nucleoside reverse transcriptase inhibitors (NNRTIs) during a high-throughput screening campaign that evaluated more than 200000 compounds for antihuman immunodeficiency virus (HIV) activity using a cell-based full replication assay. Herein, we disclose the optimization of the antiviral activity in a cell-based assay system leading to the discovery of compound 27, which possessed excellent potency against wild-type HIV-1 (EC50 = 0.2 nM) as well as viruses bearing Y181C and K103N resistance mutations in the reverse transcriptase gene. The X-ray crystal structure of compound 27 complexed with wild-type reverse transcriptase confirmed the mode of action of this novel class of NNRTIs. Introduction of a chloro functional group in the pyrazole moiety dramatically improved hERG and CYP inhibition profiles, yielding highly promising leads for further development.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1120**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The design and synthesis of 1,4-substituted piperazine derivatives as triple reuptake inhibitors

한민수 한호규[1] 남기달[2]

고려대 화학과 [1]KIST 생체과학연구부 [2]KIST 생체분자기능연구센터

Major depressive disorder (MDD) is a common and serious illness with the potential to become the leading cause of disability worldwide. Heterocyclic scaffolds represent the most promising molecules as leading structures for the discovery of novel synthetic drugs. In particular, the piperazine core is found in numerous drugs and clinical and preclinical candidates that address a broad spectrum of targets. To develop triple reuptake inhibitors which blocks synaptic reuptake of all three neurotransmitters (5-HT, NE or DA), we designed novel 1,4-substituted piperazine derivatives by fragment analysis and molecular modification of 4 selected piperazine-containing compounds which possess antidepressant activity. Herein we will report their biological activities against 5-HT, NE or DA reuptake inhibition as well as their structure-activity relationship.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1121**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Selection and Lead Optimization of Novel Anti-Tuberculosis (TB) Agents against H37Rv Strain and MDR Clinical Isolates

김재승 서민정 강선희 이세연 서무영 서정제 이수미 김영미 최인희 고윤애 이진화[1]

한국파스퇴르연구소 의약화학그룹1 [1]한국파스퇴르연구소 late discovery program(LDP)

Despite progresses in public health management and the implementation of fixed dose therapies, the epidemic and emergence of multi- and extensively-drug resistant Tuberculosis remains a serious issue worldwide. The treatment of MDR and XDR Tuberculosis requires the administration of second-line drugs for up to two years, with a success rate limited to 60% in most cases and an unacceptable mortality rate. The most urgent clinical need is to discover and develop potent agents capable of reducing the time of MDR TB therapy with a success rate at least as good as for susceptible TB. To identify novel anti-tubercular compounds, we screened various commercial chemical libraries using a high-content screening technology in/out infected macrophages. From a library of ~ 200,000 compounds, around 500 active hits were identified and reconfirmed for Dose-response. Several scaffolds of the hits were successfully optimized and one of those scaffolds is being studied for preclinical development. Next attention was focused on a series of alkyl phenyl oxazole (APO) compounds. The most active hit, compound 1, was active at an MIC of 2.2 uM and 20 uM against bacteria replicating inside and outside macrophages, respectively. In addition, compound 1 was active at an MIC of 0.6~1.25 uM against MDR clinical isolates. Lead optimization of the APO scaffold will be described.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1122**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Studies and Biological Evaluation of Oxazole Derivatives as a Novel Scaffold of HIV-1 Inhibitors

오상미 공선주 류지영 김소라 김성범 김준원[1] 이진화[2] 송릿다

한국파스퇴르연구소 의약화학 연구실 [1]한국파스퇴르연구소 의약화학팀 [2]한국파스퇴르연구소 late discovery program(LDP)

Since the discovery of the human immunodeficiency virus (HIV) as the causative agent of the acquired immunodeficiency syndrome (AIDS) in 1983, the virus has rapidly spread around the world and HIV/AIDS is currently considered a pandemic.1 According to UNAIDS 2009 report [Data.unaids.org], worldwide some 60 million people have been infected, with some 25 million deaths, and 14 million orphaned children in southern Africa alone since the epidemic began. This major global health threat triggered intensive drug discovery efforts and the first FDA-approved antiretroviral drug, AZT, was available in 1987. To date, 25 anti-HIV drugs belonging to 6 different inhibitor classes have been approved by FDA for the treatment of HIV infection, including nucleoside or non-nucleosides reverse transcriptase inhibitors (NRTIs/NNRTIs), protease inhibitors (PIs), integrase inhibitors, entry and fusion inhibitors.2 The introduction of highly active antiretroviral therapy (HAART) ? a regimen combining 3-4 antiretrovirals from different inhibitor classes ? has significantly improved the life quality of patients by delaying the progression of the disease and reducing disabilities, transforming HIV/AIDS into a chronic manageable disease. However, the lack of an effective and safe vaccine, the emergence and spread of drug-resistant viral variants3 and the inability of current regimens to eradicate the virus enforce the continuous development of novel anti-HIV drugs. As a part of our HIV program aimed at the discovery of novel antiretrovirals via HTS using a cell-based assay, we successfully identified a novel class of 5-(phenethylamino)-2-phenyloxazole-4-carbonitrile (AOZ) anti-HIV-1 agents. Initial structure?activity relationship (SAR) studies which had been done in the focused library containing around 80 compounds revealed that original scaffold itself was very important moiety for the retention of anti-HIV activity. In the mode of action study of this small molecule, it was determined that the relevance of the target to the

small molecule's anti-HIV activity was profoundly linked to the inhibition of HIV reverse-transcriptase. This work is expected to provide valuable information for the discovery of a novel anti-HIV-1 scaffold from target-free cell-based assay system.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1123**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Evaluation of Thioflavin-T Derivatives for Amyloid Plaques Imaging Agents

박용대 정순재[1] 박정훈 양승대 허민구 유국현[1]

한국원자력연구원 방사선기기연구부 [1]동국대 화학과

Alzheimer's disease (AD) is the most common form of dementia, involves accumulation of amyloid plaques. Amyloid beta (Aβ) is the main component of amyloid plaques, and thioflavin-T (ThT) is widely used to visualize and quantify the presence of Aβ found in the brains of AD patients. In this study, we synthesized the ThT analogues for detection of Aβ40 fibrils in vitro, and their biological assays to discover a fluorescence activation sensor using Aβ40 fibrils. 2-(2'-Methoxy-4'-aminophenyl)benzoxazole (1) was synthesized by the condensation of 2-aminophenol and 4-amino-2-methoxybenzoic acid in polyphosphoric acid. 2-(2'-Methoxy-4'-methylaminophenyl)benzoxazole (2) was monomethylated using the deprotonationg agent sodium methoxide, paraformaldehyde and the reducing agent sodium borohydride in methanol. 2-(2'-Methoxy-4'-dimethylaminophenyl)benzoxazole (3) was synthesized starting from 1, which was followed by dimethylation using methyl iodide and potassium carbonate. 2-(2'-Methoxy-4'-aminophenyl)benzothiazole (4) was prepared conjugation of 2-aminothiophenol and 4-amino-2-methoxybenzoic acid in phosphorus oxychloride. 2-(2'-Methoxy-4'-methylaminophenyl)benzothiazole (5) was monomethylated using the deprotonationg agent sodium methoxide, paraformaldehyde and the reducing agent sodium borohydride in methanol. 2-(2'-methoxy-4'-dimethylaminophenyl)benzothiazole (6) was synthesized starting from 4, which was followed by dimethylation using formaldehyde in the presence of sulfuric acid and powdered iron. The synthesized 6 ThT analogues were tested with synthetic Aβ40 aggregates for their fluorescence response.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1124**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Radiosynthesis of novel benzamide derivatives for malignant melanoma imaging

박정훈 김희정[1] 김동연[1] 양승대 허민구 유국현[1]

한국원자력연구원 방사선기기연구부 [1]동국대 화학과

Malignant melanoma displays a highly aggressive metastasis. Thus, early diagnosis of malignant melanoma is important for patient survival. Radiolabeled benzamides have been reported to be attractive agents for targeting malignant melanoma as they bind melanin and display high accumulation in melanoma cells. We designed and synthesized novel $Al^{18}F$ and ^{68}Ga-labeled benzamide derivatives as a potential PET agent for malignant melanoma. The novel radiotracers were synthesized in good radiochemical yields (80~90% decay corrected yield) and high specific radioactivity (5~10 GBq/μmol), respectively.

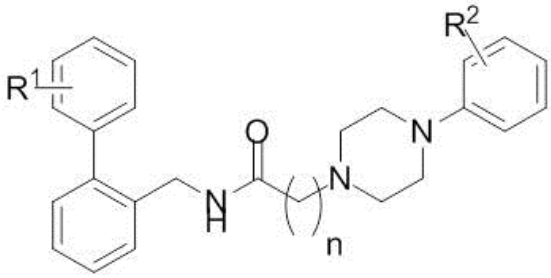
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1125**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of 5-HT7 Antagonists for Treating Depression

김영재 추현아[1]

KIST [1]KIST 생명보건본부

5-HT7 receptors, the most recently added to the 5-HT receptor family, are discretely localized within CNS such as thalamus, hypothalamus, limbic and cortical regions. Knockout animal studies have provided demonstrative proofs that 5-HT7 receptor is engaged in the pathomechanism of depression. Thus, in order to develop novel treatment for continuously increasing problematic depression, 5-HT7 receptor ligands with a biphenyl moiety were designed, and total of 76 final compounds were synthesized and biologically evaluated against 5-HT7 receptors. Binding affinity to 5-HT7 receptors, selectivity over other receptors, microsomal stability, functional assay, and in vivo animal test will be presented in detail.



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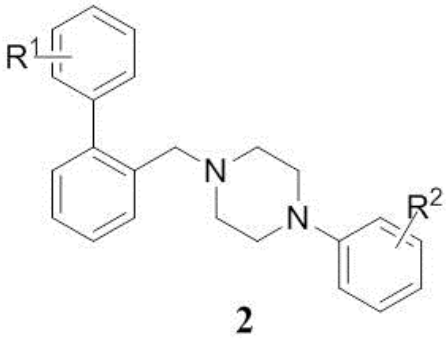

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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1126**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Triggered pH/Redox Responsive Release of Doxorubicin from Prepared Highly Stable Graphene with Thiol Grafted Pluronic

NAHAIN ABDULLAH AL 박성영

한국교통대 화공생물공학과

Strategy, to develop stable graphene and well control hydrophobic drug release from the prepared graphene, is reported to achieve a biomedical platform in drug delivery system. Reduced graphene oxide (rGO) has been prepared using quaternized 2-chloro-3', 4'-dihydroxyacetophenone to poly(ethylene glycol)-g-poly(dimethylaminoethyl methacrylate) [PEG-g-PDMA, QC-PEG] following catechol chemistry which exhibited excellent dispersibility in water. Installation of thiol grafted Pluronic (Plu-SH) results formation of disulfide bonds surrounding rGO/QC-PEG matrix and further aids to achieve high DOX loading efficiency as well as trigged responsive controlled release behavior of DOX from the matrixes by redox responsive Plu-SH and pH sensitive. The rGO/QC-PEG with Plu-SH matrix showed significant stability under different physiological conditions. In vitro DOX release was conducted against different reductive environment and at different pH to figure out the release kinetics. Investigation from MTT assay assures more biocompatible behavior of rGO/QC-PEG/Plu-SH than prepared reduced graphene oxide. Effects of introducing Plu-SH was flashed when QDs loaded rGO/QC-PEG was applied to cell and examining the emitted fluorescence behavior from the cell by confocal images. The confocal investigation showed that high quenching effect of graphene is an obstacle to trace their position if it is used in cell tracking where application of Plu-SH could minimize this.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1127**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-oxidative and Anti-inflammatory Constituents from the Leaves of *Tilia taquetii*

김수영 김상숙[1] 오태헌 양인정 이라겸 강지미 이남호

제주대 화학과 [1]국립원예특작과학원 감귤시험장

This study was designed to analyze the chemical constituents in the extract of Tilia taquetii leaves and to evaluate their biological activities. Phytochemical investigation of the ethanol extract from Tilia taquetii leaves by using repeated column chromatography with normal-phase silica gel and Sephadex LH-20 resulted in the isolation of eight compounds; phytol (1), chlorophyll a (2), oleanolic acid (3), epi-catechin(4), arjunolic acid (5), isoquercetrin (6), daucousterol (7), maslinic acid (8). The chemical structures of these compounds were confirmed by comparing their spectroscopic data to those in the literature. As far as we know, all of the compounds 1-6 were isolated for the first time from this plant.For the anti-oxidation tests, the compounds 4, 6 showed strong DPPH radical scavenging activities with SC50 of 5.41, 12.41 μg/mL, whose activities were comparable to a positive control vitamin C (SC50 5.7 μg/mL). On the screening of anti-inflammatory activities, the compounds 1, 3, 5 and 8 showed the considerable inhibition on the production of nitric oxide for the RAW 264.7 cell without any cell toxicities. Based on these results, Tilia taquetii leaves extract could be potentially applicable as anti-oxidant and anti-inflammatory agent in cosmeceutical and/or pharmaceutical preparations.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1128**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Bioassay of MAO-B Inhibitors for Treating Parkinson's Disease

김지윤 추현아[1] 문봉진 이창준[2]

서강대 화학과 [1]KIST 생명보건본부 [2]KIST 기능커넥토믹스연구단

Parkinson's disease (PD) is a gradually progressive, degenerative neurologic disorder which typically impairs the patient's motor skills, speech, writing, as well as some other functions. There is no current cure for Parkinson's disease and the treatment focuses on alleviating symptoms. Monoamine oxidase (MAO) catalyses the oxidative deamination of a range of monoamines, including serotonin (5-HT), histamine and catecholamines such as dopamine, noradrenaline and adrenaline. Monoamine oxidase B (MAO-B) acts in the brain to degrade dopamine. The level of MAO-B is increased in the brains of people with Parkinson's disease. Therefore, use of MAO-B inhibitors as dopamine-sparing agents or as adjuncts to L-dopa was considered as a treatment for Parkinson's disease. We have synthesized and biologically evaluated oxazolopyridine and thiazolopyridine derivatives as potential MAO-B inhibitors. We have identified several compounds showing high inhibitory activities against MAO-B. And also, those compounds have biologically evaluated against MAO-A and show only marginal inhibitory activities against MAO-A. Based on this study, our selective MAO-B inhibitors can be further developed as potential therapeutic agents for Parkinson's disease.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1129**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of radiopharmaceuticals using Ga-68 for tumor diagnosis

조보배 이원길 유국현

동국대 화학과

Recently, the design of surface modified nanoparticles have been interested greatly due to the major applications in nanobiotechnology (NBT). 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 focus on developing of nano-biotargeting composites using Fe_3O_4 nano particles and ^{68}Ga radioisotope that can be used for therapy in hyperthermia and diagnosis in the fields of PET and MRI applicationsFirst, spacer of Fe_3O_4 nanoparticles that are used MRI imaging and hyperthermia can be reformed by PEG(polyethylene glycol) biocompatible polymer that can increase hydrophilic property. Nano-biotageting composites can be obtained from combining Fe_3O_4 nanoparticles with Folic acid as guiding group.This bi-functional imaging media may allow to earlier detection of tumor with a high degree of accuracy

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1130**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Evaluation of Pyrazole/Pyrazoline Derivatives as Calcium Channel Inhibitors in Cancer Treatment

김정현 서선희[1] 남길수

KIST 뇌과학연구소 [1]KIST 뇌의약연구단

Calcium plays a key role in intracellular signalling and controls many different cell processes such as proliferation, differentiation, growth, cell death and apoptosis. Thus, alterations in calcium signalling can cause defects in cell growth and invasion and are associated with certain types of cancer. A role for calcium channels in tumour cell proliferation has been reported in breast, brain, colorectal, gastric, hepatic and prostate tumours, leukaemic cells and retinoblastoma cells. A number of research groups have suggested a potential role for voltage-activated calcium channels, in particular T-type, in the regulation of tumour growth and progression. We have been studying various pyrazole/pyrazoline derivatives. Here we will discussed their synthesis and biological evaluation including calcium channels (α1G, α1H) inhibitory activity and anti-proliferative activity of various tumour cells such as fibroblastoma (HT1080), prostate carcinoma (LNCap), glioma (U87-MG), which known as highly expressed of T-type calcium channels.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1131**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A study on the cosmetic ingredients from branches of *Oreocnide fruticosa*

한정환 김상숙[1] 오태헌 강다향 강승협 이남호

제주대 화학과 [1]국립원예특작과학원 감귤시험장

In our continuing efforts to find biologically active compounds from plants in Jeju island, we became interested in the ethanol extract prepared from branches of *Oreocnide fruticosa* (Gaudich.) Hand.-Mazz. Thereafter, the ethanol extract was suspended in H_2O and partitioned sequentially with *n*-hexane, ethyl acetate and *n*-butanol, respectively. The each fraction were subjected to the activity screenings on anti-oxidation, anti-inflammation, inhibitory melanogenesis and cytotoxicity. For the anti-oxidation tests, the ethyl acetate and *n*-butanol fraction showed strong DPPH radical scavenging activities with SC_{50} of 29.9 and 76.2 ?g/mL respectively, whose activities were comparable to a positive control vitamin C (SC_{50} 15.9 ?g/mL). On the screening of anti-inflammatory activities, the ethyl acetate fraction showed the considerable inhibition on the production of nitric oxide for the RAW 264.7 cell without any cell toxicities. Also the ethyl acetate fraction showed inhibited the cellular melanogenesis as effectively as arbutin for the B16F10 melanoma cell activated by α-melanocyte stimulating hormone(α-MSH). *Oreocnide fruticosa*'s cytotoxicity was determined by MTT assays using CCD-986sk and HaCaT. The ethyl acetate fraction exhibited no cytotoxicity. Based on the these results, *Oreocnide fruticosa* branches extract may be an attractive candidate as a cosmetic ingredient

일시: 2012년 10월 17~19일(수~금) 3일간
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발표코드: **MEDI.P-1132**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on bioactivities of extracts from *Corylus hallaisanensis* Nakai.

김성천 변상희 문승리 오태헌 김상숙[1] 이남호

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Corylus hallaisanensis Nakai, a deciduous shrub growing in Jeju island, was investigated for some biological activities. The dried material was extracted for 24 hour with 70% ethanol. The extract was successively partitioned with *n*-hexane (Hex), ethyl acetate (EtOAc), *n*-butanol (BuOH) and water (H_2O). For the anti-oxidation tests, the ethanol extract, EtOAc, BuOH and H_2O fractions showed good DPPH radical scavenging activities with SC_{50} of 31.69 μg/mL, 31.94 μg/mL, 23.29 μg/mL and 39.05 μg/mL, respectively, whose activities were comparable to positive control vitamin C(SC_{50} 14.49 μg/mL). On the screening of anti-inflammatory activities, EtOAc fraction showed the considerable inhibition on the production of nitric oxide for the RAW 264.7 cell without any cell toxicities. When tested in murine B16F10 melanoma cells activated by α-melanocyte stimulating hormone (α-MSH), EtOAc fraction inhibited the cellular melanogenesis more effectively than arbutin, one of the most widely applying hypopigmenting agents in cosmetics. All fractions were evaluated for their cell viability on CCD986sk(human fibroblast cell) and HaCaT(Human Keratinocyte cell line). Based on these results, *C. hallaisanensis* branch extract could be potentially applicable as anti-oxidant, anti-inflammatory, and hypopigmenting agents in cosmeceutical and/or pharmaceutical ingredient.

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Molecular design and synthesis of PLK1 kinase domain inhibitors for cancer therapeutics.

강주희 남기엽[1] 최남송[2] 안순길[3]

인천대 생명과학부 [1](주)유아이 [2](주)유아이 신약개발연구소 [3]인천대 생물학과

Polo-like kinase 1 (PLK1), a mitotic cyclin-independent serine-threonine kinase, is a member of a family of polo-like kinases involved in a wide variety of cell cycle processes. Polo kinase was first identified in Drosophila melanogaster, where mutants display abnormal mitotic and meiotic divisions caused by failure to properly organize the mitotic spindle. Human PLK subfamily includes five closely related members, that is, PLK1, PLK2, PLK3, PLK4 and PLK5. Overexpression of the Plk1 gene has also been found in multiple cancer: human glioma, breast cancer, cervical carcinoma, and non-small cell lung cancer. Inhibition of Plk1 by small-molecule inhibitors of its catalytic activity is currently being explored in clinical settings. One particularly promising compound, BI-2536, has been shown to inhibit Plk isoforms in vitro with low nanomolar potency and with high selectivity against a large panel of kinases. BI-2536 potently inhibits the proliferation of a wide variety of human cancer cell lines, causes regression of tumor xenografts in mice, and is currently undergoing clinical trials. Previously, the structure of Plk1 kinase domain in complex with BI-2536 was published. In the present study, we report on the identification of the polo-like kinase 1 (Plk1) as a potential new target for drug development. Finally, a total of 5 compounds were synthesized and evaluated enzymatic assays. We demonstrated the docking study in order to add to our understanding of activity data. The work presented here provides a framework for the structure-based design of Plk1-inhibitors.

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Development of mGluR1 Antagonists for Treating Neuropathic Pain

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연세대 화학과 [1]KIST 생명보건본부 [2]한국파스퇴르연구소 의약화학 연구실 [3]KIST 뇌의약연구단

Neuropathic pain is a complex, chronic pain, and in many cases neuropathic pain is initiated by damage to nerves. Common characteristics of neuropathic pain are chronic hyperalgesia and allodynia. The excitatory amino acids including glutamate, play a role in a variety of neurological, physiological, and psychiatric processes such as synaptic plasticity, motor control, respiration, cardiovascular regulation, and sensory perception. To exert its effect, glutamate activates two major receptor classes: the ionotropic glutamate (iGlu) and the metabotropic glutamate (mGlu) receptors. Eight mGlu receptor subtypes have been classified into three groups on the basis of their sequence homology, pharmacology, and signal transduction mechanisms. The participation of mGlu1 receptors in chronic or neuropathic pain appears to be well documented. In this study, novel compounds with a bicyclic core structure were designed and synthesized on the basis of the reference compound with tricyclic structure which was previously synthesized and biologically evaluated against mGluR1 with an IC50 value of 6 nM.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Docking Study and Synthesiss of Novel Flavonol Derivatives as JAK3 Inhibitors: Achieving Selectivity for JAK3

김미경 윤현준 조서영 신희림 정유훈

건국대 생명공학과

Development of a selective inhibitor against Janus kinase 3 (JAK3) has been anticipated to provide a novel immunosuppressive agent. However, low JAK2/JAK3 selectivity of the previously discovered JAK3 inhibitors has imposed a serious problem in developing a novel immunosuppressant with an optimal therapeutic window for the treatment of immune cell-mediated diseases. In this study, we attempted to design a novel JAK3-selective inhibitor through analysis of the characteristic binding mode of the flavonol derivatives to the ATP-binding domain of the JAK3. The results indicated that flavonol derivatives interact with the key amino acid residues at the ATP-binding cavity of JAK3 protein. The 5-OH and 7-OH of flavonol binds to the hinge part (Glu903, Leu905) of the kinase through two hydrogen bonds. In order to fill up the empty hydrophobic pocket lying next to the ligand binding site of JAK3 a substituent was attached to the B-ring of the flavonoid. The designed flavonol derivatives were synthesized and exhibited inhibitory activity against JAK3 with fairly good selectivity for JAK3 (56% ~ 63% inhibition at 10 μM) over JAK2 (no inhibition at 10 μM).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Anti-HCV Activity of 6,7-Bis-O-Arylmethyl-5,6,7-Trihydroxychromone Derivatives

윤현준 김미경 조서영 신희림 최만진 배온누리[1] 정유훈

건국대 생명공학과 [1]동의대 화학과

A series of 5-hydroxychromone derivatives have been reported to have interesting antiviral activity. Among those, galangin derivatives such as 7-O-arylmethylgalangins and 3-O-arylmethylgalangins showed potent anti-HCV (hepatitis C virus) activity, and structure-activity relationship study revealed that the arylmethyloxy group substituted to the core 5-hydroxychromone scaffold played a key role in determining the antiviral activity of these compounds. More intriguingly, when the two arylmethyloxy substituents were combined on the 5-hydroxychromone scaffold, the resulting 3,7-bis-O-arylmethylgalangin derivatives showed broad spectrum antiviral activity against SCV [Severe Acute Respiratory Syndrome (SARS) Corona Virus, SARS-CoV] as well as HCV. This interesting antiviral profile of the bis-O-arylmethyloxy-substituted 5-hydroxychromones prompted us to extend the structure-activity relationship study to include positional scanning of the arylmethyloxy substituents on the 5-hydroxychromone core structure. In this study, we designed another bis-O-arylmethyl-5-hydroxychromone scaffold with the arylmethyloxy substituents at vicinal 6 and 7 positions. In this preliminary study, the aromatic substituent R was fixed at 3′-position because it was found to be the position of choice for potent antiviral activity in a series of 5-hydroxychromone derivatives. Herein, we report synthesis and preliminary evaluation of a series of novel 6,7-bis-O-arylmethyl-5,6,7-trihydroxychromone derivatives as potential antiviral agents.

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Synthesis and SAR study of thieno[3,2-b]pyridine urea derivatives as urotensin-II receptor (UT) antagonists

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The urotensin-II ligand (U-II) as a cystein-linked cyclic undecapeptide, has been identified to be one of the most potent vasoconstrictor. U-II and its cognate receptor (UT) are proposed to be involved in the regulation of cardiorenal function and implicated in the etiology of numerous cardiorenal and metabolic diseases including hypertension, heart failure, atherosclerosis and renal failure and diabetes. Recently, we have identified a series of thieno[3,2-b]pyridine urea derivatives as UT antagonists. In continuing our efforts to optimize for these compounds, we further investigated the effects of various substituents on piperidine part linked to thieno[3,2-b]pyridine to the UT binding activity. The details of synthesis and SAR results will be presented.

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Synthesis and biological evaluation of cyclic sulfonamide derivatives as urotensin-II receptor (UT)antagonist

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한국화학연구원 대사증후군치료제연구센터 [1]과학기술연합대학원대 의약 및 약품화학부 [2]과학기술연합대학원대 의약및약품화학

The urotensin-II receptor (UT) as G-protein-coupled receptor superfamily plays an important role in the regulation of cardiorenal function through interaction of its urotensin ligand. Furthermore, UT has received a great deal of attention as potent target for cardiovascular treatment. As part of our drug discovery project in the development of potent UT antagonists, we have identified a series of cyclic sulfonamide derivatives and investigated the effects of various cyclic sulfonamide core to UT binding activity. The details of synthesis and structure-activity relationships (SAR) results will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological research of N-containing heteroaromatic compounds as mGluR5 negative allosteric modulators.

손명희 백두종 이재균[1] 배애님[2] 민선준[3] 조용서[2]

상명대 화학과 [1]KIST 케모인포매틱스연구단 [2]KIST 생체과학연구본부 [3]KIST 뇌의약연구단

Glutamate is the major excitatory neurotransmitter of mammalian in central nervous system and peripheral nervous system. Glutamate receptors are related to mediate glutamate for post-synaptic excitation in neural cell, involved in pathologies of many brain diseases. There are classified two type receptors depending on the mechanism of activation; ionotropic glutamate receptors (iGluRs) and metabotropic glutamate receptors (mGluRs). Metabotropic glutamate receptors belong to the type of C class of GPCR (G protein coupled receptors) and they are divided into three groups with eight subtypes on the basis of their sequence hormonology, pharmacology, and signal transduction mechanism. Group I consists of the mGluR1 and mGluR5, which are predominantly identified in post-synapses in the brain region, including the hippocampus, cerebellum, thalamic nuclei, and spinal cord. Recently studies 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 acetylinic N-containing heteroaromatic compounds as selective mGluR5 antagonists including in vivo study of a lead compound in animal models of neuropathic pain..

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Various Ionic Liquid Type Photosensitizers and Its Gold Nanoparticles Conjugates for Photodynamic Therapy

윤일 김정화[1] 이범희[2] 이태헌[2] 김정훈[2] 장민아[2] 심영기[2]

인제대 PDT 연구소 [1]인제대 나노시스템공학과 [2]인제대 나노공학부

Various water soluble ionic liquid type photosensitizers were synthesized and its gold nanoparticles conjugates have prepared and characterized by IR, UV-vis, and NMR spectroscopic and Mass spectrometric analyses, and transition electron microscopy. And their comparative photodynamic effect has been evaluated by in vitro test for photodynamic therapy.

THE KOREAN CHEMICAL SOCIETY

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장소: 부산BEXCO

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Second Synthetic Approaches toward Mibefradil Analogues as T-type Calcium Channel Blockers

이지은 이덕형 이재균[1] 배애님[2] 조용서[2] 민선준[3]

서강대 화학과 [1]KIST 케모인포매틱스연구단 [2]KIST 생체과학연구본부 [3]KIST 뇌의약연구단

T-type calcium channels antagonists have become considered targets for the treatment of neuropathic pain. Mibefradil (Posicor, Roche?), a novel calcium antagonist that selectively blocks T-type calcium channels, was approved in the United State as a therapeutic drug for hypertension and chronic angina pectoris. Despite it has excellent bioavailability, it was withdrawn from the market, due to it showed unfavorable side effects, which resulted from inhibition of the cytochrome P-450 isoforms CYP3A4 and CYP2D6 in the liver.The recent research on metabolic profile of mibefradil revealed that the most important metabolic process in microsomes is hydroxylation at the benzylic carbon atom of the tetrahydronaphthyl ring system. On the basis of this research, we have designed new mibefradil analogues having less oxidizable atoms at the benzylic position of the tetrahydronaphtyl ring system to prevent metabolic oxidation. Whereas we previously reported the synthesis of tetrahydrobenzopyrans via diastereoselective Reformatsky reactions, a Lewis acid-catalyzed carbonyl-ene reaction was used for construction of this structure in this study.We herein describe the overall synthetic process of mibefradil analogues and the result of their in vitro metabolic stabilities.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Size-dependent photodynamic activity of gold nanoparticles conjugate of water soluble purpurin-18-N-methyl-D-glucamine

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인제대 PDT 연구소 [1]인제대 나노시스템공학과 [2]인제대 나노공학부

Gold nanoparticles (GNPs) conjugates of water soluble ionic photosensitizer (PS), purpurin-18-N-methyl-D-glucamine (Pu-18-NMGA), were synthesized using various molar ratios between HAuCl4 and Pu-18-NMGA without adding any particular reducing agents and surfactants. The PS?GNPs conjugates showed long wavelength absorption of ranges 702?762 nm, and their different shapes and diameters depend on the molar ratios used in the synthesis. In vitro anticancer efficacy of the PS?GNPs conjugates was investigated by MTT assay against A549 cells, resulting in higher photodynamic activity than that of the free Pu-18-NMGA. Among the PS?GNPs conjugates, the GNPs conjugate from the molar ratio of 1:2 (Au(III): Pu-18-NMGA) exhibits the highest photodynamic activity corresponding to bigger size (~60 nm) of the GNPs conjugate could be efficiently transport the PS into the cells than that of smaller size of the GNPs conjugate.

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Validation of Cell-based Permeability assay in MDCK and Caco-2 System Using LC-MS/MS in Early Stage of Drug Discovery

최영선

한국파스퇴르연구소 Nano/Bio Chemistry

Predictive ADME (absorption, distribution, metabolism and elimination) assays are of great importance in screening lead compounds that lack the desired pharmacological properties in earlier stages of drug discovery. Among them, Madin Darby Canine Kidney (MDCK) cells and a human colorectal adenocarcinoma cells (Caco-2) permeability assays can provide useful information for lead optimization in the drug discovery with regard to absorption, permeation and efflux transport properties of a candidate drug. The MDCK cell monolayer system provide passive diffusion, while Caco-2 monolayer offers a selective barrier for transcellular and carrier-mediated efflux transport of different drugs. This poster describes the use of LC-MS/MS to validate MDCK and Caco-2 permeability assay in 12-well Transwell? Insert System. The permeability ranking of drug standards using the cell-based permeability assay system correlated well with the several reference compounds which are recommeded by FDA. The bi-directional transport studies using cell monolayer system verified functional P-glycoprotein efflux pump activities. In vitro permeability assys using MDCK, and Caco-2 system are robust methods for screening drug candidates with regard to their absorption properties.

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발표코드: **MEDI.P-1144**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification and preliminary characterization of a novel 7-aminopyrazolo[1,5-a]pyrimidine (7-APP) analog as a hepatitis C virus inhibitor

황종연 조수연 공선주 김영미 최지현 박동식 박은정 권정진 남지연[1] 안수진[1] 김준원 이진화[2]

한국파스퇴르연구소 의약화학팀 [1]한국 파스퇴르연구소 DMPK [2]한국파스퇴르연구소 late discovery program(LDP)

Approximately 200 million people worldwide are chronically infected with the hepatitis C virus (HCV). This pathogen is the major cause of acute hepatitis and chronic liver disease, including cirrhosis and liver cancer and thereby HCV is the leading indication for liver transplantation. Despite the recent approval of two direct acting antivirals (DAAs), telaprevir and boceprevir inhibiting the NS3/4A protease, standard of care for chronic hepatitis C is still a combination therapy of pegylated interferon-alpha (PEG-IFN-α) and ribavirin, which has limitations in HCV genotype 1 patients and causes severe side effects. Herein, we describe a novel 7-aminopyrazolo[1,5-a]pyrimidine (7-APP) derivative as a potent hepatitis C virus (HCV) inhibitor. A series of 7-APPs was synthesized and evaluated for inhibitory activity against HCV in different cell culture systems. The synthesis and preliminary structure-activity relationship study of 7-APP are reported.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The Identification of Binding Mode for Arabidopsis thaliana 7-Keto-8-aminopelargonic Acid Synthase (AtKAPAS) Inhibitors

조재은 강남숙 고영관[1]

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The 7-keto-8-aminopelargonic acid synthase from Arabidopsis thaliana plants (AtKAPAS), introduced in this research, is a novel potent herbicide target which is involved in the early steps of the creation of the biotin biosynthesis pathway. Since biosynthetic steps of biotin exist only in plants, we expect that the inhibition of the potent target AtKAPAS will not affect the human metabolic systemby any means. Inhibiting AtKAPAS leads to significant changes in the phenotypes of Arabidopsis thaliana, such as growth inhibition, severe growth retardation, and the creation of lethal phenotypes. We carried out the study of the three dimensional structure of AtKAPAS by homology modeling and the binding mode of compounds obtained from in-house library using computational docking methods. From the flexible docking study, we achieved high dock scores for the active compounds denoted in this study as compound 3 and compound 4. Thus, we highlight the flexibility of specific residues, Lys 312 and Phe 172, in active sites. Furthermore, we are going to optimizecompound 3 and compound 4 using this homology model for AtKAPAS.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

TREK1 blockers as new candidates for major depression

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TREK-1, one of the subfamily of mechano-gated potassium channels, consists of four transmembrane segments and two pore-forming domains. Human TREK1 is widely expressed in the CNS neurons, prefrontal cortex, hippocampus, hypothalamus and peripheral tissues. Recent in vivo studies revealed that TREK1 has an important role in clinical depression. In addition, correlation between TREK1 and T-type calcium channels were elucidated. Therefore molecular libraries synthesized for T-type calcium channel activity were evaluated toward TREK1. Among them, 1-(2-hydroxy-3-phenyloxypropyl)-piperidine and pyrazole amine derivatives showed promising preliminary activities.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Focused-Library Syntheses and Biological Activities of Calcium activated Chloride Channel(CaCC) Blocker Ⅱ

황석진 한호규 노은주[1]

고려대 화학과 [1]KIST 생체과학연구부

Ca2+-activated Cl- channels (CaCCs) play a role in the regulation of sensory transduction, epithelial secretion and smooth muscle contraction. Nevertheless the study of these channels is still behind because of lack of pharmacological tool compound. The development of selective and potent CaCC inhibitors will open the way for molecular investigation of the role of these anion channels in specific cell. Focused synthesis of anthranilic acid derivatives offered unprecedented promising CACC inhibitor(IC50 =0.038?M). Furthermore, the consistent SAR can be explained with these derivatives.

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발표코드: **MEDI.P-1148**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Evaluation of IKK-β inhibitors

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The transcription of several cytokines, cell adhesion molecules and enzymes involved in the inflammatory mechanism of rheumatoid arthritis is dependent on nuclear factor kB (NF-κB). Because IκB kinase (IKK) has critical role in transducing the activation of NF-κB, new derivatives as IKK inhibitors were prepared and examined. To obtain new and selective IKK-β inhibitors, thiazolidine derivatives were designed and synthesized. A series of compounds was evaluated for in vitro assay using TR-FRET method. Compounds that showed above 60% inhibitory activity at 10μM were measured the IC50 values for IKK-β and IC50 values for hERG channel. Further in vivo assay using inflammatory disease animal model and pharmacokinetic study will be performed for several derivatives that showed comparable in vitro activities with reference compound.

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발표코드: **MEDI.P-1149**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of Aurora-A inhibitors by the fragment-based virtual screening

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Aurora kinase that belongs to serine/threonine kinase having three isotypes (-A, -B, -C) plays key roles in the protein phosphorylation and regulation of mitosis. Especially, Aurora kinase A (Aurora-A) is localized to the spindle microtubules and is essential for the maturation of centrosome. Aurora-A is overexpressed in a several types of human tumors like breast, ovarian, lung, colorectal cancer and participated in the process of tumorigenesis. As the reason, Aurora-A has been studied as the anticancer drug target. We explored fragments that bind to the hinge region using 5,000 compounds collected from eMolecules database that reactive fragments are removed and molecular weight range from 200 to 350 Da. First of all, we analyzed the structural characteristics of Aurora-A by the Tanimoto coefficient using the cross-docking study. We selected five Aurora-A complex structure with low similarity between the co-crystallized ligands shown good activity. To virtually screen out the mentioned fragments, LigandFit method was used to dock structurally diverse 5000 fragments into the five diverse Aurora-A structures. Hinge region binding fragments extracted from the five co-crystal structures were used as a Control Ligand in the LigandFit protocol. From the docking result, we obtained 18 fragmental structures showing better dock score than the reference fragment and favorable docking pose among 5,000 diverse fragments. The obtained 18 fragmental structures were assayed against Aurora-A and finally 5 fragmental structures revealed more than 50% inhibition at 100 uM in the Aurora-A kinase assay.

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장소: 부산BEXCO

발표코드: **MEDI.P-1150**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Identification of Preclinical Candidate of New 11β-hydroxysteroid dehydrogenase type 1 inhibitiors

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11β-hydroxysteroid dehydrogenase type 1 (11β-HSD1) is a key enzyme that acts as an NADPH-dependent reductase capable of converting inactive glucocorticoids such as cortisone into their active form in specific tissues, such as liver, adipose, and brain. The glucocorticoids are a class of steroid hormones that bind to glucocorticoid receptor (GR), which is regulates or supports a variety of important cardiovascular, metabolic, immunologic, and homeostatic functions. Excess of active form of glucocorticoid induces metabolic syndromes like obesity, hypertension and insulin resistance. More than 20 pharmaceutical companies have been developed the 11β-HSD1 inhibitors for the obesity and diabetes improvement. To develop 11β-HSD1 inhibitors for the treatment of type 2 diabetes, we synthesized more than 300 compounds and evaluated in vitro and ex vivo activities. In this study, UI-1499 selectively inhibited 11β-HSD1 activity in human and mouse liver microsomes and in the ex vivo assay of C57BL/6 mice. In the in vivo study with KKAy mice, the oral administration of UI-1499 (10 and 30 mg/kg/day, orally for 21 days) showed good glucose levels lowering (31 %) and HbA1c (1.5 %) compare with negative control. The compound had no toxicity in normal cell-line(293) and did not inhibit several CYP P450s. Preclinical study our candidate, UI-1499, is safe and efficacious, and suggests that it may good drug candidate for the preclinical study.

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장소: 부산BEXCO

발표코드: **MEDI.P-1151**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A kinetic study on proteolysis by Cu(II)cyclen complex and Cu(II)dip complex

김경진 배형은 최원석 한슬기 박두한 정근홍[1]

삼육대 화학과 [1]육군사관학교학교 화학과

Peptide bond hydrolysis is a very challenging task because of its high stability. Synthesizing metalloproteases containing transition metal complexes is of great interest. Among them, Cu(II) has been popularly used as a key catalytic site for artificial metalloprotease. In this study, we performed the kinetic studies of Cu(II) complexes with two different chelators on proteolysis. The kinetic study showed that Cu(II) complex of new ligand, bis(pyridylmethyl)amine (dpa) can be a new promising catalytic group for preparation of catalytic drug candidates because of its enhanced catalytic activity as compared to a previously reported Cu(II)-chelator complex. The new catalytic group itself showed minimal activity toward the cleavage on non-target proteins at the low concentraiton.

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장소: 부산BEXCO

발표코드: **MEDI.P-1152**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New purine-scaffold class of Hsp90 inhibitors; design, synthesis, protein crystal and biological evaluation for cancer theraphy.

이주현 강순방[1] 정낙철 금교창[2]

고려대 화학과 [1]KIST 뇌의약연구단 [2]KIST 케모인포메틱스연구센터

Heat-shock protein 90 (Hsp90) is an ATPase-dependent protein folding molecular chaperone that plays a key role in the stability and function of many client proteins such as ErbB2, c-Raf, Cdk4, Akt. Many of its client proteins are known to play critical roles in cancer progression. Hence inhibition of Hsp90 can lead to the degradation of lots of oncogenic proteins, Hsp90 has become a target of cancer therapy. BIIB021 is in phase II clinical trial and proved to induce the degradation of Hsp90 client proteins including HER-2, AKT, and Raf-1 that is in phase II clinical trial. Since, we designed new purine-scaffolds and synthesized. Several compounds showed good % inhibitions in SKBR3, MCF-7, and HCT116 cancer cell lines. Among them, KKK5041 demonstrated a good binding interaction in the ATPase binding pocket by conformed X-ray crystallography. Therefore, We'll discuss the structure-activity relationship.

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장소: 부산BEXCO
발표코드: **MEDI.P-1153**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of novel potent anti-Hepatitis C virus agent.

염수연 강순방[1] 정낙철[2] 금교창[3]

고려대 화학 [1]KIST 뇌의약연구단 [2]고려대 화학과 [3]KIST 케모인포메틱스연구센터

Hepatitis C virus (HCV) infection is the cause of chronic liver disease such as chronic hepatitis, liver cirrhosis and hepatocellular carcinoma. Although estimated more than 180 million people worldwide are infected with HCV, a protective vaccine for the treatment of HCV is not yet available, and current standard of care, a combination of pegylated interferon with ribavirin, achieves efficay rates of 40-50% only. The FDA approved the protease inhibitors boceprevir (Victrelis) and telaprevir (Incivek) in 2011. However sustained virologic response for genotype 1 HCV is still about 70~80% when protease inhibitor was administered with standard treatment. Many antiviral agents targeting against specific HCV enzymes, such as protease, polymerase and NS5A are under development. In this study, the several potent lead compounds for the treatment of hepatitis C virus were developed. Among them, a lead compound KK6042 showed potent anti-proliferative activity against HCV cell lines with sub-nanomolar EC50. These compound displayed good human microsomal stability and exhibited similar inhibition of major human CYP enzymes compared to reference compound BMS-790052. In addition, there was no evidence of its toxic effect in the hERG, cytotoxicity, and Ames test. Especially KK6042 showed excellent PK profile with high AUC and Cmax.

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장소: 부산BEXCO

발표코드: **MEDI.P-1154**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of diacylglycerol acyltransferase 1 inhibitors as anti diabetic and obesity agents

곽현정 편유미[1] 김지영[2] 이덕형[1] 안진희[3]

한국화학연구원 대사증후군치료제연구센터 [1]서강대 화학과 [2]과학기술연합대학원대 의약 및 약품화학 [3]한국화학연구원 대사성질환연구팀

Anti-diabetic and obesity agents are currently available in the market, however, the need for the new drug is urgent due to the several side effects of existing drugs, insufficient therapeutic efficacy and rapidly increasing patients with a variety of pathology. DGAT-1 is a well known target for obesity and diabetes, therefore we are developing new preclinical candidates. We will present the discovery of new DGAT1 candidates

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1155**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Model study for solid-phase synthesis of a novel drug-like 2-thioxoimidazolidin-4-one derivatives via isothiocyanate linker

이재민 양정원 공영대

동국대 화학과

The 2-thioxoimidazolidine derivatives have attracted much attention since they have been reported to be responsible for interesting biological activities such as Hif-1α and Wnt signal path way, and various receptor antagonist. The solid phase synthesis of heterocyclic combinatorial libraries is a strategy to have drug discovery process. And solid-phase synthesis of heterocyclic core skeleton serves as the core components of a large number of substances that process very efficient for the construction of drug-like library. As a part of our ongoing drug discovery program, we have been exploring a potential of resin-bound thioxoimidazolidine-4-one derivatives since they are easily obtained from various natural amino acids. In this present, we would like to show a model study of combinatorial generation of 2-thioxoimidazolidine-4-one derivatives for solid-phase synthesis. Through making the various substituted aromatic building blocks, we could obtain linear compounds in solution-phase synthesis. We obtained the final compound in good yield and high purities from solution-phase synthetic process.

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장소: 부산BEXCO

발표코드: **MEDI.P-1156**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Regiospecific Synthesis of 2-Aminosubstiuted 1,3,4-Oxadiazole and 1,3,4-Thiadiazole Derivatives via Reagent-based Cyclization of Thiosemicarbazide Intermediate

양승주 이석형 공영대

동국대 화학과

1,3,4-oxadiazoles and 1,3,4-thiadiazoles have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas. As a result of these applications, 1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives have been targets of a number of solution- and solid-phase synthesis studies. However, preparative methods developed thus far lack diversity since they employ different intermediates for the syntheses of the oxygen- and sulfur- containing heterocyclic compounds. Although, several methods have been tried to develop an efficient synthesis of 1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives using same key intermediate, their diversity ability showed narrow spectrums to the construction of various drug-like five-membered libraries based on oxadiazole and thiadiazole core skeletons. Therefore, we undertook an investigation aimed at developing efficient and synthesis methods to produce various 2-amino-substituted 1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives. Finally, we obtained various 1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives in high yield and high purities.

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장소: 부산BEXCO

발표코드: **MEDI.P-1157**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient Solid-phase Parallel Synthesis of 2-Amino- and 2-Amido-benzo[*d*]oxazole Derivatives via Cyclization Reactions of 2-Hydroxyphenyl Thiourea Resin

정세린 공영대

동국대 화학과

An efficient solid-phase methodology has been developed for the synthesis of 2-amino- and 2-amido-benzo[*d*]oxazole derivatives. The key step in this procedure involves preparation of polymer-bound 2-amino-benzo[*d*]oxazole resins by cyclization reaction of 2-hydroxyphenyl thiourea resin. The resin bound 2-hydroxyphenyl thiourea produced by addition of 2-aminophenol to the isothiocyanate terminated resin, serve as key intermediates linker resin. This core skeleton 2-amino-benzo[*d*]oxazole resin that undergo functionalization reaction with various electrophiles, such as alkylhalides and acid chlorides to generate 2-amino- and 2-amido-benzo[*d*]oxazole resins respectively. Finally,2-amino- and 2-amido-benzo[*d*]oxazole derivatives are then generated in good yields and purities by cleavage of the respective resins under TFA in CH_2Cl_2

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1158**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Novel Solid-Phase Parallel Synthesis of *N* -Substituted-2-aminobenzo [*d*]thiazole Derivatives via Cyclization Reactions of 2-Iodophenyl Thiourea Intermediate Resin

김슬기 곽세훈 공영대

동국대 화학과

Heterocyclic skeletons serve as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. Therefore, the development of novel five-member heterocyclic core skeletons which is important to drug discovery research area. In this respect, the potential of the benzothiazole scaffold to serve as a privileged structure for the generation of drug-like libraries in drug-discovery programs has been amply demonstrated in medicinal chemistry Also solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficien.t drug discovery process. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound benzo[*d*]thiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of *N*-alkyl, *N*-acyl, and *N*-sulfonyl-2-aminobenzo[*d*]thiazole derivatives based library through resin-bound BAL linker. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

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장소: 부산BEXCO

발표코드: **MEDI.P-1159**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Parallel Synthesis of Novel 2-Quinolinyl Piperazine Derivatives as Anticancer Agents

곽현정 이은실[1] 공영대

동국대 화학과 [1]동국대 의약화학연구실

Recently we reported the anticancer activities of 5 or 6- substituted quinoxaline compounds containing piperazine groups. Especially, 1-(3,5-dimethoxyphenyl)-4-[(6-fluoro-2-methoxyquinoxalin-3-yl)aminocarbonyl]piperazine, induced G2/M arrest in cell cycle and an apoptosis in cancer cells. This hit compound has also significantly inhibited growth of drug resistant cancer cells, and has shown potential use in combination therapy with known anticancer drugs such as palcitaxel, doxorubicin, gemcitabine, 5-FU and cisplatin. However, most of the first quinoxaline hit compounds showed several hundred nM activity toward cancer cell lines as well as there were showed low water solubility. Therefore, we needed much stronger active hit compound with good physicochemical properties for the final lead compound selection process. In connection with a project for exploring the novel potent G2/M-specific cell cycle inhibitors, we have designed some target compounds for quinolinyl-piperazine-based library for optimization of the structural features of the primary screening results through high throughput screening efforts.

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장소: 부산BEXCO

발표코드: **MEDI.P-1160**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of a Novel Drug-like 2,4,5-trisubstituted Thiazole Libraries Using BAL Resin

김용상 이지형 배미선 공영대

동국대 화학과

Among organic small molecules, heterocyclic compounds have received particular attention in combinatorial chemistry, since they are important structural components of bioactive molecules. Thus as a part of an ongoing drug discovery process, we have been studying the potential of resin-bound 2,4,5-thiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. And as a result, the thiazole heterocycles are important structural components of bioactive molecules, and they serve as attractive targets for combinatorial library construction via and solid-phase synthesis. We had previously report a useful method for the solid-phase synthesis of 2,4,5-trisubstituted thiazole derivatives using a sulfone traceless linker. Herein we would like to present a novel solid-phase synthetic better than existing methods optimized method for combinatorial generation of 2,4,5-trisubstituted thiazole derivatives through resin-bound BAL linker. Also we are studying cleavage condition on solid-support under TFA. Therefore, we expect our efficient approach will be obtained many compound in good yields and high purity upon cleavage from the BAL resin.

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장소: 부산BEXCO

발표코드: **MEDI.P-1161**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Novel 3-Arylethynyl-substituted Thieno[2,4-*b*]pyrazine Derivatives as a Human Trasnglutaminase 2 inhibitor

김나연 공영대

동국대 화학과

We found that transglutaminase 2 (TGase 2) expression is highly increased in RCC cell lines and human RCC tumors. Furthermore we have observed that that TGase 2 inhibition using siRNA or TGase 2 inhibitor 3-arylethynyl-substituted thieno[2,4-*b*]pyrazine derivatives induced apoptosis in RCC cell lines. Previously we found that tumor suppressor von Hippel-Lindau(VHL) can be depleted by protein cross linking via TGase 2. However, about a half of sporadic renal cell carcinoma (RCC) cases are supposed to be related with loss of VHL expression and/or activity via epigenetic modification and/or mutations. In this study, we found another important role of TGase 2. In RCC that TGase 2 depletes p53 through autophagy via direct protein cross-linking. We also demonstrated that TGase 2 inhibitor 3-arylethynyl-substituted thieno[2,4-b]pyrazine derivatives reduced the RCC tumor in xenograft model accompanying with p53 stabilization. In clinical RCC tumor cases, TGase 2 expression is also inversely correlated with p53 expression by immune-histochemistry.

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장소: 부산BEXCO

발표코드: **MEDI.P-1162**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Computational studies of c-Met inhibitors: Docking-based 3D-QSAR and pharmacophore modeling

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c-Met (mesenchymal-epithelial transition factor) and its ligand hepatocyte growth factor (HGF), also called scatter factor (SF), are attractive targets for cancer therapy. Hence, c-Met is an attractive target for cancer treatment. In this study, docking based on three-dimensional quantitative structure?activity relationship (3D-QSAR) were performed on the 81 compounds (including in-house data), with comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). The major interaction sites were documented through calculating interaction energies between inhibitors and each residue in the active site from docking results. In addition, QSAR method on the basis of pharm-RDF molecular descriptors were compared to the other methods. The 3D-QSAR models were compared with the structural features at th active site to further elucidate the accuracy of the models.

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장소: 부산BEXCO

발표코드: **MEDI.P-1163**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure-based and ligand docking for the corticotropin-releasing factor type 1 receptor inhibitor

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한국화학연구원 신약플랫폼기술팀 분자설계 [1]한국화학연구원 화학물질연구단 [2]한국화학연구원 신물질연구본부/신약플랫폼기술팀

The corticotropin-releasing factor type 1 receptor (CRFR1) is a class B G-protein-coulple receptor (GPCR) and belong to the class B/Secretic family.The CRFR1 contains an N-termical extracellular domain which is binding site of corticotropin-releasing factor (CRF), a neuropeptide.And, experimental in vitro assay data were also collected from the public database.Fingerprint based similarity search, Bayesian classification and receptor ligand docking method were employed for virtual screening of KCB and suppliers compounds.

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장소: 부산BEXCO

발표코드: **MEDI.P-1164**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A kinked peptide using disulfide bond relieved hemolysis to generate side-effect free antimicrobial peptides

황희용 현순실 유재훈

서울대 화학교육과

Antimicrobial peptides (AMPs) are natural products of innate immunity from insects to mammals against pathogens. We have been developing synthetic antimicrobial peptides having low hemolytic activity in order to generate side effect free AMPs. Firstly, N-terminal and C-terminal modified peptide library of de novo designed model peptide LK was synthesized and its MIC, hemolytic activity and α-helical propensity were measured. A well correlated linear relationship between α-helical propensity and EC50 of hemolysis (HC50) was observed irrespective of their similar values. From this result, we thought that a transient erase of α-helical propensity by disulfide bond might possibly decrease hemolytic activity without ruining antimicrobial potency. In order to produce disulfide bond, we introduced two Cys residues at hydrophobic face of LK and oxidized two thiols. Hemolytic activity was largely decreased from these peptides, while showing compatible MIC values against gram-negative bacteria. Thus, the intended conformational stapling from α-helical to kinked peptide can generally applicable strategy for reducing toxicities of AMPs, and developed as therapeutic drugs against gram-negative bacteria.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1165**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-inflammatory effects of apolipoprotein A-mimic peptide with naphthyalanine

김예원 현순실[1] 유재훈[1]

서울대 화학교육학과 [1]서울대 화학교육과

Apolipoprotein A-I mimetic 4F is an amphipathic α-helical peptide with hydrophilic and hydrophobic spheres. Both faces of the peptide make intermolecular interactions with another molecule of the same peptide or with cholesterol/ester, forming high density lipoprotein-cholesterol (HDL-C). A variety of amphipathic peptides has been designed and synthesized as mimicry of 4F by substitution of the most important amino acids to unnatural amino acids both in hydrophilic and hydrophobic faces. These variants were screened for mimicry of apoA-? using HDL-C induced cholesterol efflux and tryptophan fluorescence intensity assays. A peptide (2s) with naphthylalanine moiety among these variants showed more than 3-fold improved cholesterol efflux than that of the reference peptide. In addition, 2s showed a strong anti-inflammatory effect that was observed by reduction of intracellular levels of TNF-alpha and nitric oxide in mice macrophage cells. In order to understand the detailed mechanism, we carried out a variety of biochemical experiments using fluorescence spectroscopy and surface plasmon resonance to observe meaningful interaction of 2s with inflammation inducers, such as lipopolysaccharides (LPS) and oxidized low-density lipoprotein-cholesterol complex (LDL). We also synthesized D-2s, in which all D-amino acids were used instead of natural L-amino acid to identify any possible intracellular target. Taken together, 2s seems to be multifunctional molecule that could interact with LPS and prohibit formation of oxidized LDL, affording strong anti-inflammatory effects.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1166**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of aryl isoxazole derivatives as metabotropic glutamate receptor 1 (mGluR1) antagonists

조경희 배애님[1]

연세대 화학과 [1]KIST 생체과학연구본부

Metabotropic glutamate receptor 1/5 (Group I) has been well-known as a novel target for treating central nervous system (CNS), especially for neuropathic pain and schizophrenia. We focused on mGluR1 antagonists in order to treat neuropathic pain. Based on known allosteric mGluR1 antagonists, we have designed, synthesized and evaluated biologically aryl isoxazole derivatives on mGluR1. Of them, although some have moderate efficacy on the in vitro test, they have moderate or excellent activities on the in vivo model for neuropathic pain. The reason may be that most of them are slightly insoluble. PCTC20045 has excellent analgesic property similar to Gabapentin, a commercially available drug, despite of moderate % inhibition.In addition, as series of improving poor solubility, we synthesized PCTC20087 and PCTC20088. All of them seems having superior inhibition of mGluR1. We have expected they also are excellent in in vivo. We will continue to study and discover allosteric mGluR1 antagonists having excellent activities in both in vitro and in vivo test.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1167**

발표분야: 의약화학

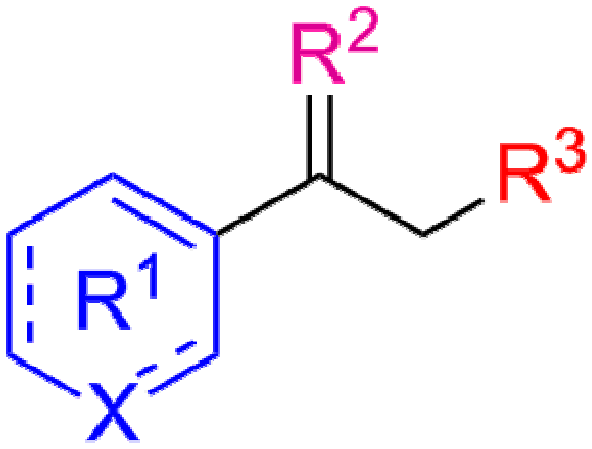
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Evaluation of Novel Compounds as mGluR5 Antagonists

최윤석 강순방[1] 금교창[2]

과학기술연합대학원대 생체분자과학 [1]KIST 뇌의약연구단 [2]KIST 케모인포메틱스연구센터

Glutamate is the predominant excitatory neurotransmitter in the brain and activates two major receptor classes: the ionotropic glutamate receptors (iGluR) and the metabotropic glutamate receptors (mGluR). mGluRs typically play a regulatory role on fast glutamatergic effects by modulating the ion channel activity and neurotransmitter release. mGluRs are a family of eight G-protein coupled receptors which are classified three groups based on their sequence homology, effector coupling and pharmacology. Group I mGlu receptors (mGluR1 and mGluR5) are positively coupled to phospholipase C; group II mGlu receptors (mGluR2 and mGluR3) and group III mGlu receptors (mGluR4, mGluR6, mGluR7, and mGluR8) are negatively coupled to adenylate cyclase. The recent research revealed that even though mGluR1 and mGluR5 are related phylogenetically, both mGluR1 and mGluR5 have a different expression pattern in the brain, which obviously suggests their different roles in nervous system function. In particular, mGluR5's over-stimulation has been implicated in several CNS disorders including anxiety, pain, depression, epilepsy, neurodegeneration, Parkinson's disease and cocaine-dependence. Therefore, mGluR5 is a potentially important therapeutic target for the treatment of several CNS diseases. 2-methyl-6-(phenylethynyl)pyridine (MPEP) and 1-(3-chlorophenyl)-3-(1-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-2-yl)urea (Fenobam) are a well known potent and selective noncompetitive mGluR5 antagonist and a negative allosteric modulator, respectively. In this study, we synthesized several novel compounds as mGluR5 antagonists and their in vitro assays were performed. The synthesis and the result of in vitro assays against mGluR5 will be discussed in detail.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1168**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The protective effect of heated ginsenoside-amino acid mixture against cisplatin-induced nephrotoxicity in LLC-PK1 cells

최필주 박순혜[1] 김희진[1] 강기성[1] 함정엽[1]

강릉원주대 화학신소재학과 [1]KIST 천연의약센터

Panax ginseng C.A. Meyer is one of the most widely used supplemental food and herbal medicines in Asia and has been used for the treatment of various human diseases. Ginsenosides are the major bioactive ingredients of ginseng, exerting many biological activities such as anti-oxidant, anti-tumorigenic, anti-fatigue, and anti-inflammatory effects. Recently, there have been reports stating that the biological activities of ginseng are fortified by heat-processing and the resulting changes in biological activities are due to the formation of a new type of ginsenosides or the increase in the content of particular ginsenosides. The aim of the present study was to verify the important role of Maillard reaction in the protective effect of heated ginsenoside-amino acid mixture against oxidative stress-induced nephrotoxicity.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1169**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

New potent and selective ligands for Dopamine receptors, aryl piperazyl 1,2,3-triazole derivertives.

곽주명 고훈영 최정화 최재이

인하대 화학과

1,2,3-Triazoles are well known heterocyclic structure as the key pharmacophore in medicinal chemistry. In continuation of our research for the discovery of potent ligands against dopamine receptor, the new ligands of substituted aryl piperazyl 1,2,3-triazole library is designed and synthesized by using of microwave synthesizer efficiently. Their binding affinities of constructed compounds were evaluated against dopamine receptors in vitro. And also, their structure-activity relationship will be discussed.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1170**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

An Amphiphilic α-Helical Peptide That Induces Apoptosis Through Interaction With Bcl-2.

허연 손미언 현순실 유재훈

서울대 화학교육과

Bcl-2 is one of the pro-survival factors of the Bcl-xl family that inhibits apoptosis signaling by interacting with Bak or Bax protein. When Bcl-2 is over-expressed, pro-survival Bcl-2 proteins can promote formation of non-apoptotic cancerous cells. Inhibitors of the interaction with Bcl-2 that are pro-apoptotic could serve as novel anti-cancer agents. Since Bak or Bax binds as amphipathic and highly α-helical peptide making extensive hydrophobic contacts with the Bcl-2, we envisaged that simple α-helical and amphiphilic peptides would be capable of binding to Bcl-2. If correct, this proposal suggests that carrying out mutations in both hydrophilic and hydrophobic faces of a simple peptide would serve as a new strategy for generating selective, tailor-made peptides against Bcl-2. A library of amphiphilic peptides, composed mainly of Arg and Leu residues, was synthesized and probed as inhibitors of Bcl-2. α-Aminoadipic acid (Aad) and Trp were incorporated into the synthetic peptide to change its hydrophilic and hydrophobic faces in order to increase conformational stability and induce more interactions with the target protein. This investigation demonstrated that one hydrophilic face mutant, 13Aad, possesses a strong pro-apoptotic propensity (EC50 = 8.4 nM). The strong binding affinity against Bcl-2 correlates with 13Aad's strong pro-apoptotic character. The results of this effort suggest that 13Aad might serve as a cancer therapeutic agent.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1171**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

New diarylureas and diarylamides possessing 1,3,4-triarylpyrazole scaffold: Design, synthesis, and anticancer evaluation (Part Ⅱ)

박이슬 Mohammed I. El-Gamal[1] 오창현[2] 지대윤

서강대 화학과 [1]과학기술연합대학원대 Medicinal Chemistry [2]KIST 바이오소재연구센터

Design and synthesis of a new series of diarylurea and diarylamide derivatives containing 1,3,4-triarylpyrazole scaffold are described. Their antiproliferative activities were tested over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). A structure-activity relationship (SAR) study was conducted for the target compounds. At a single-dose concentration of 10 ?M, most of the target compounds showed strong and broad-spectrum anticancer activity. 13 compounds have been selected for further testing in 5-dose testing mode in order to examine their efficacies and potencies over the NCI-60 cell line panel.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1172**

발표분야: 의약화학

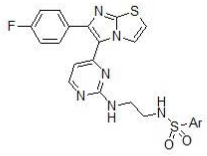
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and cytotoxicity of a new series of imidazo[2,1-b][1,3]thiazole derivatives

김미령 Mohammed Samir[1] Mohammed I. El-Gamal[2] 오창현[3] 태진성

연세대 화학과 [1]과학기술연합대학원대 Biomolecular science [2]과학기술연합대학원대 Medicinal Chemistry [3]KIST 바이오소재연구센터

A new series of imidazo[2,1-b][1,3]thiazole derivatives was designed and synthesized. Their in vitro antiproliferative activities are being tested over A375P human melanoma cell line and over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). After a single-dose concentration of 10 ?M, the most active target compounds will be further tested in 5-dose testing mode. The most potent target compounds will be tested at molecular level for inhibition of ERK pathway. The preliminary results are promising.



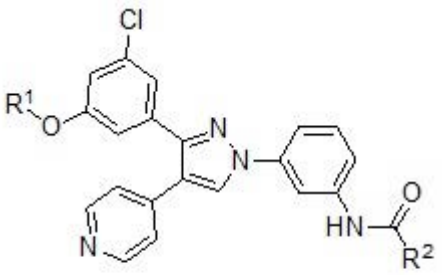
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1173**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

New diarylureas and diarylamides possessing 1,3,4-triarylpyrazole scaffold: Design, synthesis, and anticancer evaluation (Part I)

박병준 Mohammed I. El-Gamal[1] 오창현[2] 지대윤

서강대 화학과 [1]과학기술연합대학원대 Medicinal Chemistry [2]KIST 바이오소재연구센터

A new series of diarylurea and diarylamide derivatives containing 1,3,4-triarylpyrazole scaffold was designed and synthesized. Their antiproliferative activities are being tested over A375P human melanoma cell line and over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). After a single-dose concentration of 10 ?M, the most active target compounds will be further tested in 5-dose testing mode. The most potent target compounds will be tested at molecular level for inhibition of ERK pathway. This series of diarylureas and diarylamides is promising



R^1 = H, CH_3
R^2 = Ar, ArNH

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1174**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, synthesis, and biological evaluation of new diarylureas and diarylamides possessing 2,3-dihydro-1H-pyrrolo[3,2-b]quinoline scaffold

김현진 Mohammed I. El-Gamal[1] 오창현[2] 이용섭[3]

경희대 나노의약생명과학과 [1]과학기술연합대학원대 Medicinal Chemistry [2]KIST 바이오소재연구센터 [3]경희대 약학과

A new series of diarylurea and diarylamide derivatives containing 2,3-dihydro-1H-pyrrolo[3,2-b]quinoline scaffold was designed and synthesized. Their antiproliferative activities are being tested over A375P human melanoma cell line and over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). After testing at a single-dose concentration of 10 ?M, the most active target compounds will be further tested in 5-dose testing mode at the NCI. This series of diarylureas and diarylamides is promising

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1175**

발표분야: 의약화학

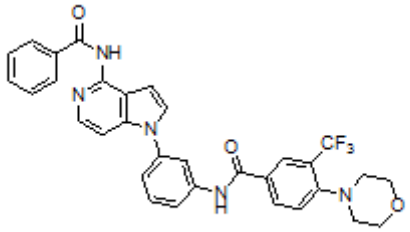
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preliminary cytotoxicity evaluation of a selective FMS kinase inhibitor possessing diarylamide and pyrrolo[3,2-c]pyridine moieties

Mohammed I. El-Gamal **Mohammed Samir**[1] **유경호**[2] **오창현**[3]

과학기술연합대학원대 Medicinal Chemistry [1]*과학기술연합대학원대 Biomolecular science* [2]*KIST 생명/보건본부* [3]*KIST 바이오소재연구센터*

A new diarylamide derivative possessing pyrrolo[3,2-c]pyridine scaffold was designed and synthesized. It was tested for kinase inhibitory activity over a panel of 47 kinases. It showed high selectivity against FMS tyrosine kinase. It was further tested over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). After testing at a single-dose concentration of 10 ?M, it was further tested in 5-dose testing mode at the NCI. Our target compound showed high potency and broad-spectrum antiproliferative activity against the tested cell lines. This compound is a promising lead for further development of new anticancer diarylamide derivatives.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1176**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and antiproliferative activity of new imidazothiazole compounds

Mohammed Samir Mohammed I. El-Gamal[1] 오창현[2]

과학기술연합대학원대 Biomolecular science [1]과학기술연합대학원대 Medicinal Chemistry [2]KIST 바이오소재연구센터

A new series of 1-(N-(substituted sulphonyl))-2-(N-(6-(3-methoxyphenyl)-5-(2-pyrimidin-4-yl)-imidazo[2,1-b]thiazole))diamino ethane, 1-(N-(substituted sulphonyl))-2-(N-(6-(4-methoxy phenyl)-5-(2-pyrimidin-4-yl)imidazo[2,1-b]thiazole))diamino ethane, 1-(N-(substituted sulphonyl))-2-(N-(6-(3-or4-hydroxyphenyl)-5-(2-pyrimidin-4-yl)imidazo[2,1-b]thiazole))diamino ethane, and 1-(N-(substituted sulphonyl))-2-(N-(6-(3-or4-hydroxyphenyl)-5-(2-pyrimidin-4-yl)imidazo[2,1-b]thiazole)) diamino ethane were synthesized and tested for their antiproliferating activity over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). Some of the target compounds showed promising results at a single dose concentration of 10 ?M. The most active compound was selected for 5-dose testing in order to determine its potency and efficacy over the NCI-60 cell line panel. This compound showed high selectivity towards melanoma subpanel in the single-dose testing.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1177**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and in vitro antiproliferative activity of new diarylamides and diarylureas containing quinoline nucleus

Mohammad Ashrafuddin Mohammed I. El-Gamal[1] 심태보[2] 오창현[3]

과학기술연합대학원대 Biomolecular science [1]과학기술연합대학원대 Medicinal Chemistry [2]KIST 생체과학연구본부 [3]KIST 바이오소재연구센터

Design and synthesis of a new series of diarylurea and diarylamide derivatives possessing quinoline nucleus are described. Their antiproliferative activities were tested over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). A structure-activity relationship (SAR) study was conducted for the target compounds. Most of the target compounds showed strong and broad-spectrum anticancer activity. After single-dose testing, 9 compounds were selected for 5-dose testing in order to determine their potencies over the NCI-60 cell line panel. Among them, a diarylurea derivative showed high potency in sub-micromolar scale over a wide range of cell lines of different cancer types.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1178**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and evaluation of (3,4,5-substituted)pyrazole derivatives as GPR 109A agonists

Vithal Jadhav 이선경[1] 송종환[2]

한국화학연구원 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 신물질연구단

3,4,5-substituted-pyrazole derivatives were synthesized and biologically evaluated as full agonists for the high affinity niacin receptor GPR 109A. The (3,4,5-substituted)pyrazole were formed by the condensation reaction of variously 3-substituted pentane-2,4-dione/benzoyl acetone and hydrazine hydrate. The 1-position of pyrazole was further diversified with (pyridine-3-yl)carbonyl and (pyrazine-2-yl)carbonyl derivatives to elucidate the structure activity relationships. Besides the effects of compounds on G-protein signal of GPR109A, the activity on ?-arrestin signal was evaluated.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1179**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Evaluation of different nonspecific binding blocking agents for SPR measurement

백철수 최은숙[1] 김은주[1] 김현철[1] 정상원[1]

대구경북과학기술원(DGIST) 나노바이오연구부 [1]대구경북과학기술원 나노바이오연구부

Au chips for surface plasmon resonance (SPR) were modified with different nonspecific binding blocking agents, namely, diethyl alcohol, mPEG350, mPEG2000 and phosphocholine (PC), by click chemistry. FT-IR measurements were carried out to confirm the successful depositions of the blocking agents. SPR measurements were performed to evaluate the degree of nonspecific adsorption of c-reactive protein (CRP), serum amyloid P component (SAP), and human serum onto the Au chips modified with different above-mentioned blocking agents. It was found that diethyl alcohol, mPEG350, mPEG2000 could completely protect the CRP binding to the concentration from 1 pM up to 400 nM (50 μg/mL in protein concentration). Because PC is specific ligand of CRP even though it is a good blocking agent against nonspecific binding of proteins, a concentration dependent binding of CRP was occurred on PC modified surface, from 5 nM of CRP. In case of SAP, SPR angle shift was observed in all blocking agents. The highest level of adsorption was observed in diethyl alcohol modified surface, to a degree of 0.162 angle shift. When 2% human serum was run through the diethyl alcohol and PC modified Au chips, PC modified surface showed the dramatically decreased nonspecific adsorption compared to diethyl alcohol modified Au surface. In conclusion, the non specific adsorption of serum proteins was effectively protected by PC than other blocking agents. Overall, the non-specific adsorption was occurred differently according to the surface characteristics of proteins, thus the blocking agent should be selected according to the target protein. PC showed very good blocking for assay using serum, but not applicable for CRP assay. Our results could be useful when one considers blocking agents for SPR-based biosensor devices.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1180**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Biological Evaluation and Molecular Docking Study of 3-(4-Sulfamoylphenyl)-4-phenyl-1H-pyrrole-2,5-dione as COX-2 Inhibitor

최민지 김경주 주동준 이재열

경희대 화학과

1H-pyrrole-2,5-dione 2l were synthesized and screened for COX-1/COX-2 inhibition. The biological results showed that 2l showed moderate inhibitory and selective profiles against COX-2, which is consistent with the molecular docking result of 2l inside the COX-2 activesite. Thus, the molecular docking results suggest us that 1H-pyrrole-2,5-dione derivatives with appropriate substitutions which can fill the adjunct pocket and interact with the other residues may be useful to propose new molecules with enhanced selectivity towards COX-2. The overall findings of this study inferred that moderate inhibition of compound 2l rendered it as a hit molecule for further development of more potent and selective COX-2 inhibitor. We are in progress of synthesizing a number of new derivatives based on this molecular docking result. Figure 1. Selection of 2l from 1H-furan-2,5-dione and 1H-pyrrole-2,5-dione library.

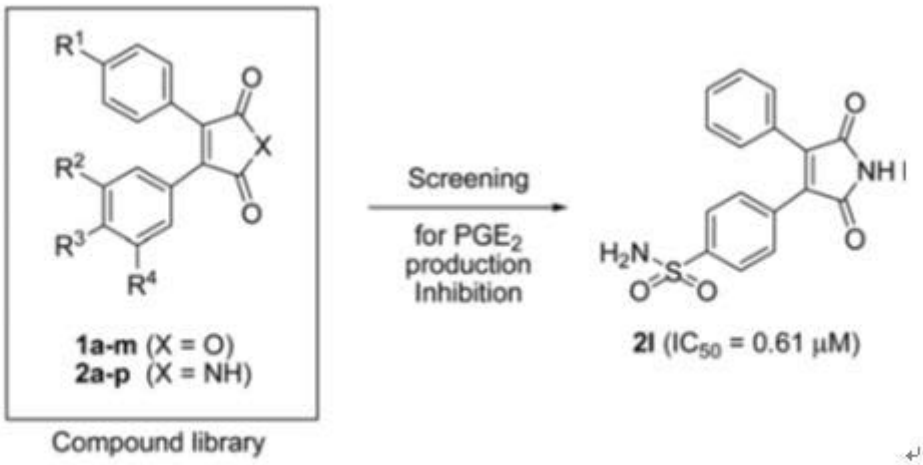


Figure 1. Selection of 2l from 1*H*-furan-2,5-dione and 1*H*-pyrrole-2,5-dione library.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

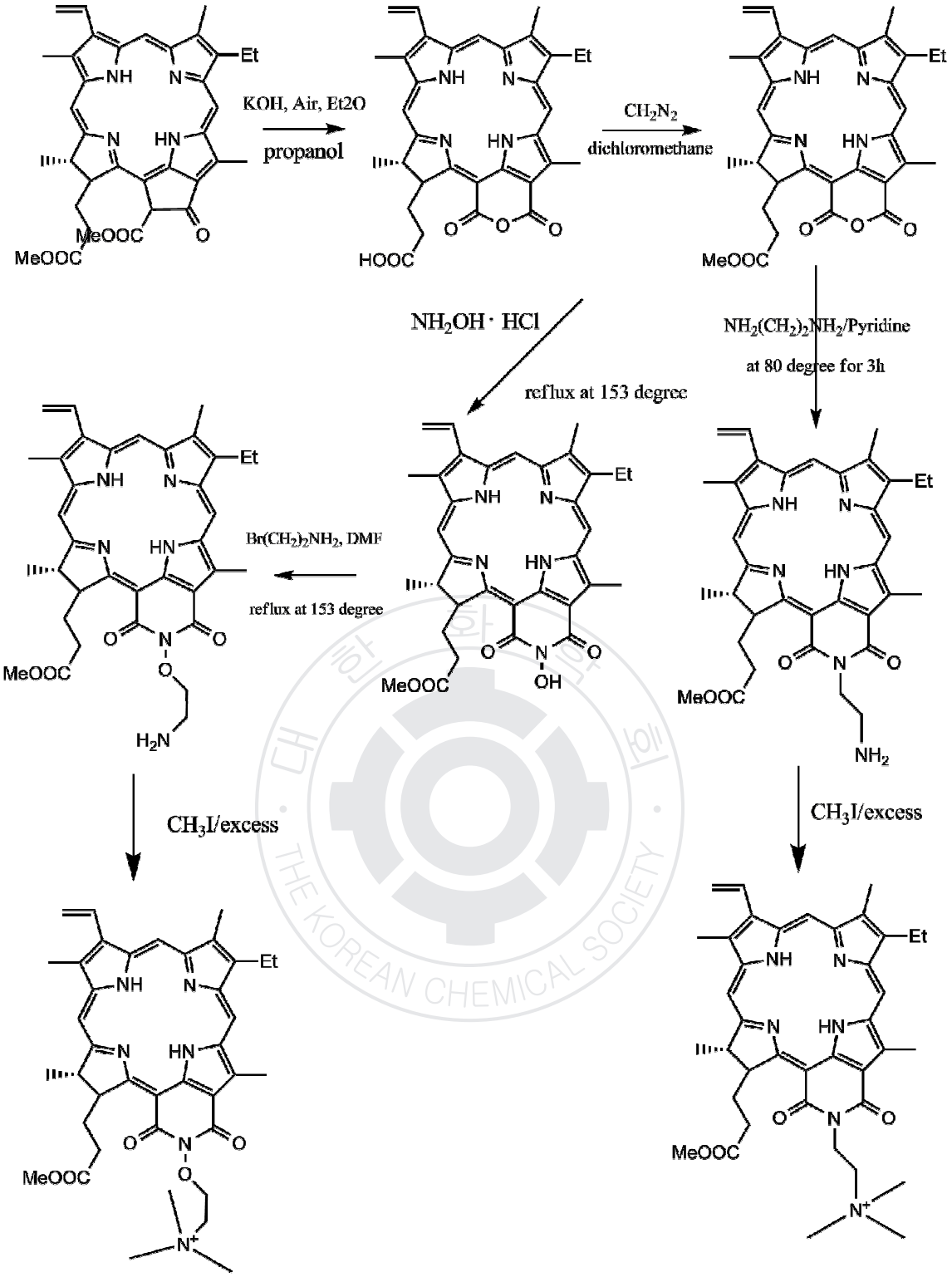
일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1181**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of synthesis and antitumor effect of cationic purpurin alkylimide

김정화 김정훈[1] 이범희[1] 장민아[1] 이태헌[1] 김병혁 류동훈 윤일[2] 심영기[1]

인제대 나노시스템 [1]인제대 나노공학부 [2]인제대 PDT 연구소

Photodynamic therapy (PDT), now well recognized treatment for the destruction of tumors, that is a modality of treating cancer based on the photosensitizer, laser light and oxygen present to generate reactive oxygen species. The high uptake and retention of such compounds and their DNA targeting capabilities have led to the synthesis of a number of novel cationic derivatives. Cationic porphyrins or chlorins have attracted considerable attention because of their remarkable ability to strongly interact with nucleotides. For the purpose of the effect, we had an idea as follows. The reactions of purpurin-18 with hydroxylamine and 1,2-diaminoethane have been investigated as a means for the synthesis of photosensitizers used in the photodynamic therapy of tumors, cationic purpurin-alkylimide.REFERENCES1. Sirish, M.; Schneider, H.J., Electrostatic interactions between positively charged porphyrins and nucleotides or amides: buffer-dependent dramatic changes of binding affinities and modes. Chem. Commun. 2000, (1),23-24.2. Fedoroff, O. Y.; Rangan, A.; Chemeris, V. V.; Hurley, L. H., Cationic porphyrins promote the formation of i-motif DNA and bind peripherally by a nonintercalative mechanism. Biochem. 2000, 30(49), 15083-90.3. Mikhail A. Grin, Rustam A. Titeev, Dmitry I. Brittal, Olga V. Ulybina, Alexander G. Tsiprovskiy, New conjugates of cobalt bis(dicarbollide) with chlorophyll a derivatives, Mendeleev Commun., 2011, 21, 84?86.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1182**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efforts to Discover Small Molecules against Hsp90 in Cancerous Diseases

박희백 서영호[1]

계명대 약학대학 신약개발 연구소 [1]계명대 약학대학

Conventional drug design in cancer embraces the “one gene, one drug, one disease” philosophy. Over the past two decades, several targeted cancer drugs, including Gleevec, Iressa and Herceptin have been discovered to eradicate tumors in more specific ways and reduce the harmful nonspecific side effects of chemotherapeutics. However, this notion of single targeted therapy has been challenged by the emergence of drug resistance. The tumor cells outsmart single-targeted drugs to escape from their destiny by mutating targeted proteins, down-regulating death signals, or up-regulating survival pathways. In this regard, the 90-kDa heat shock proteins (Hsp90) have emerged as an attractive therapeutic target in cancer research. Hsp90 is an ATP dependent molecular chaperone that is responsible for the stabilization and maturation of their substrate proteins, referred to as “client” proteins. Many Hsp90 client proteins play significant roles in six essential hallmarks of a cancer cell, including Her2, Met, Cdk4, Akt, HIF and MMP2. The therapeutic potential of targeting Hsp90 may be best appreciated by considering the possibility of simultaneously targeting the six hallmarks of a cancer cell. Besides, Hsp90 is constitutively expressed at 2-10 fold higher levels in tumor cells compared to their normal counterparts. Therefore, having a potent inhibitor targeting a cancer nodal protein, Hsp90 may be best suited to simultaneously disable multiple mechanisms of tumor maintenance and thus overcome the genetic and molecular heterogeneity of progressive cancers.As part of our ongoing efforts to discover small molecules targeting Hsp90 N-terminal ATP-binding site, we had performed a structure-based rational design of small molecule inhibitors against Hsp90. Designed inhibitors were synthesized and their anti-cancerous activities were evaluated.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1183**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

[2+1] pendanted tetraazamacrocycle for better bifunctional chelator

AJIT V. DALE 김정영[1] 이호춘[2] **Nikunj B. Bhatt** 하영수 김종희 **Nisarg R. Soni** 이웅희 안광일[3] 유정수

경북대 의과대학 분자의학교실 [1]한국원자력의학원 방사성의약품연구팀 [2]대구경북과학기술원 에너지시스템공학 [3]한국원자력의학원 방사성의약품 개발실

The stability of metal complexes, form between bifunctional chelator (BFC) and radiometal, plays a key role in ^{64}Cu-based radiopharmaceuticals. We had previously reported that TE2A is a better BFC for Cu(II) ions than widely used TETA. However, TE2A was conjugated with biomolecules in poor yields due to the involvement of acetate pendant arm and competition of its secondary amine groups with amine group of biomolecule. Here we designed and synthesized TE2A-NCS to overcome the shortcomings of TE2A while maintaining high stability of Cu-TE2A complexes. TE2A-NCS, having a third pendant arm with NCS functionality on TE2A backbone was synthesized in seven steps with excellent overall yield. The Cu(II) complex of TE2A-NH_2 was also synthesized in high yields. The X-ray crystallographic studies of Cu-TE2A-NH_2 showed that Cu(II) is strongly complexed by the BFC to form a neutral octahedral complex. Acidic decomplexation and cyclic voltammetry experiments were carried out using Cu-TE2A-NH_2 in comparison with Cu-TE2A to evaluate kinetic stability. Cu-TE2A-NH_2 showed higher stability than Cu-TE2A in acidic decomplexation studies. Cu-TE2A-NH_2 showed quasi irreversible reduction potential in cyclic voltammetry studies. TE2A-NCS was easily conjugated to antibody via its NCS functional group. TE2A-NCS-antibody was labeled with ^{64}Cu in 97% radiochemical yield within 1 min at 25°C. Overall, all above data clearly indicates that TE2A-NCS, which has two acetate group for coordination and one extra NCS group for conjugation, is very promising BFC for Cu-based radiopharmaceuticals.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1184**

발표분야: 의약화학

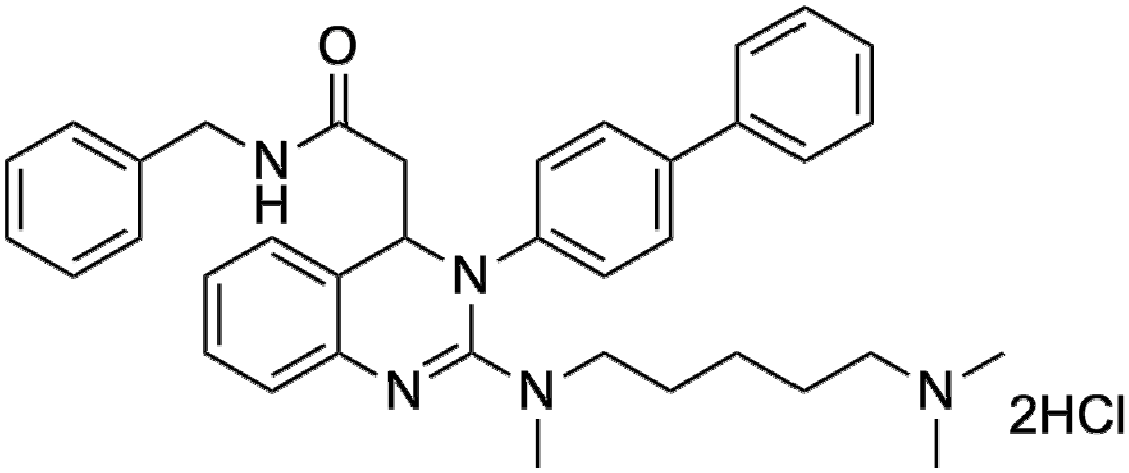
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-tumoral effect of 3,4-dihydroquinazoline derivative on solid tumor

최두리 장선정 이재열 주동준

경희대 화학과

An extension of our previously reported 3,4-dihydroquinazoline derivative is investigated. Oral antitumoral activity of 3,4-dihydroquinazoline derivative (KYS05090) as potent and selective T-type calcium channel blocker was in vivo evaluated against A549 xenograft in BALB/cnu/nu nude mice. The rate of tumor volume increment in mouse model with KYS05090-treated group was remarkably slower than that of control group. With respect to tumor weight, it exhibited 60% and 67% tumor growth inhibition through oral administration of 1 and 5 mg/kg of bodyweight, respectively, compared to control and was more potent than paclitaxel (53%). In addition, KYS05090 (10 and 50 mg/kg, po) was found to have a marked analgesic effect in acetic acid-induced writhing test, whereas it did not show any effect on hot plate test.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1185**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Antiinflammatory and Antioxidative activities of Rosemarinus officinalis L.

MORE KUNAL 이진호

계명대 화학과

Rosemary officinalis L., Mediterranean Basin herb, is well known for its antioxidant, antiinflammatory, and antiproliferative activity. The main antioxidative effects of rosemary have been reported to be due to major constituents as carnosol, carnosic acid and rosmarinic acid. In our study we studied the anti-inflammatory activity of rosemary to understand the mechanism of action. The anti-inflammatory activity of rosemary extract was evaluated by monitoring the activation of NF-kB and MAPKs, the expression of iNOS and COX-2, and the production of NO, PGE2 and cytokine in LPS-induced RAW 264.7 macrophages. The fractionation and identification were performed to find the active component other than well known. We had identified carnosol and 4’-methoxytechtochrysin by spectroscopic comparison with authentic sample. 4’-Methoxytechtochrysin, previously reported as weak in antioxidant, showed similar activity as carnosol and showed synergistic effect with carnosol in DPPH assay.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1186**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Urease and Acetylcholine esterase inhibition activities of some 1, 4-Disubstituted Thiosemicarbazides and their 2, 5-Disubstituted Thiadiazoles

Muhammad Saleem 이기환 **MUHAMMAD RAFIQ** 서승염[1]

공주대 화학과 [1]공주대 생명과학과

A new series of 2,5-disubstituted-1,3,4-thiadiazoles 6a-i was synthesized by overnight stirring various 1,4-disubstituted thiosemicarbazides 5a-i in polyphosphoric acid followed by neutralization. The structures of newly synthesized compounds 5a-i and 6a-i were characterized by IR, 1H and 13C NMR, elemental analysis and mass spectrometric studies. All the synthesized compounds were evaluated for their urease and acetylcholine esterase inhibition activities. Thiosemicarbazides 5a-i were found to possess excellent potential for urease inhibition, more than the standard drug. Thiosemicarbazides 5a-i were more potent urease inhibitor than their cyclic analogues thiadiazoles 6a-i. Almost all of the compounds were excellent inhibitors of acetylcholine esterase. The inhibition of acetylcholine esterase of compounds 5a, 5c, 5d, 5g, 5i, 6e, 6f, 6g, and 6i is much more than that of standard drug. Key words: Dehydrocyclization, Polyphosphoric acid, Urease, Acetylcholine esterase inhibition, Potent inhibitor.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1187**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of novel neuroprotective agents activating Nrf2 and inhibiting NO production

우서연

KIST

We have advanced a novel class of neuroprotective agents as Nrf2 activators for Parkinson's disease. Herein, we report a structure-activity relationship study of a series of 60 synthetic vinyl sulfone derivatives and their ability to induce HO-1 level and inhibit NO production. A representative compound 12g exerted excellent activity on HO-1 induction compared with sulforaphane, well-known Nrf2 activator. Furthermore, 12g led to more than 80% decrease of LPS-induced NO production. Collectively, the strong effects of 12g on both activities may provide a promising novel therapy for Parkinson's disease.

한국화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1188**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Activities of Some New 3,6-Disubstituted1,2,4-Triazolo[3,4-b]1,3,4-thiadiazole Derivatives

MUHAMMAD RAFIQ 서승염[1] **Muhammad Saleem** 이기환

공주대 화학과 [1]공주대 생명과학과

A series of aromatic hydrazides 3a-j were prepared by refluxing esters 2a-j with hydrazine hydrate in methanol, which were prepared by the esterification of 1a-j. Acetohydrazides 3a-j upon treatment with carbon disulfide and methanolic potassium hydroxide yielded potassium dithiocarbazate salts 4a-j, which on refluxing with hydrazine hydrate yielded substituted 4-amino-5-aryl-3H-1,2,4-triazole-3-thiones 5a-j. The target compounds 6a-j were synthesized by condensing furan-3-carboxylic acid in the presence of poly phosphoric acid under reflux. The structures of newly synthesized compounds were characterized by IR, 1H NMR, 13C NMR, elemental analysis and mass spectrometric studies. All the synthesized compounds were screened for their urease, acetylcholine esterase inhibition, antioxidant and alkaline phosphatase inhibition activity. Almost all of the compounds 6a-j showed good to excellent activities against urease and acetylcholine esterase more than the reference drugs. Compounds 6f and 6g were more potent scavenger of free radicals than the reference n-propyl gallate. Compound 6b and 6h showed excellent activities of alkaline phosphatase as compare to the reference KH2PO4. Key words: 1,2,4-Triazoles, Triazolothiadiazoles, Urease, Acetylcholine esterase, Antioxidant, Antibacterial activity.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1189**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and SAR studies of L-783277

김직녀 양한용 김환[1] 심태보[2]

서강대 화학과 [1]KIST 화학키노믹스센터 [2]KIST 생체과학연구본부

Efficient and enantioseletive total synthesis of L-783277, a naturally occurring resorcyclic acid lactone, was successfully performed by our research group. Three key steps composed of olefin cross metathesis, addition of acetylene derivative to aldehyde, and Yamaguchi macrolactonization were employed to construct the framework of L-783277. Most recently, we have successfully accomplished the modification of synthetic route of L-783277 synthesis, which resulted in a significant enhancement of overall synthesis yield. This modified synthetic route will be presented in this talk.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1190**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Antitubercular Activity of 7-Substituted-2-nitro-6,7-dihydro-5H-imidazo [2,1-b][1,3]oxazine

강민서 윤창수[1] 오태권[2] 김종승 이일영[1]

고려대 화학과 [1]한국화학연구원 신물질연구단 난치성질환치료제연구센터 [2]연세대 의과대학

Recently the re-emergence of tuberculosis (TB) in the world wide, accompanied by the rise of multidrug-resistant (MDR) strains, emphasizes the need for the discovery of new therapeutic drugs with greater efficacy, safety and novel mechanism of action against this disease. While no drugs have been introduced in the past 4 decades, only several new or redevelopment candidates are under clinical evaluation. The PA-824 ((6S)-2-nitro-6-{[4-(trifluoromethoxy)benzyl]oxy}-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazine) containing nitroimiazole has entered phase II clinical trials as novel TB therapeutics. The mechanism of action of PA-824 involved as mycolic acid synthesis inhibitors and intracellular nitric oxide (NO) release for respiratory poisoning under aerobic and anaerobic conditions. We synthesized analogues of PA-824 featuring chiral substituted at 7-position of imidazoxazine (7-substituted-2-nitro-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazine) of for seeking new drug candidates and tested for antimycobacterial activity against the H37Rv strain of mycobacterium tuberculosis. In this study, we wish to report the design and SAR(structure activity relationship) studies of 7-substituted-2-nitro-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazines as potential antitubercular agents.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1191**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of New benzooxazole and benzofuran derivatives as Aβ binding agents

김경훈 양지은 지대윤

서강대 화학과

The detection of Aβ plaques is an essential tool for the diagnosis of Alzheimer's disease (AD). In order to detect the Aβ plaques in the brain, PET imaging agent is the most effective method. Benzooxazole and benzofuran derivatives were developed as Aβ binding agents and showed good in vivo activities. We modified and derivitized benzooxalole and benzofuran to develop PET imaging agents. From the different research of benzooxazole and benzofuran we think that to design new AD probes two pharmacophores are required. First, there should be the N-methylaniline group at C-2 position of benzooxazole and benzofuran. Second, the hydroxyl group must be at C-5 position of benzooxazole and benzofuran. We designed and syntheized two molecules which has 3-fluoro-2-hydroxypropanoxy group and N-methylaniline group (Figure 1). These candidates will be good compounds for the detection of Aβ plaques and will be useful lead compounds for other chemists.

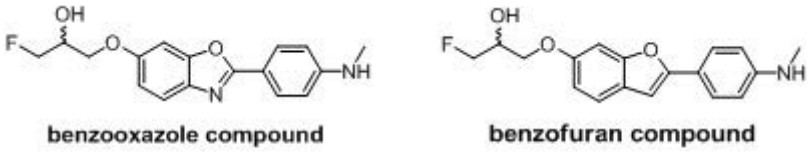


Figure 1. The structures of PET Aβ imaging agents.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1192**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Drug Release behavior of Poly(ethylene glycol)-cysteine-Poly(s-butyl cysteine) micelles.

이효정 김현철[1] 김은주[1] 정상원[1]

대구경북과학기술원(DGIST) 나노바이오연구부 [1]대구경북과학기술원 나노바이오연구부

A new amphiphilic copolymer, monomethoxy-poly(ethylene glycol)-cysteine-poly(s-butyl cysteine) (mPEG-cys-PBC) was synthesized, and cysteine group was oxidized under air. This polymer was self-assembled into micelles, which exhibited reducing agent sensitivity. Indomethacin (IMC) as a model drug was incorporated into the micelles by an oil/water emulsion method. The model drug release from drug loaded polymeric micelles was investigated as a function of glutathione (GSH) concentration in the release medium. The release study revealed that the release IMC from polymeric micelle was increased by increasing the GSH concentration and indicated that the release IMC from polymeric micelles can be controlled from (mPEG-cys-PBC-S)2 micelle by adjusting GSH concentration. In vitro cell cytotoxicity study in HUVEC cell showed non-toxicity, but in A549 (human adenocarcinoma cell) cell line showed slightly the cell toxicity with increasing polymeric micelles concentration. An anti-cancer drug, paclitaxel (PTX) was encapsulated into micelles. In vitro drug release of A549 cell for PTX-loaded micelles tested with GSH concentration.

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1193**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reduced binding of serum amyloid P component to amyloid fibril by synthetic antibody immobilized gold nanoparticles

최은숙 백철수 김은주 김현철 정상원

대구경북과학기술원 나노바이오연구부

Accumulation of amyloid fibrils in the viscera and connective tissues causes systemic amyloidosis, which is responsible for about one in a thousand deaths in developed countries. Serum amyloid P component (SAP), a pentraxin protein, is a universal constituent of amyloid deposits and contributes to their formation and/or persistence. It has been also reported that clearing of SAP in blood stream interfere the growth of the amyloid fibril, and the elimination of SAP in blood is needed for amyloidosis theraphy. In this study, we developed SAP-imprinted gold nanoparticels (SAPim-GNP), which was expected to specifically targeted to SAP, and compete with amyloid fibril for SAP binding. To prepare SAPim-GNP, 11-Azidoundecane-1-thiol (azido thiol), 1-hex-5-ynoylpyrrolidine-2-carboxylate (propargyl proline) and propargyl-mPEG350 were synthesized. GNPs were primarily immobilized on the 3-aminopropyl trimethoxysilane (APTMS) treated glass, and then azido thiol was added to form self assembled monolayer (SAM) on GNP surface. SAP was pre-incubated with propargyl-proline and click reaction was performed to conjugate propargyl proline and azide SAM, maintaining the geometry of five SAP monomer binding site on GNP. Finally, SAPim-GNP was released from glass surface by sonication. The modification of GNP surface was analyzed by XPS, and particle size and morphology was analyzed by TEM. The binding capacity of SAP to SAPim-GNP was increased three folds than non-imprinted proline immobilized GNP. The amyloid fibril was synthesized by aggregation of β-amyloid$_{1-42}$, for 3 days at RT. The SAP binding capacity to amyloid fibril was identified by SDS-PAGE. FITC-labeled SAP was used to determine the competitive binding activity SAPim-GNP with amyloid fibril. The confocal microscopy showed that SAPim-GNP inhibited the interaction between SAP and amyloid fibril. The SAP binding to amyloid fibril was decreased to 54% when SAPim-GNP was added to the solution. Anti-SAP antibody coated GNP (antiSAP-GNP) also inhibited the interaction between SAP and amyloid fibril to 68%. The

result showed that synthetic antibody prepared in this study could bind specifically to SAP, and subsequent inhibit the binding of SAP to amyloid fibril. The inhibitory effect of SAPim-GNP for SAP was increased than antiSAP-GNP.

대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간
장소: 부산BEXCO
발표코드: **MEDI.P-1194**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anticholinestase Activities of Organic Extracts of Sagassum sp.

임진아 이봉호[1] 최병욱[1] 이혜숙

한밭대 생명공학과 [1]한밭대 응용화학생명공학부

Alzheimer's disease (AD) is an irreversible, progressive neurodegenerative disorder resulting in memory loss, behavior disturbances, personality changes and a decline in cognitive abilities. It is also the most common cause of dementia among the elderly. Neuropathological studies have demonstrated that cholinergic functions in the basal forebrain and cortex decline due to senile dementia during AD. The most promising therapeutic strategy for activating the cholinergic functions has been the use of anticholinesterase agents such as Aricept? and Exelon?. But these synthetic compounds have side effects, headache, sleep disturbance, vomiting, etc. And lately, anti-butytylcholinesterase(BuChE) compounds have additionally been emerged as potential AD treating drugs. Thus, it is needed to develop safe and effective anticholinesterses from natural resources. Our previous results showed that browm algae have active secondary metabolites such as polyphenols and terpenes with many biological activities. The polyphenols from Ecklonia cava have strong AChE inhibitory, antioxidative, antiinflammatory, and antisecretase activities and are being developed antidementia agent. These led us to search for anticholinesterase compounds from brown seaweeds and we found anticholinesterase activity in the organic solvents extracts of Sargassum piluliferum and Myagropsis myagroies. From the 100 % methanol extract of S. piluliferum and M. myagroies, solvent partition fractions were prepared by using n-hexane, chloroform, butanol and water, and among them chloroform fraction showed strong BuChE inhibitory and antioxidative activity. The chloroform fraction of S. piluliferum and M. myagroies showed more than 90 % radical scavenging activity and 80 % butyrylcholinesterase(BuChE) inhibitory activity at 1mg/mL, respectively. The active compounds are being isolated by column chromatographies.

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장소: 부산BEXCO

발표코드: **MEDI.P-1195**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and antioxidative activity of 3,4,5-trihydroxyphenylacetic acid derivatives

김진아 이진호

계명대 화학과

Interest in antioxidants has been increased as researches reveal the evidence that reactive oxygen species (ROS) in the body are the main causes of diverse diseases. However, excessive uptake of synthetic antioxidants such as BHT and BHA are restricted due to risk of lipid transformation and cancer. Also, the use of natural antioxidants (e.g. ascorbic acid and tocopherol) has problems such as weak antioxidative activity and/or high cost. So, there are needs for new antioxidants which have potency, low toxicity, and low cost. Polyphenolic acids were reported to have antioxidative activity. However, highly hydrophilic character of polyphenolic acids lowers the absorbability through the lipophilic cell membrane. Based on the result that 3,4,5-trihydroxyphenylacetic acid had high potency, the derivatization of 3,4,5-trihydroxyphenylacetic acid was performed to find new antioxidant. DPPH, ABTS, FTC, TBA assays were used to evaluate antioxidative activity of the synthesized compounds. 3,4,5-Trihydroxyphenylacetic acid derivatives showed better antioxidant activity than vitamin C. Some compounds were comparable to the well-known antioxidants.

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발표코드: **MEDI.P-1196**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and evaluation of IR3535 derivative as mosquito repellents

이지훈 이진호

계명대 화학과

Diseases that are vectored by mosquitoes are encephalitis caused by Culex sp., malaria caused by Anopheles sp. and dengue fever caused by Aedes sp. These diseases infect over 700 million people each year; among these diseases, in the case of malaria, over 1 million deaths per year can be attributed to the disease, and over 3,000 people die every day due to malaria.Although as an organic compound DEET (N,N-Diethyl-meta-toluamide) is the most widely used as a general-purpose repellent ingredient, it has had problems such as safety due to its high skin permeability and issues of unpleasant odors, etc. Recently an eco-friendly natural materials IR3535 (ethyl 3-(N-butyl-N-acetyl)aminopropionate) has been used as an substitute for DEET, but it has drawbacks such as short duration time and lower activity. As a result, the development of a novel mosquito repellent which is active against mosquito while safe to human body is needed. In this study, we tried to find a new repellent ingredient with high potency and low toxicity. As an initial step, the derivatives of IR3535 were synthesized and tested for its repellency. After screening, LJH158 was found to be a promising candidate. Comparative repellent studies and toxicity tests were performed to confirm the potential of LJH158 as a new repellent ingredient.

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장소: 부산BEXCO

발표코드: **MEDI.P-1197**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, synthesis and biological evaluation of novel and potent protease-activated receptor 2(PAR) antagonists for treating arthritis

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인하대 화학과 [1]연세대 생명공학과 [2]KIST 생체과학연구본부

Protease-activated receptor 2 (PAR2) is the second number of a novel family of seven-transmembrane G-protein-coupled receptors, PARs. They are mainly expressed in platelets, but also on endothelial cells, myocytes and neurons. Activation of PAR2 is initiated through a proteolytic cleavage of serine proteases such as trypsin or b-tryptase from mast cells, exposing a tethered ligand domain which binds and activates the cleaved receptor. This receptor regulates various physiological functions including vasoregulation, arteriolar dilation, degranulation of mast cells and cell growth to inflammation. Initial observations of PAR2 knock-down mice indicated that the receptors may be useful therapeutic agents for the treatment of human diseases such as arthritis. Therefore, PAR-2 is targeted to develop as inflammatory joint disease drug. A novel series of 64 quinazoline and 2 pyrimidine derivatives were designed and synthesized as PAR2 antagonist. The synthesized 6-methoxy-quinazoline compounds showed reasonable inflammatory inhibition activity against various inflammatory cell lines. The detailed design, synthesis and biological evaluation of PAR2 antagonists as inflammatory joint disease drugs will be presented.

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장소: 부산BEXCO

발표코드: **MEDI.P-1198**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Evaluation of the Mitochondrial Permeability Transition Pore Inhibitors for the Treatment of Alzheimer's Disease

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The role of mitochondrial β-Amyloid peptide(Aβ) has been highlighted in Alzheimer's disease(AD) pathogenesis. Aβ is produced from transmembrane amyloid precursor protein(APP) by sequential actions of β- and γ-secretase. Aβ is implicated in the pathogenesis of Alzheimer's disease by interaction of Aβ with cyclophilin D(CypD). CypD, adenin nucleotide translocator(ANT), voltage-dependent anion channel(VDAC), and benzodiazepine receptor(PBR) compose the mitochondrial permeability transition pore(mPTP). The interaction of Aβ with CypD enhances the translocation of CypD to the mPTP and results in mPTP opening. After the mPTP opening, cytosolic solutes influx into the mitochondrial matrix, and then mitochondrial swelling causes cell death. Therefore, blockage of CypD or PBR can be an effective therapeutic strategy in Alzheimer's disease. Based on the pharmacophore-based virtual screening, we identified novel scaffolds KKPN0001 and KKPN0002, and the synthesis and biological evaluations of those compounds were performed. The optimization of novel mPTP inhibitors is now in progress. Approximately 90 KKPT compounds were newly synthesized and biologically evaluated.

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장소: 부산BEXCO

발표코드: **MEDI.P-1199**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Iron Oxide Nanoparticles Mediated Cancer Imaging and Therapy

채민경 이철현

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Iron oxide nanoparticles as magnetic resonance imaging (MRI) contrast agents have a variety of characteristics that penetrate effectively biological membranes, circulate for a long time in blood vessel, and conjugate with targeted peptides. We synthesized nontoxic cleaved iron oxide nanoparticles (CION) from hydrophobic FeO nanoparticles (HION) via 3 steps. It showed improved r2 relaxivities and potential application as a drug delivery system by surface modification. Peptides are valuable targeting probes and therapeutic molecules because of their small size and low immunogenicity. CION was introduced two types of peptide, RGR peptide and polo-like kinase 1 (PLK 1) targeted peptide, for targeting and therapy cancer. A tumor-homing peptide (RGR peptide) is specifically binding to PDGF receptor-beta on endothelia cells of solid tumor. It was reported that inhibition of PLK1 which is a regulator of cell growth by using PLK1 targeted peptide cause tumor cell death but not normal cell. By selectively binding to cancer cell and inhibiting PLK1, these nanoparticles could be multi-modality imaging agents.

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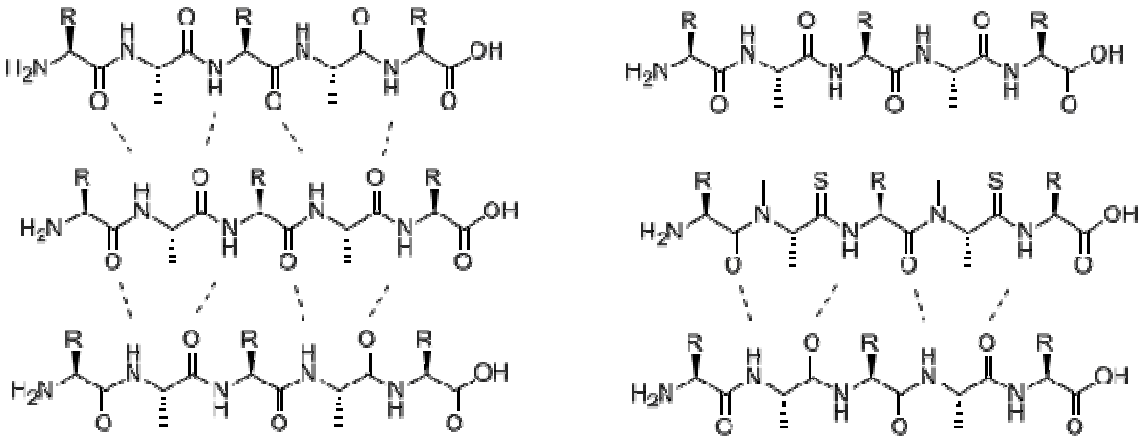
장소: 부산BEXCO
발표코드: **MEDI.P-1200**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of N-methylthioamide peptides as inhibitor of Aβ fibril formation.

양인선

충남대 신약개발학과

Neurotoxic assemblies of the amyloid-β(Aβ,39-43 amino acid), produced by the amyloid precursor protein(APP) , have been linked strongly to the pathogenesis of Alzheimer`s Disease(AD). The complicated process of conversion of Aβ peptides from their soluble to insoluble forms via oligomeric aggregates is considered a key event in the pathogenesis of AD.Inhibition of Aβ fibril formation based on the hydrophobic region of Aβ is the most ubiquitous.In this work, we utilized the KLVFF(Aβ16-20) motif, central hydrophobic core, to prevent Aβ fibril formation.N-methylthioamide modifications of the peptide backbone(KLVFF) are used to perturb secondary structure, to inhibit Aβ aggregation. N-methyl group of N-methylamide blocked hydrogen-bonding between upon Aβ amide oxygen and amide amine and can be prevented further association of β-sheets. Sulfur of thioamide is a weaker hydrogen-bond acceptor as compared to the amide oxygen. To yield potent inhibitors of Aβ aggregation , we have generated thioamide and N-methylthioamide via Fmoc-chemistry-based solid phase synthesis.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1201**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Method validation of physicochemical properties for drug optimization in early drug discovery

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The strategy to obtain lead compounds or candidates possessing good pharmacokinetic (PK) properties coupled to outstanding pharmacodynamic effects has changed the priorities in drug discovery. However, pharmacokinetic screening would be worthless if not complemented by physicochemical profiling for some reasons.Physicochemical properties such as solubility and permeability are intrinsic determinants of absorption, as shown by the Biopharmaceutic Classification System (BCS) which recognizes four types of bioavailability profile depending on whether solubility and membrane permeability are high or low. The second, a most relevant reason is that a number of physicochemical and structural properties are known to have a major influence on PK behavior and are therefore predictors of it. Therefore, accurate estimation of physicochemical properties including ionization constant (i. e., acidity and basicity), solubility, lipophilicity, and permeability are important factors for drug optimization. Aim of this study is to validate analytic method in order to gain physicochemical properties of high quality as the determinants and predictors for drug optimization in early drug discovery. It was validated analytical method for the determination of pKa and logP using 30 authentic drugs. Method validation of pKa or log P was conducted by the comparison between predicted values of which was estimated by in silico software ACD/Lab and observed values of pKa or Log P which was measured by GLpka and pKa-pro. The correlation coefficients (r2) of pKa were 0.82 and 0.80 in pKa-pro and GLpKa, respectively, showing good correlation. Log P, also, was well validated (r2=0.85).

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장소: 부산BEXCO

발표코드: **MEDI.P-1202**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Summarized report of physicochemical screening in KRICT (2009~2012)

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Drug discovery is continuously advancing due to new knowledge, methods, techniques, and strategies. Physicochemical information offers significant opportunities for enhancing discovery success. Particularly, it has been known well that solubility and permeability issues can pivotal roles for oral absorption. From 2009 to 2012, we conducted over 1200 physicochemical experiments including solubility, logP, pKa, stability, or PAMPA for early drug discovery. Here, we categorized molecular weight, logP and solubility of these compounds by the 'rule of 5' to evaluate drug-like properties. Among 452 compounds for the classification of molecular weight, compounds with M.W. ≤ 500 were present 74.7 %. About 21.6 % of 357 tested compounds had a Log P over 5. It reflects that the trends for drug discovery in KRICT are suitable well for Lipinski's rule. However, only 51.4 % of 574 compounds had acceptable solubility in the entire data set. Therefore, we suggest that it needs the strategy for the improvement of the aqueous solubility to minimize poor absorption. Finally, Our data may be useful as the first guideline for the selection of druggable compounds and ADME screening.

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장소: 부산BEXCO

발표코드: **MEDI.P-1203**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The design and evaluation of selective fluorescent coumarin conjugated derivatives that bind to WT-TTR.

명노준

충남대 신약전문대학원

TTR (trasthyretin) is a homotetrameric protein that is one of more than 30 nonhomologous human amyloidogenic proteins, whose major role is the transportation of thyroid hormone thyroxine (T4) and holo-retinol binding protein in the blood and cerebrospinal fluid (CSF). Misfolding and/or misassembly of TTR express proteotoxicity and cell degeneration thought to cause the amyloidoses. Coumarin derivatives are designed and synthesised to bind into the T4 binding site on the TTR tetramer. Coumarin derivatives are environmentally sensitive fluorophores. Of the 10 derivatives we discovered two potent compounds by fluorimetric assay with WT-TTR and acid-mediated fibrile formation assay.Inhibition of WT-TTR amyloidogenesis was evaluated using the acid-mediated fibril formation that was quantified by measuring turbidity. Also incubation of WT-TTR with compounds in Phosphate buffer (pH 7) produced blue and green fluorescence. However barely detectable fluorescece was observed when compounds were incubated with albumin. In conclusion, we synthesised 10 coumarin conjugated derivatives. Two potent derivatives selectively bind to the WT-TTR T4 binding site and fluoresce brightly (green and blue respectively).

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발표코드: **MEDI.P-1204**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Aldose Reductase Inhibitory Compounds from Xanthium strumarium

임순성

한림대 식품영양학과

As part of our ongoing search for natural sources of therapeutic and preventive agents for diabetic complications, we evaluated the inhibitory effects of components of the fruit of Xanthium strumarium on aldose reductase (AR) and galactitol formation in rat lenses with high levels of glucose. To identify the bioactive components of X. strumarium, 7 caffeoylquinic acids and 3 phenolic compounds were isolated and their chemical structures were elucidated on the basis of spectroscopic evidence and comparison with published data. The abilities of 10 X. strumarium-derived components to counteract diabetic complications were investigated by means of inhibitory assays with rat lens AR (rAR) and human recombinant AR (rhAR). From the 10 isolated compounds, methyl-3,5-di-O-caffeoylquinic acid showed the most potent inhibition, with IC50 values of 0.30 and 0.67 μM for rAR and rhR, respectively. In the kinetic analyses using Lineweaver?Burk plots of 1/velocity and 1/substrate, methyl-3,5-di-O-caffeoylquinic acid showed competitive inhibition of rhAR. Further, methyl-3,5-di-O-caffeoylquinic acid inhibited galactitol formation in the rat lens and in erythrocytes incubated with a high concentration of glucose, indicating that this compound may be effective in preventing diabetic complications.

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장소: 부산BEXCO

발표코드: **MEDI.P-1205**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Energy based phamacophore modeling and virtual screening for novel inhibitors of Cyclophilin D

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KIST 뇌의약연구단 [1]KIST 생체과학연구본부 [2]연세대 생명공학과

Cyclophilins belongs to a family of cellular enzymes that catalyze the reaction of peptidyl-prolyl cis-trans isomerase (PPIase) on their ligand proteins. One of human cyclophilin isoforms, Cyclophilin D (CypD), is a mitochondria-specific cyclophilin that is known to play a pivotal role in mitochondrial permeability transition (MPT) formation in Aβ-mediated mitochondrial dysfunction. Cyclosporin A (CsA) is a peptide analog, which is a globally used Cyclophilin inhibitor, but it has been reported unexpected side effects. Therefore, CypD small molecule inhibitors are urgently needed and developing new compounds targeting neuronal CypD can be a promising therapeutic strategy to cure Alzheimer's disease. In this study, an energy based phamacophore model was generated on the basis of protein-ligand interaction terms derived from Glide extra precision scoring function. Also, e-pharmacophore model was based on the high resolution co-crystal structure of CypD in complex with CsA at 0.96Å, used for commercially available 969,673 compounds virtual screening. Next, the qualified 84,731 compounds were processed by ADME to check drug likeness. Filtered 24,410 compounds were confirmed by 4 catalytic residues: Arg55, Gln63, Asn102, Trp121 in CypD binding analysis of Gold v5.0.1. Finally, 949 molecules were classified into 28 clusters according to chemical diversity. Out of 45 compounds have been chosen by the results of visual inspection and selected for in vitro biological evaluation.

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장소: 부산BEXCO
발표코드: **MEDI.P-1206**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Assessment for Drug Safety and Toxicity in vivo Zebrafish System

배명애

한국화학연구원 신약플랫폼기술팀

Drug discovery is a complex process, laborious, very expensive and time-consuming studies. Developing a new drug to the average costs a pharmaceutical or biotechnology company about $400 to $900 million and takes an average of 10 to 15 years. Of all the compounds entering the R&D project less than 1% will be launched to the market. In the early stages of drug development, the low correlation of the in vitro cytotoxicity studies with human toxicity makes difficult to predict. Zebrafish has relevance in preclinical trials due to its small size, transparency, easy to manipulate, rapid development, inexpensive to maintain and possibility to generate transgenic lines targeting specific organs. The zebrafish has a morphological and physiological similarity to mammals and therefore zebrafish is a widely used at various stages of the drug discovery process, such as in preclinical toxicity, safety and efficacy assessment. Therefore, we have been exploring and developing in vivo assays for assessing drug effects on toxicity and safety in zebrafish embryos. Drug Discovery Platform Technology Team (DDPT) is a biotechnological laboratory team offering drug discovery services to pharmaceutical and biotechnological laboratories and companies. DDPT offers a comprehensive range of high quality in vitro and in vivo ADMET services. Recently, we launched additional services based on the zebrafish model and the capability to offer highly efficient assays. For this purpose, we now provide a range of safety pharmacology and toxicity screens that can be used to identify and evaluate potential new drug candidates: i) zebrafish toxicity assessment ? Acute Teratotoxicity, Hepatotoxicity and Neurotoxicity. ii) zebrafish safety assessment ? Cardiac function assay. iii) zebrafish efficacy model - we have been exploring assay model chemically induced liver steatosis.

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장소: 부산BEXCO

발표코드: **MEDI.P-1207**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Prediction of the three-dimensional structure of protease-activated receptor2 by homology model based on multiple templates

조남철 차지현[1] 노경태 배애님[2]

연세대 생명공학과 [1]인하대 화학과 [2]KIST 생체과학연구본부

Protease-activated receptor 2 (PAR2), a family of G-protein-coupled receptor, is activated by serine protease such as trypsin and tryptase and play a key role in inflammatory disease like arthritis and cancers. Many x-ray crystal structures of GPCR are reported, but PAR2 is still unknown. In order to design drug, homology models of PAR2 were generated by several crystal structures of GPCR as templates. Multiple templates were employed for sequence alignments according to identity, similarity and number of gap on transmembrane between template and target protein. And then, some models were picked for structure-based virtual screening by ROC score, enrichment factor and sensitivity. Although these models need more optimization steps, multiple templates-based homology models of PAR2 may be used as the structural basis for hit identification and lead optimization.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MEDI.P-1208**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Bio-evaluation of ^{68}Ga-labeled DOTA derivative as potential PET Probe for malignant melanoma

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한국원자력연구원 방사선기기연구부 [1]동국대 화학과

Radiolabeled benzamides have been reported to be attractive agents for targeted malignant melanoma as they bind melanin and display high melanoma accumulation. Herein, we report the synthesis and bioevaluation of a novel ^{68}Ga-labeled benzamide as a potential PET agent for malignant melanoma. ^{68}Ga-SCN-DOTA-PCA was synthesized with a radiochemical yield of ~80% and a radiochemical purity of >97% by analytical HPLC. The in vitro binding of ^{68}Ga-SCN-DOTA-PCA to melanin and its cellular uptake demonstrated the selective uptake in melanin. In addition, the biodistribution and micro?PET imaging of ^{68}Ga-SCN-DOTA-PCA in B16F10 tumor models showed the specific accumulation in melanoma. These results suggest that 68Ga-SCN-DOTA-PCA would be a promising agent for melanoma diagnosis.

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발표코드: **MEDI.P-1209**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological evaluation of bicyclic amide derivatives as DGAT1 inhibitors.

이귀빈 이덕형[1] 안진희[2]

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Acyl-CoA:diacylglycerol acyltransferase-1 (DGAT-1) catalyzes the final committed step in the biosynthesis of triglycerides. The inhibition of DGAT-1 may represent an attractive target for the treatment of obesity or type II diabetes. The systhesis and biological evaluation of bicyclic amide derivatives will be presented

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Efficient access to highly pure beta-amyloid peptide by optimized solid-phase synthesis.

최지원

연세대 생명공학과

Feasible and reproducible synthesis of full-length Aβ peptides has been one of the major challenges in Alzheimer's disease research. By using dimethyl sulfoxide as an anti-aggregation solvent and as an agent to promote double-coupling of two phenylalanines that frequently experience residual deletion, we developed a reliable manual Fmoc solid phase peptide synthesis procedure to produce biologically active Aβ in large quantities at relatively high purity. The amyloidogenic activity of the synthesized Aβ was confirmed via thioflavin T assay, transmission electron microscopic analysis and electrophoresis.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **MAT.P-1211**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Morphological Tuning of Ag_2O

김명진 진다혜 정혜윤 장승호 허영덕

단국대 화학과

Various shapes of Ag_2O microcrystals were prepared by a simple precipitation reaction from a mixture of $AgNO_3$, pyridine, and NaOH at room temperature. Their morphologies were controlled by adjusting the reactant concentrations. Morphology of Ag_2O microcrystals is affected by both crystal habit formation and branching growth. The branching growth occurred at higher NaOH concentrations, whereas crystal habit formation occurred by total reactant concentration.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **MAT.P-1212**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Chemical transformation of Two-dimensional Cu-terephthalate framework structure into low-dimensional $Cu(OH)_2$ and CuO nanostructures by the concept of lamellar nanoreactor

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서울시립대 교양교직부 교양화학실 [1]단국대 화학과

In recent, we report the template-directed synthetic strategy for 1D nanostructure using lamellar precursor based on the confined crystallization, which named for the lamellar nanoreactor synthesis. Here, we demonstrate the direct chemical transformation of Cu-terephthalate with two-dimensional framework structure into low-dimensional $Cu(OH)_2$ and CuO nanostructures along the NaOH treatments. Different NaOH treatment procedures lead to the different composition of $Cu(OH)_2$ and CuO morphologies. These chemical transformations were characterized by XRD, FT-IR, and SEM data. And the magnetic properties of the obtained products also will be discussed with the data obtained from SQUID and neutron powder diffraction (NPD).

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발표코드: **MAT.P-1213**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Printable Ultrathin Substrate Using Water-Soluble Polymer Sacrificial Underlayer with dimple array structure for Stick-and-Play System

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Stick-and-play electronics have drawn a lot of attention due to its versatility for unconventional ubiquitous devices such as electronic skins and bio-implantable equipment. In order to achieve such devices, developing ultrathin structures of the devices with thickness range, i.e. less than 100 um and formulating them into printable formats to enable sticker-type devices. Here, we demonstrate one of promising methods to enable fabrication such system by introducing water-soluble sacrificial layer with two-dimensional dimple arrays on a handling substrate. Topological confinement of the sacrificial layer inside or nearby the dimple structure provides controllability of the adhesion force gently to enable high yield of transfer printing without losing the alignment of a given pattern. Successful transfer-printing of diverse patterns of ultrathin substrates on PDMS slabs reveals versatility of this method to develop membrane-type electronics that can be attached on unusual surfaces.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development and applications of carbon gold silica composite materials

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Pyrolysis fuel oil (PFO) based pitches are thermoplastic in nature and have a high carbon yield, which is the main reason why they have been commonly used in carbon industries. Gold nanoparticles unified on various materials have produced great awareness in the field of catalysis, adsorption and material science. Presently, we developed nano carbon cages, carbon gold composite and carbon gold silica composite using template methods with nano silica ball, PFO and 1% $HAucl_4$ solution. The morphology and porous structure of the silica spheres were closely shaped in the consistent hollow cores of hierarchically carbon cage. Due to their easy fabrication protocols and broad potential applications, the hybrid nanocomposites materials are choosy for specific interests. The hybrid nanocomposites was combined the excellent physical and chemical properties of gold, carbon and silica foundation. The activity and selectivity of the composites for chemisorptions capacity and catalytic oxidation were studied with excellent selectivity and higher conversion respectively. The activity of carbon gold composite for solvent-free heterogeneous catalytic oxidation of a secondary alcohol revealed with excellent conversion. The composites were characterized by various physic-chemical techniques. Keywords: Adsorption, Carbon, Catalytic oxidation, Gold composite, Oxidation, Pyrolysis fuel oil

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile one-pot synthesis of silver nanomaterials through proton beam irradiation

송재희

순천대 화학과

A facile one-pot synthetic route is presented for the preparation of silver nanocrystals via a simple proton beam irradiation process at room temperature. Size and shape of the prepared silver nanostructures were controlled just by changing the stabilizing reagents and by controlling the molar ratios of stabilizer to silver ions. The size of the resulting Ag nanocrystals was observed to be easily varied by changing the stabilizer from hexadecyltrimethylammonium bromide to sodium dodecyl sulfate. The size of the prepared silver nanocrystals was also found to be decreased as the molar ratio of hexadecyltrimethylammonium bromide to silver ion was increased.

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발표코드: **MAT.P-1216**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of CNT-Ag nanoparticle composites via proton beam irradaiation

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순천대 화학과 [1]순천대 기초의.화학부

Carbon nanotubes (CNT) are attractive candidates due to their structural characteristics and promising electronic and mechanical properties for the use as nanomaterials and nanodevices. Composites of carbon nanotube with metal nanoparticles are particularly useful for use in catalysis, energy storage, and nanotechnology. Among them, CNT-Ag nanocomposites drew significant attention due to their potential applications as catalyst, and advanced materials. In this study, a new synthetic route to decorate carbon nanotube (MWCNT) with silver nanoparticles (Ag-NPs) is presented via a simple proton beam irradiation process at room temperature. The characterization of the MWCNT/Ag composites has been done by using FE-TEM and EDS analysis.

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발표코드: **MAT.P-1217**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Platinum Nano-network Structure Using AAO Membrane via Plasma Sputtering for Stretchable Electrode

장호영 조상현 장희정[1] 이지혜[1] 문정혁[1]

성균관대 에너지과학과 [1]성균관대 화학과

Stretchable Electronics has great potential for applications in unconventional electronics. In stretchable electronic devices, there are many structures. For example, wavy structure, mesh structure, and pop-up structures. In this presentation, Platinum nano-network structure is fabricated using Anodic Aluminum Oxide (AAO) structure for stretchable electronics. Anodic Aluminum Oxide (AAO) membrane is commonly used to many fields such as nanorod growth, SERS substrates, and insulating layers. First, Platinum plasma sputtered on top of the AAO. And then, PMMA and Silver coated on platinum deposited AAO. After AAO dissolution, this structure transfer on substrate. Wall thickness of platinum nano-network structure can be easily controlled by deposition time. Platinum nano-network structures show higher transmittance than platinum films. And we investigated resistance of platinum nano-network structures by 2probe measurement. When deposition time increased, conductivity increase and transmittance decreased. In comparison with platinum film, nano-network structure shows higher durability about stretchable test.

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발표분야: 재료화학

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Pd-Pt Alloy Nanotube Arrays as Three-Dimensional anodic Catalysts for Fuel Cells

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성균관대 에너지과학과 [1]성균관대 화학과 [2]성균관대 화학

Three-dimensional (3D) alloy nanotubes on a conductive substrate are promising catalysts for various chemical reactions because the properties of nanostructures highly depend on their shape, size, and composition. In this paper, we report a one-pot synthesis of uniform three-dimensional tubular nanostructures that consist of powerful catalytic components of Pd and Pt on gold substrate by using anodic aluminum oxide (AAO) as templates. By using this convenient approach, Pd-Pt alloy nanotubes (NTs) could be successfully prepared as well as Pd-Pt alloy nanorods (NRs) and their compositions were readily tuned by adding the molar ratio of the two metal precursors. Most importantly, these prepared Pd-Pt alloy NTs and NRs especially NTs exhibited the improved electrocatalytic activity and stability toward methanol/ethanol oxidation reaction than novel Pd and Pt nanorods.

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발표코드: **MAT.P-1219**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphene-Cyclodextrin Composites: Synthesis and Characterization

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Graphene came into research spotlight due to its wide range of applications such as electrodes, sensors, transistors and solar cells. It has outstanding physical properties, e.g., high surface area, high conductivity, low cost, and so on. β-cyclo-dextrin (CD) is a bucket-shaped cyclic glucose oligomer of 7 D-glucopyranosyl units connected by alpha-(1,4)-glycosidic linkages with an hydrophobic interior cavity and a hydrophilic exterior. CD is well known for its host-guest chemistry, as it can accommodate a number of guest molecules in its hydrophobic inner cavity. In this regard, we intended to prepare graphene-CD composites, thus merging the properties of graphene and those of CD for biomedical applications, which could act as a nanocarrier for various guest molecules such as drugs. We have adopted liquid phase processing of graphite using ultrasonication to exfoliate graphene in aqueous medium. In addition, we have also exfoliated graphene by using gold and silver nanoparticles prepared by using CD. The synthesized few-layer graphene dispersions were well dispersed in water and highly soluble over a long period of time. The graphene-CD composites were analyzed by UV-Vis, Raman, and infrared spectroscopy as well as transmission electron and atomic force microscopy.

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Urea pyrolysis route to mesoporous graphitic carbon nitride

양재훈 김가인 최진호

이화여대 화학.나노과학과

Recently, graphitic carbon nitride (g-C_3N_4) materials have received a great attention due to their various roles as a visible light harvesting photocatalyst, metal-free catalyst, reactive template, nitrogen source of nitridation reaction, etc. Generally, mesoporous g-C_3N_4 could be prepared by temperature-induced polymerization of cyanamide. In this study, we utilized a synthetic method to tailor the porous texture of graphitic carbon nitrides, including pore size, and specific surface area, by pyrolyzing the urea in the presence of silica nanoparticles. At first, urea-silica nanocomposites were prepared by mixing colloidal silica with different size in the range of 7 ~ 22 nm and urea, followed by evaporating the resulting mixture. Mesoporous g-C_3N_4 samples were prepared by calcinating urea-silica nanocomposite at ~ 500 ^oC for 4 hrs and removing the silica nanoparticles by using ammonium hydrogen fluoride. The formation of g-C_3N_4 was confirmed with the x-ray diffraction pattern showing the (002) peak at 27.4^o for graphitic interlayer stacking, and the (100) peak at 12.9^o for in-plane repeating unit in the x-ray diffraction patterns. According to N_2 adsorption-desorption analysis, the pore size of mesoporous carbon nitrides was similar to the size of colloidal silica which was used as hard template (7 ~ 22 nm). The analysis also revealed that the specific surface area of mesoporous g-C_3N_4 decreases with the size of silica nanoparticles, while the total pore volume of the carbon nitride increases with the size of silica nanoparticles.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric Detection of Hydrochloric Acid at 10 ppm by Electrostatic Attraction of Size-controlled Au Nanoparticles

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Hydrophobic gold nanoparticles have been synthesized in gram scale by reduction reaction of HAuCl4?4H2O in the solution containing 1,2-dichlorobenzene, oleylamine, and oleic acid. Controlling the volume ratio between oleylamine and oleic acid led to size change of 540 % of the nanoparticles from 10 nm to 54 nm. After phase transfer of the particles, the water-soluble Au particles were employed to colorimetric system for detection of hydrochloric acid in water. Consequently, the system showed color change of the gold-aqueous solution from the analyte of 10 ppm and also high selectivity among other acid and salt species. The careful investigation with changing one experimental parameter could demonstrate that the Au nanoparticles assembly and the consequent precipitate formation by electrostatic attraction is a decisive mechanism for color transition.

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종양세포 표지를 위한 엽산이 결합된 형광 금-실리카 나노 복합물질의 개발Development of folate conjugated fluorescent silica gold nanocomposites for labeling neoplastic cells

이준영 고성현 마야니 위샬 김상욱

동국대 신소재화학과

실리카와 금을 이용한 나노복합물은 의약 화학분야, 불균일 촉매분야 등에 다양하게 이용되어 왔으며, 쉽고 안정적인 제조 방법과 잠재적인 광범위한 이용으로 재료 과학 분야에서도 다양한 연구가 수행중이다. 금-실리카 나노복합물질의 우수한 화학적, 물리적 특성을 기반으로 이 복합물에 다양한 화학물질을 결합시킴으로써 다기능 하이브리드 나노복합물의 합성이 가능하다. 본 연구에서는 새로운 방법으로 엽산 (folic acid) 및 형광 (FITC) 물질이 결합된 다양한 크기의 실리카 금 나노 복합물을 합성 하였다. 엽산은 모든 세포기능에 필수적인 비타민으로 정상세포와 마찬가지로 암세포도 평균이상의 엽산을 필요로 하며, 가능한 많은 엽산을 이용하기 위해 어떤 암세포는 세포막에 수용체를 가지게 된다. 이러한 원리를 이용하기 위해 엽산수용체가 발현된 마우스 대장암세포 (CT-26)를 대상으로 하여 생물학적 평가를 수행하였고, 나노복합물질과의 친화력이 있음을 확인하였다. 본 나노복합물질은 향후 F-18 등과 같은 방사성동위원소를 표지 해 질병의 진단에 이용 할 수 있는 새로운 방사성 나노복합물질로 개발 될 수 있을 것으로 기대된다. 나노복합물질의 합성은 XRD, DLS, TEM, SEM, UV-Vis, Fluorescence Spectroscopy, ^{13}C CP MAS Solid State NMR 로 확인 하였고, CT-26 세포의 친화력 실험은 Confocal Lazer Scanning Microscopy 를 이용해 관찰하였다.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Transformation of pyrolysis fuel oil based pitch into metal incorporated composite carbon materials

마야니 수란자나 마야니 위샬 김상욱

동국대 신소재화학과

Mesoporous carbons (MC) have high surface area and pore volume, inert nature and easy regeneration properties, therefore widely used in adsorption, energy storage, super capacitors, and catalyst support. An innovative approach was carried out towards synthesis of mesoporous carbons using thermally modified pyrolysis fuel oil based pitch and nano silica ball as carbon precursors and pore generators. Copper, nickel, potassium and manganese were incorporated on mesoporous carbon material. The metal incorporated composite carbon materials are helpful in chemisorptions of different gases for energy conservation and reversing “green house” effect. The newly synthesized carbon materials were well characterized by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), thermo-gravimetric analysis (TGA), elemental analysis, inductive coupled plasma (ICP) and N_2 sorption isotherm analysis. Keywords: Adsorption, Mesoporous carbon, Nano silica ball, Pyrolysis fuel oil, Pitch

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장소: 부산BEXCO

발표코드: **MAT.P-1224**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of functional nanomaterial using matal oxide and silica금속 산화물과 실리카를 이용한 기능성 나노물질의 합성

고성현 이준영 마야니 수란자나 김상욱

동국대 신소재화학과

나노 사이즈의 금속 산화물은 열전도성, 전기전도성, 항균 효과, 광촉매능 등에 우수한 특성을 가지는데 그중 SnO_2 는 산화되어 견고한 산화막을 형성해 부착방지 효과가 뛰어나 방오페인트의 재료로 사용되고 ZnO_2 는 태양광 중에 적외선을 차단하여 냉난방 효율 증대 및 눈부심 방지에 효과가 있고 TiO_2 는 재료 고유의 광촉매능, UV 차폐능, 표면 자체 정화 효과가 있어 백색 페인트에 주로 사용된다. 금속 산화물은 나노 사이즈로 합성될 경우 응집되거나 산화 될 수 있는 단점을 가지므로 이를 극복하기 위해 금속산화물 외부를 실리카로 코팅하였다. 나노물질의 특징은 크기에 따라 다양하게 나타나므로 금속과 환원제의 다양한 조합을 통해 크기를 조절하는 방법을 연구 하였으며 전자현미경 (SEM, TEM 등) 으로 나노 금속 산화물의 크기와 합성 여부를 확인하였다. 향후 금속 산화물의 크기에 따른 항균, 항곰팡이 능력 등을 평가할 것이며 합성된 나노물질의 산업용 응용 가능성에 대해 연구해 보고자 한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1225**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Chromatography using mesoporous thin film as stationary phase.

최서영 권영욱

성균관대 화학과

Highly ordered mesoporous thin films are synthesized using evaporation induced self-assembly method with structure-directing agents and metal oxide precursors. These mesoporous thin films have repetitive pores and regular pore sizes. Mesoporous thin films with various wall materials and various pore sizes could be synthesized by changing several conditions and used as stationary phases in chromatography. In this research, PDMS channels are made using photoresist and these channels are attached on mesoporous thin films. In microfluidic channels, fluidic rates depend on interaction between interfaces. In case of this research, because we fabricated the microfluidic channels on mesoporous thin films, interactions between wall materials and fluidic materials determine the rates. The properties of mesoporous thin films such as pore size and wall material and the properties of fluidic material such as molecular size and charge will affect the fluidic rates.

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장소: 부산BEXCO

발표코드: **MAT.P-1226**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A thermally stable diimide derivative as an organic electron-injecting material for organic light-emitting devices

이혜나

경북대 화학공학과

Organic light-emitting devices (OLEDs) have been extensively studied for the last two decades. Since 1997, small size OLED displays have been commercialized for use in mobile phones, MP3 players, smart pads, etc. However, large-size OLED displays for monitors and televisions are still under development because of immature technology for effective heat-sinking control and large-area coating, lifetime/stability, etc. Of these various issues the stability/lifetime of organic materials that consist of key parts in the large-size OLED system is one of the last hurdles to overcome. In order to achieve this goal, the unstable organic-inorganic interfaces should be reconsidered. In this regard, we synthesized new diimide materials that have a rigid aromatic ring in the center unit as well as an electron-deficient phenanthroline unit. These materials have been applied as an organic electron-injecting material in OLEDs. The detailed results will be discussed by combining materials aspect and device performances.

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장소: 부산BEXCO

발표코드: **MAT.P-1227**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polydopamine Formation Shares Two Pathways: Non-covalent Self-assembly and Covalent Oxidative Polymerization

홍선기 김우연 이해신

KAIST 화학과

Polydopamine coating is an emerging method to control surface properties of materials, which was inspired by the adhesive properties of marine mussels. Although it has been widely used for the modification of biomaterials and medical devices, the mechanism of dopamine polymerization is not yet clearly demonstrated. Covalent, oxidative polymerization via 5,6-dihydrxoyindole (DHI) similar to the mechanism proposed in synthetic melanin synthesis has been the only clue. Here, in contrast to the widespread understanding of covalent polymerization, we report that a physical trimer of (dopamine)2/DHI is the main intermediate during polydopamine formation. We also found that the dopamine was tightly bound, barely escaped from the polydopamine complex explaining previously reported in vitro and in vivo compatibility. Our study reveals a different picture of polydopamine formation in which it is formed in part by self-assembly of dopamine and DHI, suggesting a new clue to understand melanin structures.

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장소: 부산BEXCO

발표코드: **MAT.P-1228**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation, characterization and photocatalytic activity of ZnO-decorated carbon nanotubes

김유현 최현철

전남대 화학과

Recently, photocatalysis method has played an important role in the environmental procedures such as air purification, water disinfection and purification. Among the various semiconductors applied, zinc oxide (ZnO) has been employed in photocatalytic method to decompose many organic pollutants under ultraviolet light irradiation. In this work, we demonstrate a novel and simple method for the synthesis of CNT-ZnO hybrid materials. The prepared CNT-ZnO was characterized by X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM), which have indicated uniform hybrid structure of 2.9 nm diameter ZnO decorated on MWCNT surface. The photocatalytic activity of CNT-ZnO was tested by methylene blue degradation process under ultraviolet light irradiation. The results showed that CNT-ZnO displayed much higher photocatalytic activity than that of pure ZnO. In addition, CNT-ZnO exhibited excellent stability in the photocatalytic process.

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장소: 부산BEXCO

발표코드: **MAT.P-1229**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic oxidation of hydrazine on Pd-decorated graphene.

김지당 최현철

전남대 화학과

Graphene is one of the most exciting materials today. Graphene, by definition, is a single-layer, two-dimensional material. Recently, graphene has extensively studied as catalyst supports in both heterogeneous catalysis and electrocatalysis, due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. In this study, we prepared Pd-decorated graphene by introducing thiol groups on graphene surfaces. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and scanning electron microscope (SEM). The Pd-decorated graphene exhibits higher activity in electrochemical reactions of hydrazine oxidation than that of the reference systems. This synthetic approach should be broadly applicable for preparing graphene-supported metal catalysts and markedly improves the catalytic activity.

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장소: 부산BEXCO

발표코드: **MAT.P-1230**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation & electrochemical characteristic of Pt-decorated graphene.

김지당 최현철

전남대 화학과

Graphene is a two-dimensional material with a single atomic layer of carbon atoms arranged in a hexagonal lattice. Due to its unique structure, graphene exhibits unusual optical and electronic properties. In this study, we prepared Pt-decorated graphene by introducing thiol groups on graphene surfaces. Surface thiolation is an effective way to obtain dispersed metal nanoparticles on the surface of graphene. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and Transmission electron microscopy (TEM). Electrochemical characteristic of methanol oxidation is also investigated via Cyclic voltammetry (CV) measurement.

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장소: 부산BEXCO

발표코드: **MAT.P-1231**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mesoporous gallium oxide-platinum nanocomposite thin films for CO-poison free methanol oxidation electrocatalyst

홍정은 권영욱

성균관대 화학과

we synthesized mesoporous Ga2O3 thin films (MGTFs) by using a non ionic surfactant (F127) as a structure directing agent and investigated their applications.Nevertheless none of the previously reported the mesoporous Ga2O3 has a thin film structure. We can control the film thicknesses in the range of 40 ? 340 nm depending on the composition of gallium source (GaN3O9) and F127 of the coating solution. Mesostructural studies of the products were carried out by transmission electron microscopy (TEM) and Scanning electron microscopy (SEM). The elemental composition was determined by X-ray photoelectron spectroscopy (XPS). For electro-oxidation of methanol, we prepared Pt-MGTFs from the electrodeposition of Pt into the pores of MGTFs. We confirm that Pt-MGTFs increased catalytic activity and was not poisoned by CO because MGTFs could adsorb CO and oxidized CO to CO2, while Pt replica removed MGTFs by HF solution show CO poisoning. Hence, we demonstrated that MGTFs could be used as a co-catalyst for the electro-oxidation of methanol on Pt.

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장소: 부산BEXCO

발표코드: **MAT.P-1232**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photoresponsive Covalent Metal-Organic Network Material by Molecular Layer Deposition from Titaniumchloride and Hydroquinone

한규석 성명모

한양대 화학과

We demonstrated covalent metal-organic networks using molecular layer deposition. Titanium chloride and hydroquinone were used as precursors to deposit the covalent metal-organic films named titanium aryloxide (Ti-AO). UV-VIS spectroscopy showed new emerging peak due to ligand metal charge transfer (LMCT). Infrared spectroscopic and X-ray photoelectron spectroscopy were invited to determine the chemical composition. Photo transistor was fabricated adopting Ti-AO and ZnO with nanohybrid superlattice structure thin film as active layer. The fabricated photo transistor exhibited good photo sensitivity and responsivity compared with ZnO transistor.

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장소: 부산BEXCO

발표코드: **MAT.P-1233**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and properties of halogen doped graphene nanosheets via ball milling

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We reported new method to make graphene nanosheets (GNs) which is very simply, eco-friendly and economic. Using this method, we have first achieved a high yield of edge-selectively halogen doped graphite (EHG) by a simple ball milling of pristine graphite in the presence of halogen materials such as Cl2, Br2 and I2. We have confirmed that graphene nanosheets were well doped with halogen elements by using XPS, SEM, TEM and EDAX. Besides, we also showed that it was possible for graphene to be doped with other various materials by using ball milling method. The resultant EHG displayed to have very high surface area and highly dispersion into various solvents. And also, EHG had outstanding electrocatalytic activity for oxygen reduction reaction (ORR).

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장소: 부산BEXCO

발표코드: **MAT.P-1234**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Edge-functionalized graphene nanoplatelets as catalysts for oxygen reduction reaction

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울산과학기술대 친환경에너지공학부 [1]울산과학기술대 에너지공학부

Edge-functionalized graphene nanoplatelets were simply prepared by eco-friendly method via ball milling in the presence of hydrogen, carbon dioxide, sulfur trioxide and carbon dioxide/sulfur trioxide mixture. The resultant hydrogen- (HGnP), carboxylic acid (CGnP), sulfonic acid (SGnP) and carbocylic acid/sulfonic acid (CSGnP) functionalized graphene nanplatelets were studied with TEM and SEM, EA, EDX, FT-IR, TGA, and XPS. The electrocatalysis of the oxygen reduction reaction (ORR) on HGnP, CGnP, SGnP and CSGnP were evaluated in 0.1 M KOH by cyclic voltammetry and rotating disk electrode system. The electrocatalytic activity is in the order of SGnP > CSGnP > CGnP > HGnP > pristine graphite, suggesting that the efficiency of oxygen reduction reaction (ORR) is significantly attributable to the edge nature of graphitic structure. These results indicated that electrocatalytic activities follow well the polarity, indicating diffusion control also plays an important role.

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장소: 부산BEXCO

발표코드: **MAT.P-1235**

발표분야: 재료화학

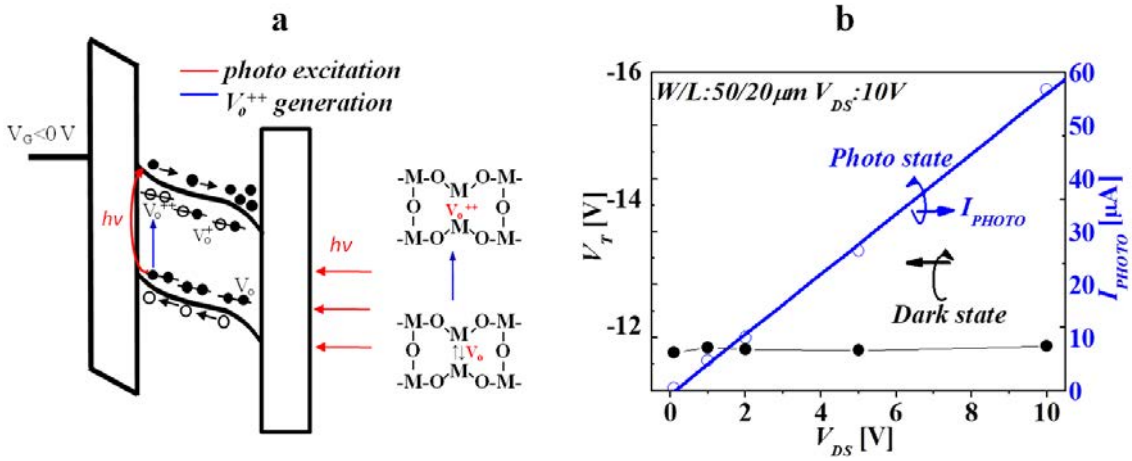
발표종류: 포스터, 발표일시: 수 16:00~19:00

The photo-sensor device utilizing InZnO thin film transistor

박서경 박성호 채원석 한만소

대진대 화학과

We demonstrate a marked photosensitivity of amorphous InZnO (IZO) thin film transistor (TFT), where the active channel is passivated with SiO2. The illumination yields an increase in the off-current rather than a negative shift of the threshold voltage, and thus photosensitivity(IPhoto/IDark) can be maximized by adjusting a reading bias. In addition, it was significantly influenced by the active thickness, device dimension and operation condition. In particular, for 1500?-thick IZO TFT, the IPhoto/IDark was increased to nearly 8 orders of magnitude. The photo induced Vo++ generation in the active semiconductor screens the gate field and it causes the current flow at back-channel of IZO TFT.



일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1236**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyelectrolyte/Graphene Composites as Metal-Free Electrocatalyst for Oxygen Reduction Reaction

김민정 전인엽 백종범[1]

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Graphene is one-atom thick two-dimensional atomic crystal having sp2 carbon atoms in the honeycomb crystal lattice. It has unique physical properties such as high carrier mobility, mechanical strength, elasticity, superior thermal conductivity and Young's modulus. Heteroatom-doped graphene has demonstrated high electrocatalytic activity as metal-free cathode in fuel cell (FC), which is an electrochemical cell that converts chemical energy into electric energy. However, the syntheses of heteroatom-doped graphene involve tedious procedures and harsh conditions. Hence, to replace existing precious metal-based FC catalysts, we study poly(pyridinium salt)/graphene (PSS/G) composites as a low cost and high performance metal-free electrocatalysts for oxygen reduction reaction (ORR) in FC. The PPS can play as not only dispersing agent for graphite into graphene by π-π interactions with graphitic layers, but also intermolecular charge transfer agent with high electrochemical stability to facilitate efficient ORR.

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장소: 부산BEXCO

발표코드: **MAT.P-1237**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Diels-Alder Reaction of Graphite in the Presence of Maleic Anhydride via Ball-Milling

서정민 전인엽 백종범[1]

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Since the first experimental observation in 2004, graphene has been attracted a lot of attention due to its outstanding properties such as high transparency, high electron and hole mobility, and so on. In particular, graphene shows ballistic charge transport, making it to be an ideal material for electronic devices. Despite of the characteristics of high mobility, graphene has limitations for using in electronics due to a vanishing band-gap. There are several attempts to open band-gap of graphene including graphene nanoribbon, bilayer graphene and functionalization of graphene. All these approaches do not resolve fundamental problems. Here, we reported edge-selective functionalization of graphite with maleic anhydride via Diels-Alder reaction to open band-gap. The process involves a very simple mechanochemical reaction in ball-milling apparatus in solid state. Edge-functionalized graphene can be efficiently afforded by dispersing in polar solvents.

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발표코드: **MAT.P-1238**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Graphene nanoplatelets with edge-chloride prepared *via* ball milling

정선민 전인엽 백종범[1]

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Graphene is one layer of graphite composed of sp_2 carbon bond, having one-atom thick flat honeycomb lattice. Graphene is one of the most promising materials for various applications due to its outstanding properties such as good electric conductivity, thermal conductivity, high electron mobility and mechanical strength. It has been spotlighted to make carboxylated graphene nanoplatelets *via* ball milling production, because of simplicity and scalability. Applying ball milling method, edge-functionalization of graphite with carbon tetrachloride was achieved. Multiplicity of chloride substitution reaction is expected to make edge-chlorinated graphene nanoplatelets to be useful in many applications. We report a number of properties of edge-chlorinated graphene nanoplatelets.

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장소: 부산BEXCO

발표코드: **MAT.P-1239**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

With Stability and Dispersibility silica photosensitizers nanoparticle

송미령 김준성 박수진 정민숙

(주)바이테리얼즈 부설연구소

Photodynamic therapy (PDT) is a novel treatment modality, which produces local tissue necrosis with laser light.But, to date, most of the available photosensitizing agent is insoluble in water and photobleaching. To overcome these problems, various polymers conjugated for photosensitizing agent have been investigated. This polymer conjugated has provided high solubility of photosensitizing agent in aqueous solution. However, most polymer conjugated do not provided photo stability.In this report, we capsulated photosensitizing agent by silica for provide solubility and stability.

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장소: 부산BEXCO

발표코드: **MAT.P-1240**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile and Fast Synthesis of Flower-like ZnO Nanostructures

PARTHIBAN 김진권

공주대 화학과 및 GETRC

Nanostructured zinc oxide (ZnO) an exceptionally important semiconductor materials to study due to its attractive physical properties such as wide band gap (3.37 eV) and large exciton binding energy (60 meV) at room temperature. Because of its unique optical and electrical properties it has potential applications in UV lasers, light-emitting diodes (LED), field-effect transistors, solar cells, and sensors . The tremendous interest in ZnO is due to its unique ability of possessing structure-dependent properties. Therefore, the design and synthesis of ZnO nanomaterials with different structures are very important. Herein we report a fast and facile method to synthesis flower-like ZnO nanostructures at room temperature without using any capping agent. The products were characterized by field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD) and transmission electron microscopy (TEM) Raman and Photoluminescence studies.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1241**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Synthesis of SnO_2 Nanotubes using Selenium Nanowires as Templates

김정수 **PARTHIBAN** 김진권

공주대 화학과 및 GETRC

One-dimensional (1D) nanostructures have been the focus of intensive research because they provide an ideal system to investigate the dimensionality and size dependence of the electrical and optical properties of nanomaterials. As an n-type wide-bandgap semiconductor (Eg = 3.6 eV), SnO_2 is one of the most intensively studied materials owing to its technologically important applications such as gas sensors anode materials in lithium rechargeable batteries and solar cells. Herein we report the facile synthesis of SnO_2 nanotubes using selenium nanowires as template. First Se NWs with uniform lengths and diameters were prepared in water and these nanowires are used as templates to synthesize SnO_2 nanotubes with preserved morphologies via a simple hydrothermal route. The as synthesized nanotubes are well characterized by SEM, TEM, EDS and XRD.

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장소: 부산BEXCO

발표코드: **MAT.P-1242**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Single Source Precursors for Sb2Te3

LIRICHENG 김진권

공주대 화학과 및 GETRC

Antimony tellurides (Sb2Te3), which belong to the layered semiconductors with tetradymite structure are promising candidates for near room-temperature thermoelectric applications due to their high zT values in the temperature range of 300?500 K. Antimony telluride nanostructures with well-de?ned morphologies can be synthesized by gas phase processes such as chemical vapor deposition and vapor transport growth, as well as in solution by hydrothermal processes. Herein we report the synthesis of novel single source precursors for the preparation of Sb2Te3 nanoplates. Decomposition of these precursors in oleylamine at 250 ℃ gives uniform nanoplates. The as synthesized nanoplates are characterized by XRD, SEM and TEM.

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장소: 부산BEXCO

발표코드: **MAT.P-1243**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

인쇄 전자용 전극 재료를 위한 구리염과 아민 리간드의 착화합물 연구

김신희 황재은 김홍두

경희대 정보전자신소재공학

공기 중에서 안정하며 낮은 온도에서 공정이 가능한 구리염과 아민 리간드의 착화합물은 진한 청색을 띠며, 150 ℃에서 완전히 구리로 분해되고 14.4 wt%의 구리함량을 가진다. 이 착화합물은 구리의 벌크 저항(1.68 μΩ?cm)에 가까운 1.84 μΩ?cm 을 나타내며 높은 점도를 가진다. 하지만 열처리 시, 온도 상승으로 인해 점도가 급격히 떨어져 패턴 고정을 방해하고 접착성이 떨어지는 성질을 보여 첨가제를 넣어 이를 개선하고자 하였다. 첨가제가 들어간 구리 잉크는 27.4 ~ 18.5 μΩ?cm 정도의 비저항값을 나타내며, 패턴이 고정되며 박리가 발생하지 않아 이를 이용한 인쇄전자용 전극으로 사용될 수 있음을 보였다.

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Effects of a pre-thermal treatment on PbS quantum dots for photovoltaic devices with improved fill-factor, efficiency, and air stability

최민재 정연식

KAIST 신소재공학과

Colloidal quantum dot photovoltaics (CQD PVs) are of great interest due to their cost-effectiveness and solution-based processability. However, the relatively low power conversion efficiency (PCE) of CQD PVs has been an important issue. We employed a simple pre-thermal treatment on PbS quantum dot (QD) films prior to metal electrode deposition. It significantly enhances a fill factor up to ~ 60% and improved the capability of PCE retention in ambient condition. Highly monodisperse (average diameter ~ 3.5 nm) PbS QDs with a first excitonic peak at ~ 900 nm were synthesized with an organometallic method and schottky-junction-based CQD PVs were fabricated via the layer-by-layer spin-coating of the PbS QDs, followed by metal electrode deposition. The device, with a 160-nm-thick QD layer, exhibited a PCE of 1.82% under AM1.5G illumination. Interestingly, a short thermal treatment significantly improved both fill factor and air stability. The best results showed increases of fill factor and PCE by ~50% and ~35%, respectively, compared to the device without thermal treatment. To analyze this phenomenon, X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM) analyses and current-voltage measurements were performed. We found that the improvements of device characteristics are due to the formation of thin oxygen compounds such as PbSO3 and PbSO4 at the outer shell of the QDs. These results suggest a simple, but effective processing strategy to overcome the reliability issues of CQD PVs.

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A new bottom-up approach to fabricate size-controlled graphene quantum dots over large area using self-assembled silica nanostructures

김경호 박운익[1] 정연식

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Size-controllable graphene quantum dot (GQD) structures over large area have attracted interests due to their quantum optical and electronic properties. So far, most researches for fabricating GQDs have been performed based on conventional top-down lithography to pattern graphene reduced from graphene oxide, which is difficult to control the size of GQDs and to decrease size distribution. As a new approach to resolve this issue, we introduce a novel methodology for GQD fabrication by using the self-assembly of diblock copolymers. In this study, we used a diblock copolymer of poly(styrene-b-dimethylsiloxane) because this polymer shows excellent etch selectivity, uniformity in size, small size distribution. Moreover, the self-assembled morphology can easily be converted to silica nanostructures, which serve as a useful etch mask for patterning underlying graphene layers prepared by chemical vapor deposition. Electron microscopy techniques were used to analyze the sizes of silica nanostructures as well as GQDs. Raman and photoluminescence (PL) analyses were performed after each patterning step to investigate their effects on the optical properties of GQDs. In the PL measurement, the emission peak of GQDs on the SiO2 substrate was shown at ~395 nm. Furthermore, oxygen contents in GQDs were controlled by air plasma treatment, and the effect of oxygen contents on PL property was analyzed in detail.

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Fabrication of Iron Oxide Nanoleaf via Electrostatic Anodization for Immobilized Fenton-like Process

장준원 김혜란 김령주 박재우[1]

한양대 건설환경공학과 [1]한양대 토목공학과

Iron oxide nanotubes (INTs) were fabricated with potentiostatic anodization of iron foil in 1M Na2SO4 containing 0.5 wt% NH4F electrolyte, holding the potential at 20, 40 and 60 V for 20 min, respectively. Field Emission Scanning Electron Microscopy (FE-SEM) and X-ray Diffractometer (XRD) were used to evaluate the morphology and crystalline structure of the INT film. From the attained results, the potential of 40 V for 20 min was observed to be sufficient to produce an optimal catalytic film. Cyanide dissolved in water was degraded through the Fenton-like reaction using INT film with hydrogen peroxide. In case of INT-40V in the presence of H2O2 3 %, the first-order rate constant was found to be 1.7 × 10-2 min-1, and indicated to be 1.2 × 10-2 min-1 on commercial magnetite powder. Therefore, this process proposed in this work can be an excellent alternative to the traditional catalyst for Fenton-like reaction.

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3-Dimensionally ordered macroporous plasmonic metal skeletons by electrochemical routes

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한국기초과학지원연구원 강릉센터

Plasmonic metal nanomaterials are of great interest in the fundamental and applied sciences due to tunable visible light absorption, localized electric fields enhancement, ultrasensitive molecular sensing efficiency, and enhanced fluorescence. Recently, porous plasmonic metal nanomaterials have been synthesized and applied to study localized field-enhanced molecular sensing and fluorescence behaviors. In this study, we have prepared 3-dimensionally ordered macroporous (3DOM) plasmonic metal (Au, Ag, AuAg) skeletons by electrochemical deposition using polystyrene synthetic opal as structure-guiding templates. Pulsed routings of electrochemical deposition is useful to fabricate 3DOM skeletons minimizing template delamination from gold substrates. The resulting 3DOM skeletons were characterized using SEM, TEM, absorption microscope, and fluorescence lifetime imaging microscope.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Multisegment Metal Nanowires and Near-field Spectroscopic Study on Their Surface Plasmons

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조선대 화학과 [1]Institute for Molecular Science

Surface Plasmons (SPs) have attracted increasing attention for past decade, because of their basic scientific interest and potential applications in a variety of fields, such as a tool for diagnosis, sensor, and plasmonic devices. In the previous studies, detailed properties of SPs had been discussed only for nanostructures consisting of single material. Recently, multi-component systems such as core-shell structures have been studied, because some of multi-component structures show not only simple addition of their functions but also new interesting properties. In this study, we prepared multicomponent structures of nanowire (35 ? 5 nm in diameter and 650 ? 50 nm in total length) consisted of Au-Ni-Au using anodized aluminum oxide templates, and successfully dispersed onto surfaces of cover glasses for scanning near-field optical microscope (SNOM) and scanning electron micrograph (SEM) measurements. We are now measuring near-field optical images of nanowires and analyzing the result.

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

저온 소성이 가능한 reverse-offset printing용 silver nano-ink 제조 및 성질

김경영 공명선

단국대 나노바이오의과학과

인쇄전자 기술은 차세대 전자소자 제작 공정으로서 저가, 대량생산, 친환경 공법의 장점을 가지고 있으며 최근 TFT, 디스플레이, 바이오, 에너지 소자 등 다양한 분야에서 개발이 진행 되고 있다. 특히 Reverse offset printing 공정은 대면적 패턴 형성이 가능하고 미세 패턴구현에 이점을 가진 프린팅 공정 기법이다. 기존의 포토리소그라피(photolithography)에 의한 패턴형성 공정에 비하여, 인쇄전자 기술은 액체 상태에서 인쇄 가능한 소재들을 사용한다. 특히 이런 소재는 나노 기술의 발전과 접목되어 다양한 나노 입자 등을 함유한 기능성 잉크 소재로 개발이 진행되고 있다. 본 연구에서는 reverse-offset printing 공정에 적합하고, 저온 소성이 가능한 전도성 silver nano-ink 를 제조하였다. 은 나노입자의 전구체로 silver 2-ethylhexyl carbamate complex 에 수소 환원법을 이용하였으며 안정제로는 Polyvinylpyrrolidone 을 사용하여 silver nanoparticles (Ag NPs)를 제조하였다. 이렇게 제조된 Ag NPs 에 습윤 분산제를 첨가하고, binder 및 유기 용제을 혼합하여 Siver nano-ink 을 제작하였다. Siver nano-ink 의 분산 및 저장안정성, 비저항, blanket 과의 호환성 및 전이-전사력, 표면 morphology 등을 TEM, SEM, TGA, XRD, Zetasizer 을 이용하여 분석 확인 하였다.

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Synthesis of ZnO nanoparticles with controlled shapes and sizes using one-pot thermal reduction method

김경아 차재령 공명선

단국대 나노바이오의과학과

ZnO has been one of the most promising materials for electrical devices, including transparent conductive films, light emitting diodes and photocatalyst. Unfortunately, because aggregation of ZnO nanoparticles (NPs) occur well, low dispersibility has been limited to the use. In this study, ZnO NPs enhanced dispersibility were prepared using one-pot thermal reduction method. Zn(Ⅱ) isobutylcarbamate was used as a precursor of ZnO. ZnO NPs dispersions were prepared by varying the concentration of the precursors and the amount of polyvinylpyrrolidone as a stabilizer to control the shape and size of ZnO NPs. The formation of ZnO NPs were confirmed by the UV-vis, scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD) and energy dispersive X-ray spectroscope (EDS).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Humidity Sensors based on grephene/polyelectrolyte composite materials and their Properties

차재령 공명선

단국대 나노바이오의과학과

Polymeric humidity sensor using varying nature of water adsorption and desorption on the electrical properties of the conductive polymer can be used in the area of fast response time and wide humidity. Currently polyelectrolyte has a small problem in a durable, because it contain quaternary ammonium salts and high humidity in the dissociated or swelling up repeatedly. In this study, conventional polymer electrolytes and grephene composite material made good electrical conductivity sensors were fabricated. Characteristics as temperature dependency, hysteresis, frequency dependence and response rate were investigated as a humidity sensor using humid temperature chamber and impedance analyzer.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Ag nanoparticles with controlled sizes on graphene seets using microwave reduction method and their properties

윤상우 차재령[1] 공명선[1]

단국대 화학과 [1]단국대 나노바이오의과학과

Graphene is a monolayer of carbon atoms that are tightly packed into a two-dimensional, honeycomb crystal structure. This extremely thin nanomaterial has shown fascinating properties and holds the promise for future carbon-based device architectures, owing to characteristics such as high mechanical stiffness, extraordinary electronic transport properties and excellent antibacterial activity. So we consider that if nanoparticles with high electric conductivity such as silver were deposited onto the graphene sheets, graphene sheets with good dispersity and conductivity could be maintained.In this work, Ag nanoparticles with controlled sizes were deposited on graphene sheets by microwave reduction method. Ag-graphene nanocomposites were dispersed in hydrophobic solvents after treatment of 1-dodecanethiol. The successful synthesis of the Ag-graphene nanocomposites was confirmed by SEM, TEM, EDS and XRD and dispersion stability was determined by Uv-vis.

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Electrodeposition of PbSe in Mesoporous Thin Films for the Near-IR Abosorption Materials

이기림 홍정은 권영욱

성균관대 화학과

PbSe is a IV-VI semiconductor material having a narrow band gap (Eg = 0.278 eV for bulk PbSe) that has near infrared absorption ability. Therefore, this material is or interest for near infrared detectors, biomolecule imaging sensors, photovoltaic devices and thermoelectric materials. We deposited PbSe in mesopores of mesoporosu silica thin films using electrodeposition method. As the working electrode, mesoporous silica thin films (MSTFs) were synthesized by spin-coating precursor solutions composed of tetraethylorthosilicate (TEOS), non-ionic surfactant F-127 ((EO)106(PO)70(EO)106, EO = ethylene oxide, PO = propylene oxide), absolute ethanol, and HCl in water, followed by aging and calcination. PbSe nanostructed films were obtained by electrodeposition of the PbSe precursor solution into pores of MSTFs at the potential range of -0.4 and -0.5 V for Pt substrate and FTO substrate, respectively and removing MSTFs. Electrodeposited PbSe nanostructured films were composed of polycrystalline PbSe and had a stoichiometric elemental ratio, near infrared absorption and fluorescence ability.

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Biodegradable Polyurethanes Containing Isosorbide and Polycaprolactone: Physical Properties and Biocompatibility.

박형석 공명선

단국대 나노바이오의과학과

Biocompatible and biodegradable polyurethanes were prepared with fixed aliphatic diisocyanate level and varying ratios of isosorbide, and PCL diol via a simple one-shot polymerization without a catalyst. The successful synthesis of the polyurethanes was confirmed by gel permeation chromatography, 1H-nuclear magnetic resonance and Fourier transform-infrared spectroscopies and the thermal properties were determined by differential scanning calorimetry and showed glass transition temperatures of around 30-35oC. The degradation tests were performed at 37oC in phosphate buffer solution (approx. pH 7.3) and showed a mass loss of around 5 % after 12 weeks, except for the polymer with the highest isosorbide content which showed an initial rapid mass loss. The in vitro cytocompatibility test results following culture of osteoblasts on the polymer surface showed that relative cell number on all of the polyurethane films after 5 days of cultured on polymer films was lower compared to proliferation rate on the optimized tissue culture plastic. These polymers offer significant promise due to the simplicity of the synthesis and the controlled degradation.

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Metal Nanoparticle-Based pH Indicators in High Alkaline Region

임종국 정병규

조선대 화학과

Since the pH is very important property which determines performance of systems, measurement of pH is frequently conducted in everywhere around us, such as hospital, factory, laboratory, and so on. The change of pH in a system can be monitored using a pH indicator in a wide range of pH spanning 0 to 14. However, only a few pH indicators are known to have working range in high alkaline region between pH 11 ~ 14. Since most of pH indicators working in high alkaline region are made of organic molecules that have complex molecular structure, these indicators can be easily destroyed at high temperature or under intense ultraviolet light, and their price is quite expensive. In addition, some of indicators are biologically poisonous or explosive in ambient conditions. In here, we propose that metal nanoparticles (e.g. Au, Ag, and Cu) can be used as a pH indicator in high alkaline region. Each nanoparticle shows different working pH range depending on the size, the reducing agent, and the materials of nanoparticles. The difference of working pH range is explained as destabilization of nanoparticles and their aggregation property.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Hierarchically Structured Functionalizable Mesoporous PEDOT-Derived Materials

홍진연 황용경[1] 허성

한국외국어대 화학과 [1]금호석유화학(주) 고무TS팀

Shape-controlled poly(3,4-ethylenedioxythiophene), or PEDOT, was shown to display shape-dependent electrical conductivities. Compared with PEDOT, the morphology control of polyanilines (PANIs) have been intensively studied. The interfacially polymerized PANI nanofibers showed a Brunauer-Emmett-Teller (BET) surface area up to 54.6 m^2 g^{-1}. Thus far, however, the morphology control of functionalizable PEDOT/PSS derivatives with high surface area has not yet been achieved, where PSS is poly(4-styrenesulfonic acid). The development of a new preparation method for these functional conductive materials is expected to provide opportunities for diverse applications based on PEDOT-derived polymeric materials. In this presentation, chemically functionalizable carboxy group-containing mesoporous PEDOT derivatives, C1-CT/PEDOT/PSS and C4-CT/PEDOT/PSS, with hierarchical particle morphology were prepared in the presence of the sacrificial acid-labile $ZnO/Zn(OH)_2$ hard template. The hard template could be effectively removed by acid etching. The electrical properties and surface texture of the mesoporous PEDOT derivatives were investigated. The chemical accessibility of the carboxy group in the PEDOT derivatives was demonstrated by conjugation with green fluorescent 5-aminofluorescein (AFL). AFL-conjugated AFL-C4-CT/PEDOT/PSS particles exhibited uniform green fluorescence under a fluorescence microscope.

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발표분야: 재료화학

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Liquid Crystalline Molecule of Bent-core type with Sulfur unit and Acryloyl Derivative : Synthesis and Physical Properties

김두헌 송호준 문두경

건국대 신소재공학과

We propose advanced film patterned retarder (FPR) through reactive crystal materials using UV curable reactive mesogen (RM). Reactive Mesogen (RM) solutions can either be coated onto flexible plastic substrates by a roll-to-roll coating process, or used to inside the display to form incell optical elements, either as patterned or monolithic retarders. It has been known that achiral banana-shaped(bent-core) molecules may form polar smetic layers with ferroelectric or antiferroelectric behavior. In this study, we synthesized the novel bent-core molecule based on sulfur unit and acryloyl derivatives. Bent-core molecule was investigated physical and optical properties.Keywords: bent-core molecule, sulfur unit, liquid crystal, compensation film

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High photocatalytic activity of 3-dimesional mesoporous TiO2 inverse opal under UV irradiation

QUAN LINA 장윤희 장유진 김동하

이화여대 화학나노과학과

TiO2 has been recognized as representative semiconducting metal oxide material with excellent photocatalytic activity due to its good stability, nontoxicity, and UV absorbance. In this work, enhanced photocatalytic efficiency under UV light irradiation was achieved by structuring a mesoporous TiO2 inverse opal nanostructures. The mesoporous TiO2 inverse opals were fabricated by using polystyrene beads and amphiphilic triblock copolymer as templates and sol-gel infiltration method. The photodegradation of 4-nitrophenol was chosen to evaluate the photocatalytic activity of thus-obtained samples. 4-nitrophenol is considered one of the most refractory substances present in industrial wastewaters because of their high stability and solubility in water. The purpose of this study is to investigate the enhanced photocatalytic degradation of 4-nitrophenols by optimizing TiO2 morphology. Concretely, the photocatalytic activity of three different types of TiO2 inverse opals were compared to find an optimized nanostructured photocatalyst.

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Synthesis of Germanium sulfide and Tin sulfide nanoparticles by laser ablation and their Electrochemical Application

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Laser ablation of Germanium sulfide and Tin sulfide nanoparticles synthesis by gas-source has been performed using a Nd:YAG laser in a vacuum. The NPs were synthesized by the photolysis of a tetramethyl germanium/hydrogen sulfide and tetramethyl tin/ hydrogen sulfide gas mixture, respectively. The as-grown NPs are sheathed with thin (1-2 nm) carbon layers. 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), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Both Germanium sulfide and Tin sulfide exhibit excellent cycling performance and high capacity of the lithium ion battery as promising anode materials for the development of high-performance lithium batteries.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1260**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid State Reactions of Carbamates with Aldehydes to Form Imines

임병욱 이병노 이규형 최종명 허남회

서강대 화학과

A wide range of solid carbamates were prepared from the reactions of liquid amines with supercritical CO_2, which were isolated as white crystalline solids in yields greater than 97%. The resulting carbamates are free of smell and are easy to handle in the lab. They turned out to be novel solid alternatives for toxic liquid amines. We found that solid-state grindings of carbamates and aldehydes yielded imines as the sole products in yields greater than 97%. Moreover, the solid state reactions showed higher selectivity than conventional solution-based synthesis. The grinding methodology also exhibited the possibility of large-scale production of organic solids with a very small vessel, which could thus be utilized for industrial applications. We will present newly developed solid carbamates as well as their solid state reactivities towards aldehydes.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1261**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Sonochemical Synthesis of Pd-Mn (M = Ni, Co, Fe and Mn) Nanoparticles for the Electrooxidation of Formic Acid

Matin Md Abdul 권영욱

성균관대 화학과

The bimetallic Pd-M (M = Ni, Co, Fe and Mn) nanoparticles (NPs) were synthesized by sonochemical precursor materials of $Pd(acac)_2$, $Ni(acac)_2$, $Co(acac)_2$, $Fe(acac)_2$, $Mn(acac)_2$ in ethylene glycol. The Pd-M NPs were characterized by XRD, TEM, and ICP-AES to determine their particle size, morphology and elemental composition. The NPs were applied to electrocatalysis for formic acid oxidation reaction (FAOR) in 0.1 M $HClO_4$ containing 0.5 M HCOOH. Their activities followed the trend of $Pd_5Co/C>Pd_4Co/C>Pd_3Co/C$. All compositions of PdCo/C catalysts demonstrated higher catalytic activity in FAOR than that of Pd catalyst which was synthesized by the same procedure. The synthesis procedure was also extended to prepare the PdNi/C, PdFe/C and PdMn/C nanoparticles when $Co(acac)_2$ was replaced by $Ni(acac)_2$, $Fe(acac)_2$, and $Mn(acac)_2$, respectively. We found Pd-M nanoparticles on FAOR follow direct oxidation pathway which was evidenced by the CO-stripping. The order of reactivity toward FAOR with respect to onset potential and maximum current density among Pd-M nanoparticles is PdCo/C>PdNi/C>PdFe/C>PdMn/C.

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장소: 부산BEXCO

발표코드: **MAT.P-1262**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Solid-State Synthesis of Silver Nanoparticles in the Presence of Poly(3-hexylthiophene) and its Effect on the Active Layer of Polymer Solar Cells

정희영 K. E. Geckeler[1]

광주과학기술원 나노바이오재료전자공학과 [1]광주과학기술원 신소재공학과,나노바이오전자재료공학과

Metal nanoparticles have been recently used as additives in polymer solar cells due to their plasmonic effect for improving their efficiency. Poly(3-hexylthiophene) is one of the conjugated polymers used as an electron donor material in the active layers of polymer solar cells. Thus, silver nanoparticles were synthesized in the presence of poly(3-hexylthiophene) using a solid-state synthesis method for the direct application in polymer solar cells. The size of the nanoparticles thus produced was in the range of 2.5 - 3 nm. Thereafter, the silver nanoparticles were added to the active layer of the solar cells, based on poly(3-hexyl-thiophene) and [6,6]-phenyl-C61-butyric acid methyl ester as an additive. When employing a 100 nm thickness of the active layer in the solar cells, they showed the highest power efficiency, reflected in a higher open circuit voltage and higher fill factor. Finally, the cells with silver nanoparticles in the active layer exhibited an increase of 1.8% of power conversion efficiency in comparison to those without the nanoparticles.

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장소: 부산BEXCO

발표코드: **MAT.P-1263**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on InGaZnO nanoparticles for preparation of oxide thin film

이기라 이유진[1] 이계행[2]

성균관대 고분자시스템공학과 [1]성균관대 고분자공학과 [2]한국기초과학지원연구원

Indium-galium-zinc-oxide (IGZO) semiconductors have been investigated as an active layer in thin-film transistor for high-definition liquid crystal display (LCD) device and organic light-emitting diode (OLED). Recently, IGZO layers have been prepared by sol-gel process at relatively low temperature for the flexible electronics, in which stable and homogeneous solution of sol-gel precursors were prepared with several organic additives as ink. Their nanoparticles suspension can be used as ink for the low-temperature fabrication of thin film transistor. We have prepared aqueous IGZO nanoparticles suspension from sol-gel reaction of their hydroxide. By changing the reaction scheme, particle size was controlled and also crystallinity was controlled inside reactor. Then, their particulate thin film was prepared by spin-coating on p-doped silicon wafer with silicon oxide layer (~200nm) and annealed. Finally, simple bottom-gate thin-film transistor were fabricated and their TFT performance was investigated.

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장소: 부산BEXCO

발표코드: **MAT.P-1264**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Robust superomniphobic surfaces prepared from silica/polymer core/shell particles

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한국생산기술연구원 [1]연세대 화공생명공학과

A novel procedure for the preparation of omniphobic surfaces with good robustness is described. TLRIP method was used to synthesize silica/poly(Zonyl? TM-co-styrene) core/shell particles. The method employs fabricating the surface by spray coating of silica /poly(Zonyl? TM-co-styrene) core/shell particles followed by drying process. The water and oil contact angle of the core/shell particle surfaces were 170? and 140?, respectively. The surfaces presented herein also exhibit the highest rating of 5B as determined by adhesion test ASTM D-3359-02 (American Society for Testing and Materials).

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1265**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Phosphorescent Blue Host Materials with Sulfur Compounds for Organic Light-Emitting Diodes

빈종관 홍종인

서울대 화학부

Two novel host materials based on carbazole derivatives were synthesized with benzo[b]thiophene (B2tCz) or dibenzothiophene (DB2tCz) for use in evaporation-processed blue phosphorescent organic light-emitting diodes. Both host materials exhibited high glass transition temperatures (Tg = 179 °C for B2tCz and Tg = 185 °C for DB2tCz) and triplet energy levels (ET= 2.84 eV for B2tCz and ET = 2.93 eV for DB2tCz). Multilayer devices fabricated using B2tCz or DB2tCz as hosts for the phosphorescence emitter, iridium(III)bis[(4,6-di-fluorophenyl)pyridinato-N,C2′]picolin-ate (FIrpic), showed maximum current efficiencies of 43.3 and 35.6 cd/A, power efficiencies of 34.0 and 29.4 lm/W, and external quantum efficiencies of 24.6% and 20.0%, respectively.

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장소: 부산BEXCO

발표코드: **MAT.P-1266**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of Opal Silica Photonic Crystals

한송이 유정보 박규리 채원식[1] 허남회

서강대 화학과 [1]한국기초과학지원연구원 강릉센터

Highly uniform core/shell silica microspheres whose diameters are in the range of 200 to 500 nm were successfully synthesized by modifying the Stober method. Colloidal photonic crystals composed of core/shell silica microspheres having the same diameters were prepared by self-assembly from colloidal silica suspensions in water, which are arranged on a face-centred cubic lattice. The core/shell silica opals were fully characterized by SEM, TEM, XRD, BET, and UV-visible measurements. They behaved as 3-dimensional photonic crystals, with a wide range of photonic band gaps (PBGs). The PBGs depend on the diameter of the silica microspheres. The core/shell silica opals showed enhanced thermal stability, which can be useful in applications operated at high temperature.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1267**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasound-Induced Synthesis of Pt Nanoparticles on the surface of Layered Double Hydroxide Nanoplates

나정운 이종현[1] 문지원[1] 황지예[1] 조혜란[1]

가톨릭대 화학 [1]가톨릭대 화학과

Ultrafine Pt nanoparticles were successfully synthesized on exfoliated layered double hydroxide nanoplates without aggregation of Pt nanoparticles by using a ultrsound treatment with sodium borohydride, ascorbic acid and hydrazine hydrate as reducing chemicals in formamide solution. TEM measurements clearly demonstrated the uniform distribution of Pt nanoparticles on the surface of hydroxide nanoplates. A colloidal solution of the resulting Pt and hydroxide composites had a remarkable stability in solutions such as formamide, alcohols and water, without a phase segregation, which also supported the tight bindings of the Pt nanoparticles on the hydroxide nanoplates. Control experiments clearly showed that the absence of exfoliated layered double hydroxide nanoplates prevent the formation of Pt nanoparticles under the formamide conditions, which revealed that the metal hydroxide surface strongly induced a nucleation of Pt nanoparticles. This unique and facile synthetic procedure can be extended to prepare other important series of noble metal based nanostructures.

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장소: 부산BEXCO

발표코드: **MAT.P-1268**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Methyl-functionalized MIL-125 with enhanced water stability

임지혁 고낙은[1] 김자헌[1] 박종래

서울대 재료공학부 [1]숭실대 화학과

Metal-organic frameworks (MOFs) are extended crystalline materials with regular arrays of metal ions, or metal clusters and organic linkers. Their controllable porosity allows MOFs to have specific functions for gas storage and separation, catalysis, sensing, or drug delivery. However, most MOFs are moisture-sensitive because their metal-oxygen coordination bonds can be attacked by water molecules, resulting in the destruction of the framework. The poor stability for hydrolysis limits the practical applications of MOFs. Here we report that methyl-modified MIL-125 showing the same topology with MIL-125 exhibits much more excellent water stability than that of MIL-125. We will discuss these results by representing the PXRD and gas adsorption measurement data for a series of water-treated MOF samples.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1269**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Convex Polyhedral Au@Pd Core-Shell Nanocrystals with High-Index Facets and Study of Their Electrochemical Property

김동흔 한상우[1] 이상복[2]

KAIST 나노기술대학원 [1]KAIST 화학과 [2]KAIST 나노과학기술대학원

Through the simultaneous reduction of Au and Pd ions in the presence of octahedral Au nanocrystal (NC) seeds, hexoctahedron-like convex Au@Pd core?shell NCs, enclosed predominantly by high-index {12 5 3} facets, were synthesized under aqueous room-temperature conditions. The synthesized convex Au@Pd NCs were characterized with scanning electron microscopy (SEM), transmission electron microscopy (TEM), and UV-vis spectroscopy to confirm the shape, composition and structure evolution of NCs. Electrocatalysis experiments unambiguously showed that high-index-faceted convex polyhedral Au@Pd core?shell NCs displayed much higher catalytic activity and stability compared with cubic and octahedral Au@Pd core?shell NCs bound by low-index {100} and {111} facets, respectively.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1270**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Au triangular-shaped nanostructure based Sensitivity Enhancement of Surface Plasmon Resonance for Biosensor

성소희 김효섭 김재호

아주대 분자과학기술학과

The Surface Plasmon Resonance (SPR) can be used to analyze the real-time response to the changes in surface properties on a metallic film. The resonance phenomenon results in energy loss of the incident radiation when it reflected from the surface of the chip. SPR has been widely employed for biosensor applications because of the capability for label-free detection of biomolecular interactions. Since the resonance condition is sensitive to a refractive index change of dielectric environments in the vicinity of a metal film, the SPR technique has been employed to sense the signals originated from biomolecular interactions. However, despite a lot of efforts on improvement of coupling efficiency between biomolecules, it has been difficult to measure a resonance shift at very low concentrations, implying that a thin film based SPR biosensor has critical limitations on sensitivity.Noble metal nanoparticle pairs effect enhance nanosensing sensitivity. Individual gold nanocrystal dimers appear plasmon hybridization. Localized surface plasmon (LSP) result from distance changes depending on the direction of the incident is different.Many different researches have been performed for sensitivity enhancement. The Nanosphere lithography (NSL) has been established as an efficient tool for preparation of nanostructured substrates.In this study, periodic particle array surfaces have been prepared using identical single-layer NSL template made by Langmuir-Blodgett (LB) method of silica nanospheres with a variety of diameter(D = 150, 300 and 500 nm). We study improvement the sensitivity of SPR by Inducing LSP-SPP conjugation and investigation of the size effect of nanostructure on SPR effect.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1271**

발표분야: 재료화학

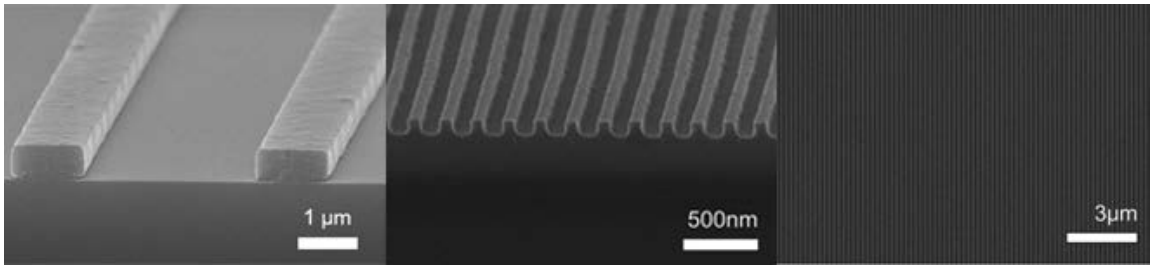
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Single Crystal Poly(3,4-ethylenedioxythiophene) Nanowires by Liquid-Bridge-Mediated Nanotransfer Molding for use as electrodes for Field-Effect Transistors

백장미 조보람 성명모

한양대 화학과

We have studied a fabrication of vapor phase polymerized Poly(3,4-ethylenedioxythiophene) (PEDOT) nanowire arrays for the first time. The vapor-phase polymerization (VPP) technique is a bottom-up processing method that utilizes the organic arrangement of macromolecules to easily produce ordered aggregates, including on the nanoscale, or prepare thin films of self-assembled molecules, micropatterns, or modified microstructures of pure conducting polymers. Also, liquid-bridge-mediated nanotransfer molding (LB-nTM), which was reported as a new direct patterning method recently, is for the arrayed formation of two- or three-dimensional structures with feature sizes as small as tens of nanometers over large areas up to 4 inches across and is based on the direct transfer of various materials from a mold to a substrate through a liquid bridge between them. We observed this PEDOT nanowire, which we fabricate, has a very high quality of crytallinity. We analyzed this by using selected area electron diffraction (SAED). Also, PEDOT single-crystal nanowires are directly transferred on specific positions of substrates to generate nanowire arrays as pure PEDOT not including any FeCl3. The PEDOT nanowires grown by VPP method and transferred on a substrate to use LB-nTM method have been fabricated to single crystal PEDOT nanowires. We fabricate arrays of the PEDOT nanowires acting as source and drain electrodes for 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-PEN) nanowire field-effect transistors. We thus promise the PEDOT nanowire would have high conductivity comparable to inorganic materials although it is an organic material. So, it has the possibility of of using it instead of metalas as electrodes.



대한화학회
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일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1272**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Nickel-Graphene Hybrids for Electrochemical Hydrogen Storage Applications

최문형 백승민

경북대 화학과

In this study, nickel-graphene nanosheet (Ni/GNS) hybrids were successfully prepared through a soft chemical synthetic process. The nanohybrid materials were investigated by X-ray powder diffraction (XRD) and scanning electron microscopy (SEM) measurement. According to the XRD analysis, we found that the nickel particles were hybridized with the graphene nanosheets. Also, SEM images of these hybrids show that nickel particles were deposited on the surface of graphene nanosheets. In addition, electrochemical analysis indicated that Ni/GNS hybrids showed the increased hydrogen storage capacity compared to the starting materials. Therefore, the present nanohybrids materials could be potentially useful for application in electrochemical hydrogen storage.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1273**

발표분야: 재료화학

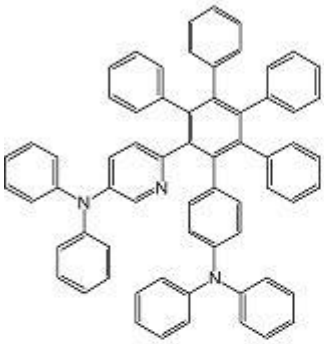
발표종류: 포스터, 발표일시: 수 16:00~19:00

New Hole Transporting Materials Based on Tetraphenylbenzene and Aromatic Amine Derivatives for OLEDs

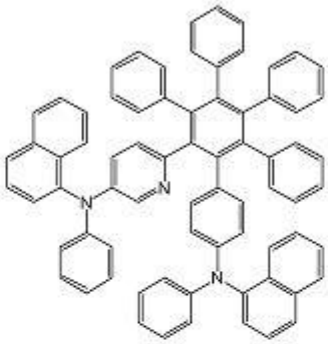
김승호

가톨릭대 화학과

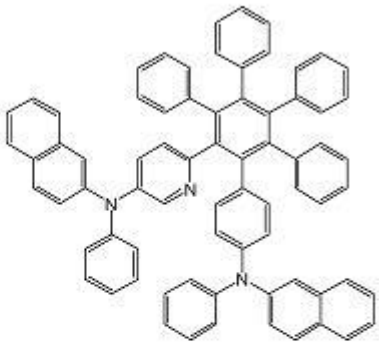
Three different new hole transport compounds, namely, 2-[1-{4-(N, N-diphenylamino)phenyl}-3, 4, 5, 6-tetraphenylbenzene-2-yl]5-N, N-diphenylaminopyridine(DPAP-TB), 2-[1-{4-(N-phenylnaphthalene-1-amino)phenyl}-3, 4, 5, 6-tetraphenylbenzene-2-yl]5-(N-phenylnaphthalen-1-amino)pyridine(1-PNAP-TB) and 2-[1{4-(N-phenylnaphthalen-1-amino)phenyl}-3, 4-,5, 6-tetraphenylbenzene-2-yl]-5-(N-phenylnaphthalen-2-amino)pyridine(2-PNAP-TB) were synthesized. Optical and electronic properties were examined by UV-Visible absorption spectrum and cyclic voltammetry. Luminance efficiencies and external quantum efficiencies of DPAP-TB, 1-PNAP-TB and 2-PNAP-TB were 3.72, 2.82, 3.30 cd/A, and 1.29, 0.97, 1.12 % at 10mA/cm2, respectively. Synthesized materials exhibited high Tg in the range of 118 to 125℃. These values are higher than that of NPB which is commonly used as a hole transporting material.



DPAP-TB



1-PNAP-TB



2-PNAP-TB

Scheme 1. Chemical structures of the synthesized hole transporting compounds of DPAP-TB, 1-PNAP-TB, and 2-PNAP-TB.

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장소: 부산BEXCO

발표코드: **MAT.P-1274**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Doped TiO_2 and Application to Dye-Sensitized Solar Cells on Flexible Substrate

윤용태 김영일

부경대 화학과

Doped TiO_2 was synthesized by hydrothermal process, using metal and non metal precursors to enhance photovoltaic properties of dye-sensitized solar cell(DSC). Prepared TiO_2 powders were mixed into alcoholic solution with acid which was adjusted increase viscosity of the coating solution and thickness of the TiO_2 photoanode. Because of weak heat-resistance of flexible substrate, any organic compounds were excluded the coating solution and every sintering process was under way at low temperature. The electrode was coated on PEN/ITO, using 3M Magic tape as a spacer. The deposited electrode was dried in air and sintered below 150 ^{o}C for a short period.Doped and undoped TiO_2 based DSC fabricated for comparison of the photovoltaic properties. Finally, some strip cells were connected in series, known as a Z-connected type on a sheet of a film and DSC module was fabricated with Pt counter electrode.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1275**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Crystalline Organic Semiconducting Nanorods through Epitaxial growth

임현민 명지은 강영종[1]

한양대 화학과 [1]한양대 자연과학대학 화학과

One-dimensional (1D) nanomaterials have been fascinated in recent years due to their optoelectronic properties as well as promising applications in nanoscale devices. The intrinsic properties of organic nanorods are usually dictated by their crystallinity, packing density and molecular level assembly. However, the fabrication of organic semiconducting nanostructures has not been well established yet comparing with their inorganic parts. Herein, we present fabrication and characterizations of well-defined organic semiconducting nanorods, which can be applied for patterning and alignment.In order to take an easier way, we fabricated nanomaterial with highly crystalline by using epitaxial growth, and its crystallinity and optical properties could be controlled. The physical properties were characterized by electron and optical microscopies, MALDI-TOF, XRD and CV.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1276**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation of CdSe quantum dots using various capping ligands

강미재 김상욱

아주대 분자과학기술학과

양자 점은 양자 제한 효과로 인해 다양한 전기적, 광학적 특성을 지니며 이러한 특성을 이용하여 디스플레이, 바이오 이미징, 태양 전지 등에 적용하려는 연구가 활발히 진행되고 있다. 양자 점은 유기 리간드에 둘러 쌓인 무기 나노 입자로써 고효율을 나타내고 안정한 양자 점을 만들기 위해서는 유기 리간드에 대한 연구가 필요하다. 우리는 Cd(acac)2 와 TOP-Se 를 전구 체로써 사용하고 순수한 리간드의 역할을 보기 위해 용매를 Octadecene 으로 고정 시킨 후 리간드만 바꿔서 CdSe 나노 입자를 합성하였다. TOP, TOPO, 1-dodecanethiol, Oleic acid, Oleylamine, Octadecylamine, Alkyl acid 를 사용하여 CdSe 양자 점 합성 후 양자 점의 특성을 살펴보았다. 이 연구를 통해 리간드에 대한 연구의 중요성은 물론 각 리간드로 양자점을 합성했을 때 양자점의 특성을 알 수 있었다. 감사 : 이 연구는 2012 학년도 경기과학고등학교의 R&E 프로그램으로 지원되었으며 김홍기, 유환옥 학생이 이 연구의 실험과 토의에 참가하였습니다.

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장소: 부산BEXCO

발표코드: **MAT.P-1277**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effects of magnesium content on the physical properties in a MgO-CaO-Na_2O-P_2O_5 glass system

이인호 공명선 Jonathan C. Knowles[1]

단국대 나노바이오의과학과 [1]Division of Biomaterials and Tissue Engineering, Eastman Dental Institute, University College London

Glasses with composition 20Na_2O-(30-X)CaO- XMgO-50P_2O_5 (X = 30, 25, 20, 15, 10, 5 and 0 mol %) have been successfully synthesized by the melt-quenching technique. This paper presents the development of this system by introducing magnesium oxide as a partial calcium oxide substitute and solubility behaviors. Degradation study has been carried out by means of measuring their chemical durability against buffer solution with initial pH values of 7.00 at 37°C for up to 21 days. The dissolution rate(DR) was obtained by calculating the measured weight loss of the glasses per unit surface area per unit immersion time. This study shows that whilst there is little change structurally as seen from the NMR, FTIR and thermal measurements, the glasses have an inverse exponential relationship between solubility and MgO content and there is a possibility to create soluble phosphate-based glass with a selective range of solubility from highly soluble to relatively stable glass for the potential applications in orthopaedic biomaterials.

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발표코드: **MAT.P-1278**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesize enhancement Nb_2O_5 NWs for photovoltaic cell using SILAR method

백승혁 김한성 장동명 박정희 안재평[1]

고려대 소재화학과 [1]KIST 산업화지원센터

Niobium pentoxide's band gap is 3.0 eV. So, It is absorbed 380nm-450nm wavelength like ultra-violet light. We aim to prepare photovoltaic cell of hybrid core-shell Nb_2O_5 nanowires using SILAR method. The products of these reactions were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), UV-vis Spectrophotometer (UV).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile preparation of two-dimensional arrays of Iron oxide nanoflakes with visible light induced photocatalytic activity

이선영 정현민

금오공과대 응용화학과

Nano-structured iron oxides have attracted attention due to wide usefulness in catalysis and uses. Especially two-dimensional arrays of iron oxide particles on substrate have interested in photocatalytic reactions which were usually fabricated by electrodeposition method. Although, well-defined and effective structures of arrays hane been obtained via electrodeposition, more direct and facile method are still required to provide controlled structures in large scale production without limitation in instrument and scale. In this work, we present the facile synthesis of iron oxide nanoflakes which were assembled into 2-D arrays and its application as visible light-driven photocatalysis. The arrays of iron oxide nanoflakes were synthesized by a simple solvothermal reaction and sequential calcinations without employing templates or matrices for self-assembly. The flake size of hematites could be easily controlled by changing the concentration of Fe(CO)5 and reaction time, respectively, and also this technique can potentially be extended for large-scale synthesis of iron oxide nanostructures. The resulting iron oxide nanoflakes were characterized by X-ray diffraction (XRD), brunauer?emmett?teller (BET), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The results indicate that the as-prepared samples are hematite (α-Fe2O3) nanoflakes, and were compared in shape and nanometer-dimension of flake. These hematite nanoflakes were investigated for studying the flake size-dependent photocatalytic degradation of methylene blue in an aqueous solution under visible light. The difference in photocatalytic activity of these hematite nanoflakes is discussed in terms of nano-size of flakes.

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발표코드: **MAT.P-1280**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced exfoliation of graphite using gold nanoparticles for the production of graphene

김승현

아주대 분자과학기술학과 나노재료실험실

Graphene, a single-layer allotrope of carbon, has been receiving great attention due to its high conductivity and mechanical strength. Several methods to obtain graphene including direct growth from carbon or the reduction of graphene oxide have been previously reported. However, these methods result in defects across the graphene layer. In addition, the use of hazardous and explosive reducing agents hampers the application to mass production. In this context, exfoliation from graphite by sonication seems to have the most potential for synthesizing graphene. We developed a new exfoliation method using polyethylene glycol(PEG) as a surfactant and a gold-organic complex as a precursor of nanoparticles. It is expected that the formation of Au nanoparticles from the Au ions between the carbon layers at a proper condition enhances the exfoliation of graphite. The graphene produced were observed by transmission electron microscopy(TEM). [Acknowledgement]This work was partly supported by the 2012 R&E program of Gyeonggi Science High School. Jeongmin Yim and Donghyun Ahn at Gyeonggi Science High School participated in the experiments and discussion.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ordered Mesoporous Carbon-Carbon Nanotube Nanocomposites as Highly Conductive and Durable Cathode Catalyst Supports for Polymer Electrolyte Fuel Cells

천재영 주상훈

울산과학기술대 나노생명화학공학부

Highly interconnected ordered mesoporous carbon-carbon nanotube (OMC-CNT) nanocomposites were synthesized via a nanocasting method, using SBA-15 mesoporous silica as a template and nickel phthalocyanine as a precursor, respectively. The OMC-CNT nanocomposites as well as two other OMCs were used as fuel cell catalyst supports for preparing highly dispersed Pt nanoparticles (below 2 nm in diameter). The Pt/OMC-CNT catalyst exhibited superior oxygen reduction reaction activity and durability, compared with two Pt/OMC catalysts. In single cell tests for proton electrolyte membrane fuel cell, the Pt/OMC-CNT-based cell showed much higher current density after high-voltage degradation test. The high activity and stability of the Pt/OMC-CNT catalyst was ascribed to its novel interconnected OMC-CNT nanocomposites structure, which induce improved electrical properties.

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장소: 부산BEXCO

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of a New Mixed-metallic Phosphate Chloride, $Li_{4.35}Na_{0.65}Nb_{10}P_6O_{42}Cl$

기용호 윤호섭[1]

아주대 에너지시스템학부 응용화학과 [1]아주대 화학과

Transition metal phosphates have been widely investigated due to their potential applications for secondary batteries. In attempts to design a new mixed-metallic phosphate from the known system, Li/Na/V/Nb/P/O, single crystals of $Li_{4.35}Na_{0.65}Nb_{10}P_6O_{42}Cl$ have been prepared and characterized through X-ray diffraction. The structure of the title compound consists of infinite chains of trans-corner-sharing NbO_6 octahedra, which are linked together by tetrahedral PO_4 groups. The polyhedra share O atoms to form a three-dimensional framework with large empty channels along crystallographic b- and c- axis. The Li ions stay in the b-axial channels and the Na ions stay in the c-axial channels with interjacent Cl ions. The presence of alkali metal and chloride ions in the channels involves the idea of synthesis on new materials that could play an important role as a cathode of secondary batteries. The classical charge balance of the title compound can be represented as $[Li^+]_{4.35}[Na^+]_{0.65}[Nb^{5+}]_{10}[P^{5+}]_6[O^{2-}]_{42}[Cl^-]$.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot supercritical ethanol process of ruthenium selenide nanoparticles as electrocatalyst for direct methanol fuel cells

이은직 권영욱[1]

성균관대 나노과학기술협동학부 [1]성균관대 화학과

In this study, we report that the synthesis of carbon supported ruthenium selenide nanoparticles prepared via supercritical ethanol process and their electrochemical properties toward oxygen reduction reaction. To prepare the electrocatalyst, the $RuCl_3xH_2O$ and SeO_2 are used as reagents along with carbon support. Decomposition of the reagents occurs under supercritical ethanol at 350 °C for 1 h and facilitates the rapid homogenous nucleation, growth and crystallization of the desired nanoparticles on carbon support. Structure analysis of materials is investigated by X-ray diffractometry (XRD) and transmittance electron spectroscopy (TEM). Elemental composition and oxidation state of materials are also verified by energy dispersive X-ray spectroscopy (EDXS) and X-ray photoelectron spectroscopy (XPS). Electrochemical studies show the ruthenium selenide nanoparticle has suitable electrocatalytic activity and methanol insensitivity during oxygen reduction reaction.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymerization and Physical Properties of Functional Hydrogel Lens containing Flouoroaniline Group

강인중 성아영

세한대 안경광학과

The copolymerization of 5-Flouoro-2-methoxyaniline, 5-Flouoro-2-methylaniline, EGDMA (ethylene glycol dimethacrylate as a cross-linker), HEMA (2-hydroxyethyl methacrylate), MMA (methyl methacrylate), NVP (n-vinyl pyrrolidone) was performed in the presence of AIBN (2-2'-azobisisobutyronitrile) as an initiator. Measurement of the physical properties of the resulting copolymers showed that water content, refractive index, visible ray and UV transmittance were in the range of 37.63~38.45%, 1.436~1.439, 24.0~76.8%, and 76~89%, respectively. The UV blocking effect of 5-Flouoro-2-methoxyanilin copolymers were higher than those of the copolymers containing 5-Flouoro-2-methylanilin. From the results we came to the conclusion that the produced copolymers are suitable for the application of ophthalmic contact lens with high UV blocking effect.Key words : 5-Flouoro-2-methoxyaniline, 5-Flouoro-2-methylaniline, UV block effect.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of Ophthalmic Copolymer Containing 2-(Trimethylsilyloxy)ethyl methacrylate and 2,4-dihydroxybenzophenone

김동현 성아영

세한대 안경광학과

The physical and optical characteristics of polymerized hydrophilic ophthalmic lenses with addition of 2-(Trimethylsilyloxy)ethyl methacrylate(2TMS) and 2,4-Dihydroxybenzophenone(DHB) in the traditional hydrogel lens materials such as HEMA, NVP, MMA, EGDMA and the initiator AIBN were measured and assesed. The resulting mixture containing 2TMS and DHB were copolymerized by heating 30 min for 60℃, 30 min for 70℃ and then 90℃ for 30 min. The measurement of physical properties of the produced copolymers exhibited that refractive index, water content, visible transmittance and oxygen transmissibility were in the range of 1.4346~1.4305, 35.39~36.48%, 90.2~91.0%, 13.29~14.09 × 10-11(cm2/sec)(mlO2/ml×mmHg) respectively. And also, the measurement of UV transmittances of hydrogel polymer containing DHB showed that UV-B, UV-A transmittances were in the range of 0.2~0.6% and 4.0~4.6% respectively. The produced polymer satisfied physical properties required to manufacture ophthalmic hydrogel contact lenses, and were suitable to be applied as a functional material for ophthalmological purposes.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of full color emitting liquid crystal display module using highly stable QDs-polymer composite film

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한국기초과학지원연구원 강릉센터 [1]서울대 화학부

Semiconductor QDs nanocrystals have been successfully developed and commercialized as a wavelength converter for LED due to their highly efficient luminescent efficiency, negligible light scattering and narrow emission. In spite of these remarkable properties, it was disclosed that QDs nanocrystals could not show enough stability as phosphor in LED under long term irradiation. The PL decay and wavelength shift of QDs nanocrystals are usually explained by defect site formation and oxidation. Such as, these problems would be mitigated through the metal oxide on the surface. Here, we proposed new approach to metal oxide coating on the surface of QDs nanocrystals. The synthesized CdO coated QDs nanocrystals were shown the highly stability and photoluminescent efficiency. In addition, it confirmed application as phosphor for LED through fabrication of liquid crystal display module using CdO coated QDs-polymer composite film.

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발표코드: **MAT.P-1287**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, structural and photoelectrical properties of $MgSb_2O_6$ for application to dye-sensitized solar cells

배지희 장지연 김승주

아주대 에너지시스템학부

Mesoporous nanocrystalline films of wide-band gap semiconductor oxides play an important role in dye-sensitized solar cell (DSSC). In this work, we have prepared $MgSb_2O_6$ nanoparticles and investigated their electrical properties for application to DSSCs. The crystal structures of $MgSb_2O_6$ prepared at different temperature were monitored by means of powder X-ray diffraction and analyzed by the Rietveld refinement method. The compounds prepared below 500°C exhibit rutile structure. When the compounds were heated up of 600°C, the rutile structure began to change to trirutile-type in which Mg ion and Sb ion are ordered with 1:2 ratio in the lattice. The cation ordering ratio increases as the annealing temperature increases. The $MgSb_2O_6$ powders were deposited onto F-doped SnO_2 glass and subsequently heated at 500°C. After dye adsorption with the conventional ruthenium dye (N719). The highest power conversion efficiencies of MgSb2O6 based solar cell was 1.97% under AM1.5, 100mW/cm^2 illumination.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure and photoluminescence of the tetranuclear copper(I) cluster $Cu_4I_4C_8N_4O_4H_{28}$

김재겸 김필수[1] 윤호섭[2] 김승주

아주대 에너지시스템학부 [1]아주대 에너지시스템학부 응용화학과 [2]아주대 화학과

A single crystal of new tetranuclear copper(I) cluster $Cu_4I_4C_8N_4O_4H_{28}$ was synthesized via solvothermal method. Crystal structure of $Cu_4I_4C_8N_4O_4H_{28}$, is orthorhombic with the lattice parameters of a = 15.278(6) Å, b = 7.941(3) Å, c = 10.187(5) Å. (space group = *Pban*, and Z = 2) This compound composes of distorted cubic cluster where copper and iodine atoms are alternatively located on the corners of the cluster. Each copper atom is coordinated with nitrogen-donor ligand. We prepared the compound with powder form by dropping organic solution into CuI dissolved in acetonitrile. The X-ray diffraction pattern of the synthesized powder is corresponded with single crystal simulation data. The copper(I) tetranuclear cluster $Cu_4I_4C_8N_4O_4H_{28}$, showed photoluminescence character of orange color in range of λ^{ex}_{max} = 367nm and λ^{em}_{max} = 572nm at room temperature. We compared the photophysical properties of the titled compound with several analogues of general formula $Cu_4I_4L_4$.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of iron nitrides by ammonolysis of iron oxide nanoparticles.

손혜진 김승주

아주대 에너지시스템학부

Iron nitrides, Fe_xN (x=2,3,4), exhibit the structural variance depending on their compositions; Fe_2N crystallizes in the α-PbO_2 structure type. Iron atoms show the motif of a slightly distorted hexagonal close packing as also found for Fe_3N. Fe_3N, only corner sharing octahedra of Fe are occupied in an ordered way by nitrogen. In Fe_2N, nitrogen occupies corner and edge sharing octahedral. Fe_4N crystallizes in the perovskite structure type that the arrangement of Fe was cubic close packing. In Fe_4N structure, nitrogen occupies only corner sharing octahedral of Fe. In this work, iron nitride powders were synthesized by ammonolysis of iron oxide (Fe_3O_4) nanoparticles. We investigated the composition, size and morphology of iron nitrides under various synthetic conditions (temperature and reaction time).

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발표분야: 재료화학

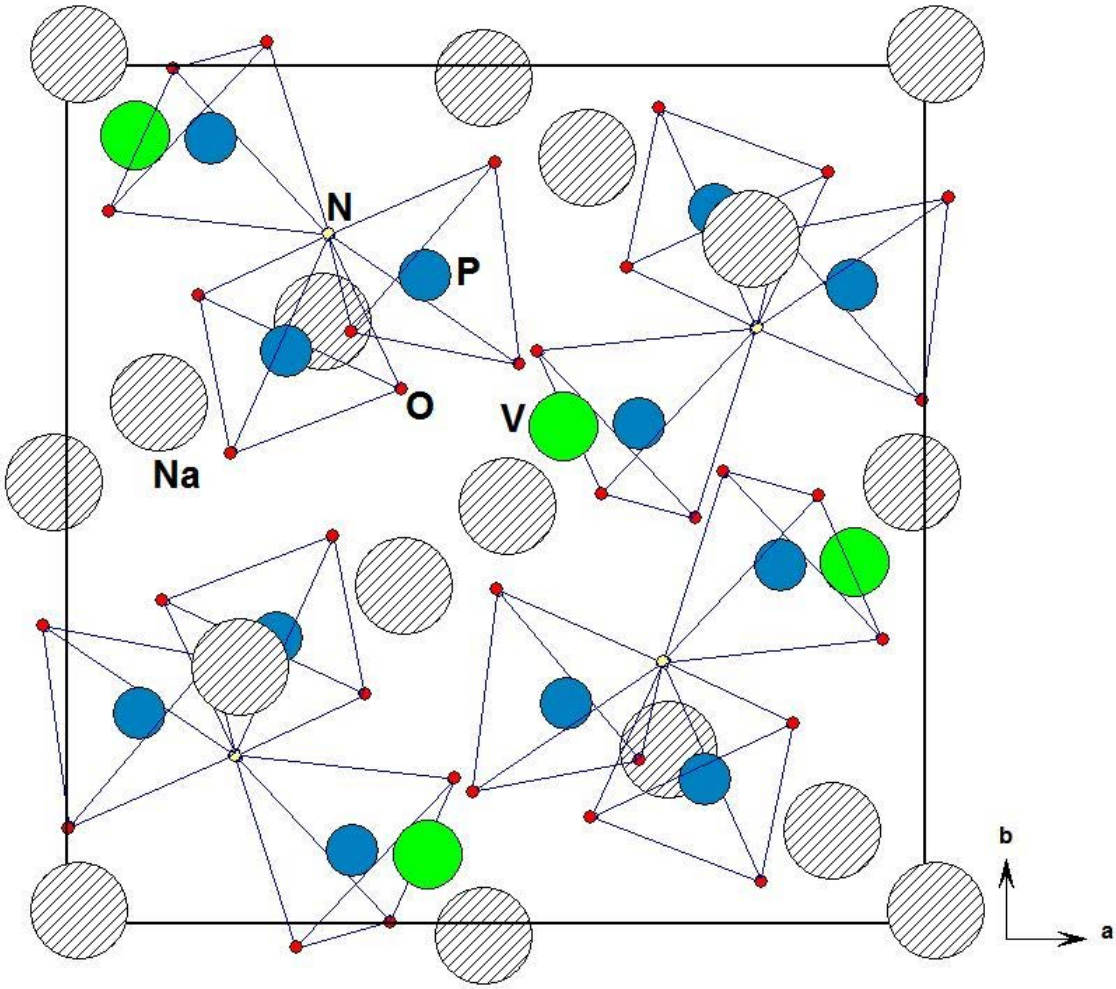
발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal structure of $Na_3V(PO_3)_3N$ refined by synchrotron X-ray diffraction method

김민웅 김승주

아주대 에너지시스템학부

The crystal structure of $Na_3V(PO_3)_3N$ was investigated by means of Rietveld refinement based synchrotron X-ray powder diffraction data and bond valence sum calculation. $Na_3V(PO_3)_3N$ was synthesized by the thermal nitridation of stoichiometric mixture of $NaPO_3$ and V_2O_5 in flowing ammonia gas at 700°C. The synchrotron powder diffraction patterns for $Na_3V(PO_3)_3N$ showed the cubic symmetry with lattice parameter a = 9.4414(5) Å. Systematic absences, $h = 2n+1$ for $h00$ observed in the intensity data, suggested the space group of $P2_13$. As an initial model for Rietveld refinement, we adopted the structural parameters of a single crystal $Na_3Al(PO_3)_3N$. Refinement of atomic positions and isotropic displacement parameters were carried out using the Fullprof program package. In the structure of $Na_3V(PO_3)_3N$, phosphorous atom is coordinated to three oxygen atoms and one nitrogen atom to form a PO_3N tetrahedron. The $(PO_3)_3N$ entity is formed by three PO_3N tetrahedrons sharing a common corner occupied by the nitrogen atom.


N
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O
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Na
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a

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **MAT.P-1291**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and characterization of TiO_2-decorated carbon nanotubes for photocatalytic applications

김성필 최현철

전남대 화학과

TiO_2 is one of the most investigated photocatalysts, and it has been found to be capable of decomposing a wide variety of organic and inorganic pollutants in both liquid- and gas-phase systems. The photocatalytic efficiency of TiO_2 is greatly influenced by crystal structure, particle size, surface area and porosity. One of the strategies to improve the photocatalytic efficiency is to increase the surface area of the catalyst. Thus, fixing TiO_2 particles of high surface area on inert support will simplify the recovery of TiO_2 from the treated effluent. In this study, we prepared TiO_2-decorated carbon nanotubes using multi-walled carbon nanotubes as a starting material and titanium n-tetrabutoxide as titanium source. The obtained samples were characterized by using XRD, XPS, TEM, and FTIR methods. The photoactivity of the prepared materials was evaluated by the conversion of methylene blue in aqueous solution under UV irradiation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Au/semiconductors Hybrid Mesoporous Films for Enhanced Photoelectrochemical Performance based on the blocking of electrons capature by Au

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Au modification has been demonstrated to be an efficient strategy to improve the photoelectrochemical (PEC) performance of semiconductors due to the plasmon-induced charge carriers and effective electron-hole separation at the interface. However, the PEC performance can be dramaticly effected by loading the amount of Au on the semiconductors surface attributed to the electron captures by Au. Herein, two approaches, i.e electrochemical deposition and UV photoreduction were designed to load the amount Au on the mesoporous semiconductors (TiO_2, Fe_2O_3) surface. We observed that the more significant enhancements in photocurrent can be achieved for Au/Semiconductors by using electrochemical deposition method. It can be explained that the Au not only helps the electron-hole separation, but also contributes to the effective electrons transfer in case of Au produced by electrochemical deposition method.

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발표분야: 재료화학

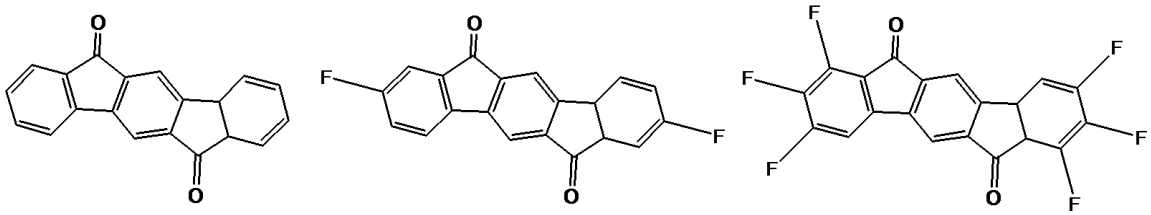
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorine Effect Using New Indenofluorenedione Derivatives for Electron Transporting Layer in OLED Devices

이재현

가톨릭대 화학과

Many attempts have been widely investigated in organic light emitting diodes (OLED) materials field. Especially, in order to balance hole and electron carriers, hole transporting layer (HTL) and electron transporting layer (ETL) are used with different thickness in OLED device.1In this study, new three indenofluorenedione derivatives were synthesized and proposed for ETL. Three compounds are indeno[1,2-b]fluorene-6,12-dione (NoF-IF-dione), 2,8-Difluoro-indeno[1,2-b]fluorene-6,12-dione (MonoF-IF-dione), and 1,2,3,7,8,9-Hexafluoro-indeno[1,2-b]fluorene-6,12-dione (TriF-IF-dione) as shown in figure 1.We report optical and electrical properties of three compounds such as UV-Vis. absorption spectrum, cyclic voltammetry, and OLED device performance, etc. In figure 1, MonoF-IF-dione and TriF-IF-dione include fluorine halogen group at compound, which can withdraw electron from aromatic ring. The changes of electro-optical properties of compounds caused by the change of fluorine number were examined. Especially, three compounds were used as an ETL in OLED device.



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Highly enhanced luminescence property of Tb-doped layered yttrium hydroxynitrate by antenna effect of tungstate anions

이기룡 변송호

경희대 화학과

Intense green-emission of $Y_2(OH)_5NO_3 \cdot nH_2O$:Tb (LYH:Tb) was induced by 'antenna effect' of tungstate anions (WO_4^{2-}). The adsorption of tungstate anions has been completed within a few minutes on LYH:Tb surface. No shift of (*0 0 l*) reflections in X-ray diffraction patterns and observed W-O vibration modes from infrared spectra indicated that highly enhanced green-emission of LYH:Tb results from an surface adsorption of tungstate anions instead of ion-exchange process in the interlayer space. Based on photoluminescence (PL) spectra, the luminescence property of LYH:Tb is generally quenched by hydroxyl groups coordinated to Y atoms in the intralayer, while the tungstate adsorbed on the surface of LYH:Tb shows a bright green-emission due to the energy transfer from the oxygen to metal charge transfer (OMCT, $O^{2-} \rightarrow W^{6+}$) band. Thus, the tungstate groups located on the surface of LYH play a role as light harvesters (such as antenna). These WO_4^{2-}/LYH:Tb hybrid compounds obtained by simple surface adsorption would have potential applications for various fields, such as optical device, catalyst, and sensor.

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발표코드: **MAT.P-1295**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Low-cost fabrication of graphene quantum dots using thermal plasma jet

김주한 서정쌍

서울대 화학부

We report a new low-cost method to fabricate graphene quantum dots (GQDs) using thermal plasma jet. A carbon atomic beam was generated by injecting a relatively large amount of ethylene gas (2.5 L/min) continuously into Ar plasma; the beam was then flowed through a carbon tube attached to the anode, and then dispersed into a chamber. The production rate of carbon soot was 30 g/hour. Almost all of carbon soot was dispersed in ethanol by sonication. Carbon soot consisted of GQDs and some onion type carbon materials. When the soot was dialyzed, GQDs were only extracted. The size of the extracted GQDs was in the range of 8 to 18 nm . GQDs were made by a gas phase collision reaction during flowing through the attached carbon tube. We have measured their TEM and SEM images, and UV-visible absorption and PL spectra.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Polydopamine Microfluidic System toward a Two-Dimensional, Gravity-Driven Mixing Device

유인성

KAIST 나노과학기술학과

A new type of microfluidic system called polydopamine microfluidics is reported. It is a pump-free, two-dimensional surface-tension-confined-microfluidic system, energy efficiently operated with gravity. The device is fabricated by hydrophilic polydopamine micro-patterns on nanostructured, superhydrophobic anodized aluminum oxide (AAO) surfaces on which liquid droplets move along the predetermined paths of polydopamine with no residuary liquid trace. Polydopamine coating, inspired by mussels' robust adhesion on versatile substrates, was utilized to stably modify the superhydrophobic AAO surface. The flow rate of polydopamine microfluidics was about 30 uL/s, faster than that used in conventional microfluidic systems (~0.5 uL/s), which is suitable for large volume applications. A rapid mixing device to monitor structural changes of photoactive yellow protein (PYP) and a micro-reactor for the synthesis of gold nanoparticles were fabricated to demonstrate the utility of the polydopamine microfluidic device. The polydopamine microfluidic device is a promising candidate for a new type of microfluidic systems that is potable with extremely low energy consumption for operation.

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Azo 화합물이 층간 삽입된 층상 구조 물질의 합성 및 특성 규명

길현석 양지윤 이석우

공주대 화학과

본 연구에서는 층상 구조 물질의 층간에 아조 화합물을 층간 삽입한 복합 재료를 합성하여 특성 규명을 위한 연구를 수행하였다. 층상 구조 물질로 음이온성 코발트 착물과 4,4'-bipyridine 을 이용한 MOF, Mg-Al 형태의 LDH 를 사용하였으며, 양이온성 계면 활성제를 사용하여 지질층을 모사하였다. 아조 화합물은 4,4'-dihydroxyazobenzene (DHAB)과 sodium 5,5'-azotetrazolate (SADT)를 사용하였으며, 층상 구조 물질의 층간에 삽입하였다. 합성된 화합물은 원소 분석을 이용하여 조성을 확인하였고, FT-IR 을 통해 작용기를 확인하였다. 분말 X-선 회절 분석을 통하여 층간에 존재하는 아조 화합물의 빛과 열에 의한 가역적인 구조 변화를 관찰하였다.

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발표코드: **MAT.P-1298**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

실리카 비드 표면에서의 BALB/3T3 섬유아세포의 성장과 이동

김지희 이석우

공주대 화학과

본 연구에서는 PDMS 몰드와 실리카 비드를 이용하여 패턴이 형성된 기판을 제작하고, 패턴 위에서 성장된 세포의 거동을 관찰하고자 하였다. 실리카 비드는 TEOS 를 NH4OH 조건에서 반응시켜 600~800 nm 크기로 제조하였다. APTMS 로 처리된 유리 기판 표면에 TESPSA 로 처리하여 반응성이 있는 유리 기판을 제조하였으며, PDMS 몰드와 산소 플라즈마를 이용한 건식 식각 방법으로 일정한 패턴을 형성하였다. 식각된 부분에는 세포 부착을 막기 위하여 OTS 로 처리하였으며, TESPSA 부분에 APTMS 로 처리된 실리카 비드를 고정하였다. 제작된 실리카 비드 패턴 위에 BALB/3T3 섬유아세포를 배양한 후, 일정 시간 간격으로 광학 현미경 이미지를 분석하여 세포 성장과 이동에 대하여 모니터링하였다. 대조군 유리 기판, APTMS 처리된 유리 기판, 실리카 비드 처리된 유리 기판에서 BALB/3T3 섬유아세포를 배양하여 성장 곡선과 이동 속도를 분석하여 표면 특성이 세포의 성장과 이동에 미치는 영향을 조사하였다.

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발표코드: **MAT.P-1299**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Cadmium Oxide Nanocrystals with Size and Shape Controll

최동혁

아주대 분자과학기술학과

Metal oxide nanocrystals have attracted considerable attention owing to their specific properties and potential application in various fields. For instance, metal oxide nanocrystals are used as catalysts, biomedical diagnosis and therapy, electro-chemical device, and bioseparation because it has good chemical stability, simple synthesis method, and easily Large-Scale Synthesis.Cadmium oxide(CdO), which are a II-VI binary oxide semiconductor with a direct bandgap of 2.27 eV and an indirect bandgap of 0.55 eV in the bulk state, is a promising candidate for a transparent conducting oxide material because it has a simple rock-salt crystal structure, high carrier mobility, and high conductivity, which is due to the nonstoichiometric property which resulted from oxygen vacancies in cadmium oxides. Although CdO have numerous potential applications, very less research has been carried out on the synthesis and application of these nanocrystals. We report the simple synthesis of colloidal CdO nanocrystals with various sizes and shapes. Size- and shape-controlled CdO nanocrystals were obtained via a simple thermal decomposition method in which the decomposition temperature and surfactant composition (oleic acid/oleylamine ratio) were appropriately adjusted. Oleic acid facilitated the formation of octahedral CdO nanocrystals by effecting growth rate control in a given crystal plane through selective binding.

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발표코드: **MAT.P-1300**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of highly luminescent Cd-free core-shell quantum dot

김성우 김상욱

아주대 분자과학기술학과

Considerable research has been carried out on colloidal semiconductor nanocrystals on account of their size dependent electronic and optical properties, which are the key issues in many applications, such as biomedical fluorophores, LEDs and photovoltaic devices. Among them, a group of II-VI semiconducting NCs, CdSe QDs exhibit excellent photostability, quantum yield, and a tunable emission wavelength, however, because they are highly toxic and thus pose a potential threat to the environment. As an alternative to CdSe QD, InP QD has been suggested as it shows a broadband emission spectrum comparable to that of CdSe yet is much more environmentally compatible. however, InP QDs emitters include poor emission efficiency, poor control of size distribution, poor size tenability, and poor stability. Furthermore, the synthetic procedure of InP QDs are more complicated than that for CdSe QDs. To overcome these problems, it is important to control their surface properties, including defects by core-shell structures. However, because of the thin shell thickness, InP based core-shell quantum dots have not obtained a high QY, narrow FWHM, and photochemical stability.To solves this problems, we report on the InP/GaP/ZnS core-shell-shell QDs.

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발표코드: **MAT.P-1301**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of iron-based quantum dots

마오샹

부산대 나노과학기술학과

.Quantum dots (QDs) is one kind of fluorescent materials and used in many areas, such as bio-chemistry, sensor devices, solar cell and so on. Generally speaking, along with different element attending in synthesized works, different kind of QDs are fabricated in organic solvent by adjusting the amount of precursor reagents or changing the elemental precursors in the reaction. Timely, the method synthesize hydrophilic QDs is also been developed. Among information, to the best of our knowledge, there are many the previous reports to show the different consisted Iron chalcogenide materials. The preparation of iron based QDs have not been reported in synthesized works. In our tentative actions, upon thermal annealing, organic solvent and surfactant functionalized with NC cores forming well-crystallized pure phase. The crystalline and semiconducting properties can be characterized by conventional devices, such as UV-Vis spectrophotometry, Thermo Gravimetric Analyzer (TGA) and so on. Corresponding to the band gap characterization, along with different mole ratio used in synthesized work, the main value is being tunable and it can be showed in optical property completely. Moreover, the synthetic approach demonstrated here shows potential for the controlled synthesis of other metal chalcogenides.

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장소: 부산BEXCO

발표코드: **MAT.P-1302**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhancement of the Electrode Performance of Nanocrystalline $LiMn_2O_4$ upon Immobilization on the Surface of Graphene Nanosheets

조경연

이화여대 화학나노과학과

The intimately-coupled nanocomposites of LiMn2O4?reduced graphene oxide (RGO) are synthesized by solvothermally-assisted immobilization of lithium manganate nanocrystals on the surface of RGO nanosheets. A solvothermal treatment with the mixed water/ethanol-based suspension of graphene oxide (GO) nanosheets gives rise not only to the reduction of GO to RGO but also to the immobilization of LiMn2O4 nanoparticles on the surface of RGO nanosheets. According to powder X-ray diffraction and electron microscopy, the crystal structure and morphology of lithium manganate remain intact upon the composite formation with RGO nanosheets. Micro-Raman and X-ray absorption spectroscopy clearly demonstrate the homogeneous hybridization of LiMn2O4 and RGO in the nanocomposites. The present LiMn2O4?RGO nanocomposites display promising cathode performance for lithium ion batteries, which is superior to the pristine LiMn2O4 nanocrystal. This finding clearly demonstrates the usefulness of the present solvothermal method to improve the electrode performance of lithium intercalation electrode materials through the coupling with RGO nanosheets

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Building of bamboo-like conducting carbon nanotubes ornamented with Au nanoparticles by the thermal decomposition of sucrose in an AAO template

이명순 홍성철 김돈

부경대 화학과

An easy method is reported for the preparation of bamboo-like conducting carbon nanotubes decorated with Au nanoparticles (Au-CNT), by carbonization of sucrose inside of anodic aluminum oxide (AAO) nanochannels (~80 nm and ~30 μm in diameter and length, respectively). First, the AAO membrane nanochannels were coated with Au nanoparticles (~10 nm in diameter) and the carbon nanotubes were then formed in the same channels below 973 K. Electron microscopy shows long bamboo-like carbon nanotubes, ~30 μm in length, decorated with crystalline gold nanoparticles, ~50 nm in diameter. The coalescence of the precoated small Au nanoparticles inside the channel results in the attached large Au nanoparticles. The apparent resistivity of the Au-CNT prepared at 973 K, was ~16.8 Ωcm. The electrical conductivity of the structure is discussed with relation to electrochemical and micro Raman experiments.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of hematite using the hydrothermal and functionalization of silica coated hematite.

허지수

충남대 화학과

Hematite cubes, was prepared using the aqueous solution containing formic acid and ferric chloride in a Teflon-lined autoclave at 180°C for 30h. Silica coating was carried out by mixing the as prepared hematitie, tetraethoxysilane (TEOS) and ammonium hydroxide followed by stober method. The 3-(2aminoethylamino) propylmethyldimethoxysilane (APMS) and succinic anhydride (SA) are graft carboxyl group at prepared hematite@SiO_2 nanoparticles. For amino functionalization, hematite@SiO_2-NH_2, 3-(2aminoethylamino) propylmethyldimethoxysilane (APMS) was grafted onto the prepared hematite@SiO_2 nanoparticles surfaces in their aqueous suspensions. The carboxyl functionalization was obtained in the surface amines at the functionalized, hematite@SiO_2 nanoparticles, with succinic anhydride (SA) in non-aqueous medium. In this, the SA only reacted with the terminal primary amino groups of the surface-grafted APMS molecules. The characterization of the samples by X-ray powder diffraction (XRD) confirmed the formation of α-Fe_2O_3 (hematite). Scanning electron microscope (SEM) analysis was carried out to study the morphology and particle size of the hematite prepared. The presence of the terminal primary amino groups and carboxyl groups on the surface of hematite@SiO_2 was confirmed by FT-IR.

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발표코드: **MAT.P-1305**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and Raman analysis of graphitized carbon nanotubes decorated with Gold nanoparticles by conversion of sucrose assisted template.

이명순 홍성철 김돈

부경대 화학과

We investigated a facile route to prepare the AuNPs attached carbon nanotubes(Au@C) by a thermal decomposition method. This method consists of the thermal decomposition of HAuCl4 followed by the carbonization of sucrose in the AAO channel with a diameter of ~80 nm and a length of ~30 μm. This synthetic route produces the conductive and graphitized CNTs with a relatively large AuNPs. The size variation of the attached AuNPs at Au@C was discussed with optical and diffraction methods. The degree of crystalization and the size of carbon crystals in the graphitized carbon phase were discussed with Raman shift.

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발표코드: **MAT.P-1306**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of High-*k* Dielectric Thin Films via Electrophoretic Deposition of Layered Metal Oxide Nanosheets

박수혜 김수정

이화여대 화학나노과학과

As precursors, nanometer-thick nanosheets of several dielectric metal oxides such as titanoniobate (Ti_5NbO_{14}, Ti_2NbO_7), calcium niobate, and strontium niobate are prepared by soft-chemical exfoliation process of the pristine alkali metal titanoniobates and alkali metal niobates. The thin films of these layered metal oxides can be successfully fabricated by a facile electrophoretic deposition of the precursor colloidal nanosheets. The formation of uniform and dense films consisting of well-stacked metal oxide nanosheets is confirmed by field emission-scanning electron microscopy and transmission electron microscopy. Elemental mapping analysis clearly demonstrates negligible change of the chemical composition of component nanosheets upon the electrophoretic deposition. The obtained thin films of titanoniobates and niobates show much higher dielectric constant than do the corresponding bulk materials, underscoring the merit of the present deposition method for preparing the high-*k* dielectric films. Moreover, the dielectric property of these films is easily controllable by changing the composition and structure of the exfoliated nanosheets. The present electrophoretic deposition method can provide a facile and economic methodology to fabricate the high-*k* thin film with exfoliated nanosheets. In terms of processibility, fabrication time, and energy consumption, the present electrophoretic deposition is much superior to the previously reported deposition methods such as Langmuir-Blodgett deposition and layer-by-layer deposition.

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

A Linker-Mediated Route to Porous Nanohybrids of CdS-Layered Double Hydroxide with Highly Efficient Photocatalytic Activity

이장미 김인영[1] 황성주[1]

이화여대 화학나노과학부 [1]이화여대 화학·나노과학과

Isocharged nanospecies of cationic CdS quantum dots and cationic Zn-Cr-layered double hydroxide (Zn-Cr-LDH) nanosheets can be successfully hybridized using inorganic anion as a linker. The effects of the charge and electrical property of linker species on photocatalytic activity of the resulting CdS-Zn-Cr-LDH nanohybrids are investigated with several anionic species. The maintenance of the crystal structure of CdS and Zn-Cr-LDH components upon hybridization is confirmed by powder X-ray diffraction and X-ray absorption spectroscopy. The formation of mesoporous structure with expanded surface area of ~100 m^2 g^{-1} is attributable to the house-of-cards-type stacking structure of sheet-like LDH crystallites. A strong electronic coupling between CdS and Zn-Cr-LDH is obviously evidenced by diffuse reflectance UV-vis spectroscopy and photoluminescence spectroscopy. The CdS-Zn-Cr-LDH nanohybrids display high efficient photocatalytic activity for visible light-induced O2 production, which is much higher than those of the pristine Zn-Cr-LDH and CdS. All the findings presented here clearly demonstrate the usefulness of the anionic linker not only in hybridizing two kinds of positively charged nanomaterials but also in exploring new efficient hybrid-type photocatalysts.

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A Study on Single-layered White Organic Light-emitting Diodes based on Co-Host System using Solution Process

김범진 박종욱

가톨릭대 화학과

The interest in organic light-emitting diodes (OLEDs) based on White OLEDs (WOLEDs) has been rapidly growing in display and lighting application fields. WOLEDs device has been generally fabricated by using a vaccum evaporation method, but the vacuum evaporation method has disadvantages such as high manufacturing cost and difficulty in large-area production.Solution process such as spin-coating and inkjet-printing method has also attracted much attention due to its potential advantage of easy production for large-area lighting and extremely low production cost. However, multilayer is difficult to be made with solution process, which means low device efficiency compared to that of evaporation method.In this paper, we report high-efficient single emitting layer based on co-host system by using solution process. The device configuration is as the following: ITO / PEDOT: PSS (40nm) /EML (50nm)/TPBi (20nm)/LiF/Al. Double host (NPB and TATa) and dopant (DPAVBi and Ruburene) in emitting layer were used. These devices show two-colored white emission having a CIE (0.307, 0.409). α-NPB and β-NPB were used to compare the effects of energy transfer mechanism from host to dopant. As a result, the device using α-NPB as host shows 3.87 cd/A, which leads to higher efficiency than that of device using β-NPB. α-NPB showed more efficient energy transfer effect than β-NPB.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Thermoelectric Properties in Bismuth Chalcogenide Multicomponent Nanocomposites by Scalable Surfactant-Free Synthesis

민유호

연세대 신소재공학

Thermoelectric materials have been intensively investigated in order to realize highly efficient power generation and eco-friendly refrigerating systems. Bismuth telluride (Bi2Te3) is a narrow band-gap semiconductor, when alloyed with antimony or selenium is an effective thermoelectric material near room temperature. Bi2Te3 based thermoelectric materials are widely used for small-scale cooling applications such as CCS (climate control seat), however, wider applications including power generation from low-grade heat (

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The encapsulation layer for Organic Light Emitting Diodes made up of Aluminium oxide and F-Alucone

권덕현 김홍범 성명모

한양대 화학과

Active Matric Organic Light-Emitting Diodes (AMOLEDs) draw people interests due to their vivid full color, perfect video capability, light weight, low driving power, and potential flexibility. Due to the absence of backlight source, AM-OLED can be flexible compare to the Liquid Crystal Display (LCD). However, the absence of powerful and flexible encapsulation layer of AM-OLED that can prevent the water and oxygen molecules which degrade the AM-OLED is the huge obstacle of realization for flexible AM-OLED. Therefore, our group makes the encapsulation layer by Inorganic-Organic hybrid thin film with Atomic Layer Deposition (ALD) and Molecular Layer Deposition (MLD) techniques. This hybrid layer with 110nm has the $2.04*10^{-6}$ g/m^2 day of Water Vapor Transmission (WVTR) value that is tested by Ca sensor and requirement value for AM-OLED is 10^{-6} g/m^2 day of WVTR. More tests about flexibility will be needed, nevertheless this kind of hybrid film can be used in flexible devices.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Bipolar resistive switching in vapor phase polymerized poly (3, 4-ethylenedioxythiophene) organic memory

Pranav Kalode 성명모

한양대 화학과

We report nonvolatile memory properties of poly (3, 4-ethylenedioxythiophene) (PEDOT) thin films grown by vapor phase polymerization using FeCl3 as an oxidant. Liquid-bridge-mediated transfer method was employed to remove FeCl3 for generation of pure PEDOT thin films. Electrical measurement of organic memory device showed voltage induced bipolar resistive switching behavior with ON/OFF ratio of 103 and reproducibility of more than 103 dc sweeping cycles. ON and OFF states were stable up to 104 seconds without significant degradation. Cyclic voltammetry data illustrates resistive switching effect can be attributed to formation and rupture of conducting paths due to oxidation and reduction of PEDOT. The maximum current before reset process was found to be increase linearly with increase in compliance current applied during set process.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Photovoltage by the Modification of Counter Electrode in Dye Sensitized Solar Cells

강태연 채원식 고민재[1]

한국기초과학지원연구원 강릉센터 [1]KIST 광전하이브리드연구센터

Three different kinds of Pt electro-catalytic counter electrodes including tin oxide (SnO2), zinc oxide (ZnO), and mixed zinc-tin oxide (ZnSnO) films on FTO, were fabricated by the atomic layer deposition (ALD) technique and then their photoelectrochemical performances in dye sensitized solar cells (DSSCs) were investigated. The open circuit voltage (Voc) of DSSCs with the ZnO and ZnSnO film counter electrodes was enhanced by approximately 11% and 3%, respectively, as compared with that of traditional Pt/FTO counter electrode. However, such an increment in Voc was not observed for the cell with the SnO2 film counter electrode. We will report the origin of Voc change depending on the types of counter electrode from the electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) measurements.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Metal/Ceramic Hybrid Particles Composed of Nanoneedle Iron oxide core and Armor Calcium carbonate shell with Superior Capability for Water Treatment

남보라 이하진[1] 최원산[2]

한국기초과학지원연구원 [1]한국기초과학지원연구원 전주센터 [2]한밭대 응용화학과

탄산칼슘 (CaCO3)은 CO2 흡수제, 오-폐수 흡착제, 약물 전달체, bone cement 와 같은 골격구조제등으로 활용되는 매우 중요한 물질로서, 다양한 합성방법에 대해 많은 연구와 결과들이 보고되고 있다. 그러나 탄산칼슘의 특성상 일정한 구조를 갖는 복합체 형태로 합성하는 일은 쉽지 않아 많은 연구가 필요하다. 본 연구에서는 매우 간단한 실험방법을 통하여 일정한 크기와 모양의 자성 탄산칼슘 입자를 합성하였다. 산화철 전구체와 염화칼슘, 탄산나트륨을 용매 내에서 섞고 일정한 조건에서 반응하면 코어 부분은 자성을 띄는 나노니들로 쉘 부분은 갑옷과 같은 탄산칼슘 블록으로 구성되는 구형의 입자를 합성할 수 있었다. 이때, 반응조건을 조절함에 따라 자성의 특성과 입자의 크기 및 구조를 제어할 수 있었다. 또한, 이 입자는 구조의 특성상, 중금속 흡착 및 오-폐수 제거에도 매우 뛰어난 성능을 보여주었다.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyelectrolyte-Coated CNTs as a Three-Dimensional Nanonecklace Support for Embedding High-Density of Metal Nanoparticles

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한국기초과학지원연구원 [1]한국기초과학지원연구원 전주센터 [2]한밭대 응용화학과

We have reported a very simple approach (sequential sonication techniques) for synthesizing well-defined nanonecklace structure of polyelectrolytes (PEs)-coated multi-walled carbon nanotubes (MWCNTs) without prior chemical modification. Initially, MWCNTs were coated with anionic polystyrene sodium sulfonate (PSS) PE. Then, cationic poly(allylamine) hydrochloride (PAH) and anionic poly(acrylic) acid (PAA) PEs in to nonstchiometric ratio were assembled on top of the PSS modified nanotubes in aqueous solution. After sequential coating, nanonecklace shaped CNTs, functionalized with both NH2 and COOH groups (denoted as MWCNT/PSS/PAH/PAA) was obtained. The surface coating was verified with zeta potential measurements, Raman spectroscopy, SEM and TEM. Subsequently, MWCNT/PSS/PAH/PAA was employed as a three-dimensional support for loading ultra-high-density of individual Au, Ag, Pt, Pd metal nanoparticles (NPs) or multi-metallic hybrid NPs such as Au/Pt, Au/Ag, Ag/Pd, and Au/Pt/Ag/Pd. Moreover, tunable and side specific controlled loading of metal NPs on MWCNT/PSS/PAH/PAA have been characterized successfully. As future prospects, these hybrid materials could be used for constructing electrochemical devices as well as powerful SERS substrate for biological tags and molecular detection.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Li^+ extraction/insertion properties of $Li_{1.6}Mn_{1.6}O_4$ and $LiM_{0.5}Mn_{1.5}O_4$ (M=Ni, Co) in aqueous solutions

권지희

충남대 화학과

The spinel-type lithium manganese oxides are interesting materials because of their extremely high affinity toward lithium ions. Especially $Li_{1.6}Mn_{1.6}O_4$ is the most suitable for recovery of lithium from seawater, because it has a high chemical stability, high selectivity for lithium ions and large adsorptive capacity. It is also known that the chemical stability of transition metal substituted spinel materials is expected to be improved compared to the unsubstituted ones. We have prepared the transition metal substituted spinels with Ni, Co in order to improve the lithium adsorptive capacity of the $LiMn_2O_4$. In this work $Li_{1.6}Mn_{1.6}O_4$ and $LiM_{0.5}Mn_{1.5}O_4$(M=Ni, Co) are prepared using sol-gel method. And then the Li^+extraction were performed in a acidic solution. The Li^+ uptake experiments were progressed to evaluate the lithium adsorption capacity. The physicochemical properties of the product were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), brunauer-emmett-teller(BET) and inductively coupled plasma atomic emission spectroscopy (ICP-AES).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Properties of ordered mesoporous spinel $Li_{1.6}Mn_{1.6}O_4$and Li^+ uptake capacity as a lithium adsorbent

전현철

충남대 화학과

Spinel lithium manganese oxides can be used as Li^+ adsorbent with extraction of lithium. In this work, the sol-gel methods were introduced to prepare spinel lithium manganese oxides. The ordered mesoporous Li-Mn spinels are of great interest as the material of lithium adsorbent because it has good selectivity and high efficiency towards Li^+ ion. We have preapred mesoporous $Li_{1.6}Mn_{1.6}O_4$ using KIT-6 and SBA-15 as the template. Li and Mn acetates were mixed simultaneously adding the mesoporous silica(KIT-6, SBA-15), and precursors was calcined in air at 500℃. The uptake of lithium from artificial seawater was performed and compared with $Li_{1.6}Mn_{1.6}O_4$. The conventional physicochemical properties of the mesoporous Li-Mn spinels were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), thermogravimetric analysis (TGA)/differential thermal analysis(DTA), inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and brunauer-emmett-teller(BET)

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of spinel $LiM_{0.5}Mn_{1.5}O_4$ (M = Co, Ni, Cu) from needle-like β-MnO_2 using flux method and its lithium uptake capacity for lithium adsorbent

채창완

충남대 화학과

Ion-sieve type manganese oxide spinels for the selective adsorption of lithium from seawater were prepared and their properties were examined. Needle-like $LiM_{0.5}Mn_{1.5}O_4$ are prepared using needle-like β-MnO_2. We have proven that the morphology control of the precursor compounds such as β-MnO_2 can provide a route to control the morphology of the final products. In this work, the $LiM_{0.5}Mn_{1.5}O_4$ has been synthesized from needle-like β-MnO_2 through flux method using relatively low reaction temperature, which prevents β-MnO_2 from the phase transition occurred at more than 500°C owing to the loss of oxygen. For the purpose of evaluating the as-prepared $LiM_{0.5}Mn_{1.5}O_4$ as lithium adsorbent, manganese oxide adsorbent ($HM_{0.5}Mn_{1.5}O_4$) was made by acid treatment, and then the Li^+ uptake was carried out in lithium-enriched solution. SEM observation showed that the needle-like morphology of β-MnO_2 was maintained through the whole processes. The physicochemical properties of the needle-like $LiM_{0.5}Mn_{1.5}O_4$ and needle-like $HM_{0.5}Mn_{1.5}O_4$ were characterized by X-ray powder diffraction (XRD), brunauer-emmett-teller(BET), inductively couple plasma-atomic emission spectroscopy (ICP-AES) and thermogravimetric analysis (TGA)/differential thermal analysis (DTA).

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장소: 부산BEXCO

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Investigation of Cell Morphology on Hierarchical Nanostructures of Conducting Polymer

경민규

광주과학기술원 신소재공학부

Recent years have witnessed that cell morphology is highly dependent on physical environments such as substrate rigidity/topography and electric field which dramatically affect cellular functions in many cases. However, there have been relatively few systematic studies on the relation between cell morphology and substrate topographical parameters while electrical stimulation is applied. In this presentation, we report how cell morphology is affected by the nanoscale topography of underlying substrates and the applied electrical field. First, we fabricated vertical silicon nanowires (SiNWs) via metal-assisted chemical etching and deposited poly(3,4-ethylenedioxydithiophene) (PEDOT) on SiNWs by electrochemical polymerization. Subsequently, mouse embryonic fibroblast cells (NIH-3T3) were cultured on the bare and PEDOT-modified SiNW substrates, and cell viability and morphology were examined. In contrast to the flat and star-like morphologies of cells grown on the control flat substrates, those on the PEDOT-coated SiNW substrates exhibit three-dimensional and round morphologies as revealed by confocal fluorescence microscopy. Additionally, we observed that the simultaneous application of electric field effectively controls cell viability and morphology on the vertical nanostructures. We expect that our study contributes to a fundamental understanding of external stimuli-induced tissue regeneration and wound healing mechanism.

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Branched and Three-Dimensional Transformed Nanochannels through Anodization of Pre-Patterned Aluminum Surface

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KAIST(KAIST) 나노과학기술대학원 [1]KAIST 나노기술대학원 [2]KAIST 나노과학기술대학원

Anodic aluminum oxide (AAO) membrane composed of highly ordered hexagonal nanochannel arrays has been attractive due to its structural potential as a template material for metal/metal oxide nanowires and also as a host material for energy storage, catalysts and sensor system. We studied the growth mechanism of pre-patterned nanochannel arrays with 100-240 nm interpore distances at intervals of 10 nm using focused ion beam lithography. Nanochannels developed in accordance with the interspacing of concaves and that affects the morphological change of both the pore diameter and the depth from top to the branched site. As induced interpore distance changed from the range of 100, 110-150 nm, 150-180, and 190-240 nm, the three-dimentional transformation of nanochannels occurs differently with distinct conditions. Our approach will be helpful for fundamental studies which describe the effects on interpore distance variation in AAO synthesis procedure.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of single-crystal organic nanowire field-effect transistors from solution-processed indolocarbazole derivatives

박경선 정진원 성명모

한양대 화학과

We fabricated single-crystal organic nanowire field-effect transistors from solution-processed novel indolocarbazole (IC) derivatives. The direct printing process was utilized to generate single-crystal organic nanowire arrays enabling the simultaneous synthesis, alignment and patterning of nanowires using molecular ink solutions. These new molecules are particularly suitable for p-channel organic field-effect transistors (OFETs) because of the high level of crystallinity usually found in IC derivatives. Selected area diffraction (SAED) and X-ray diffraction (XRD) experiments on these solution-processed nanowires showed high crystallinity. Transistors fabricated with these nanowires gave a hole mobility as high as 1.0 cm2V-1s-1 with nanowire arrays with the direct printing process.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon coated iron oxide core-shell nanostructures as a anode material in lithium ion batteries

박지은 김경[1] 김성진[2]

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Iron oxides have been extensively investigated as an anode material in lithium ion battery due to its high theoretical Li ion storage capacity (900 ~ 1000 mAh/g), low cost and high cycling stability. However, the practical use of this material has been frustrated by its fast capacity fading due to the phase transformation during the lithium alloying and dealloying. To circumvent these problems, we have synthesized the carbon coated magnetite core-shell nanostructure by polymer convert and nitrogen-doped carbon coated magnetite core-shell nanostructures. Structural characterization, such as SEM, TEM, XRD, Raman and XPS measurements clearly shows that the products are monodispersed and the thickness of carbon coating layer is about 5 nm. In addition, preliminary electrochemical study indicated that the present nanostructures showed the enhanced electrochemical property compared to the pristine iron oxide. It is, therefore, concluded that such a carbon coated magnetite core-shell material could be an excellent candidate as an electrode material for lithium ion battery.

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The annealing effect of thermoelectric properties of Ge-doped Bi_2Te_3

유혜인 한미경[1] 김성진[2]

이화여대 화학나노과학과 [1]이화여대 화학나노과학부 [2]이화여대 화학과

Thermoelectric materials are suitable for renewable energy sources due to the ability of converting waste heat into electricity. Among many kinds of materials, Bi_2Te_3-based compounds are the most widely used thermoelectric materials near room temperature but need more enhancement of efficiency. It has been known that the substitution or intercalation with other proper elements in Bi_2Te_3-based compounds can increase the thermoelectric figure-of-merit (ZT) by modifying their morphology, crystal structure or electronic structure. We prepared p-type Ge doped Bi_2Te_3-based bulk samples with various composition using Bridgman method, and studied thermoelectric properties as a function of Ge doping in Bi_2Te_3. To optimize the thermoelectric properties of Ge_x Bi_2Te_3, we tried to annealing samples at 773K for 100 hours. The structure and composition of the samples are characterized by using XRD and EDS. To understand the effect of annealing on the thermoelectric properties, we investigated the temperature dependence of Seebeck coefficient and the electrical conductivity of annealed and non-annealed Ge_x Bi_2Te_3 . Among the as prepared Ge_x Bi_2Te_3 ($0.005 < x < 0.02$) samples, the $Ge_{0.01}Bi_2Te_3$ showed the highest power factor of 25μW/cmK^2 at room temperature, while $Ge_{0.005}Bi_2Te_3$ had a power factor of 23μW/cmK^2 at room temperature. However after annealing at 773K, power factor of $Ge_{0.005}Bi_2Te_3$ showed the highest power factor of 30μW/cmK^2 at room temperature.

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장소: 부산BEXCO

발표코드: **MAT.P-1323**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of thermoelectric PbTe nanoparticles and its ligand substitution

성은규 한미경[1] 김성진[2]

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Lead telluride (PbTe) is one of the promising thermoelectric materials in mid-range temperature. Recent research in thermoelectric materials has involved decreasing lattice thermal conductivity with nano-scaled morphology. Typically, synthesized nanoparticles are protected by organic capping materials which have low electrical conductivity. To enhance electrical properties, ligand substitution with inorganic ligand is designed. We obtained mono-dispersed lead telluride nanoparticles with different size distribution, the size of the particles is around 10-25nm. Ligand substitution with metal chalcogenide complexes was carried out by two-phase heterogeneous reaction. In this case, oleic acid was exchanged with SnS4-. PbTe-PbS heterogeneous nanostructures were found after spark plasma sintering (SPS) and generated coherent interface that cause enhanced phonon scattering. The synthesized nanostructures are investigated by using HR-TEM and XRD analysis. Thermoelectric characterization was also performed. Surface-modified PbTe nanostructures are expected to contribute to improvement of the thermoelectric performances.

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장소: 부산BEXCO

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발표종류: 포스터, 발표일시: 수 16:00~19:00

n-Type Nanostructured Bulk Thermoelectric Materials Prepared from Chemically Synthesized Cu doped Bi2Te3 Nanotubes

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Highly uniform Bi2Te3 and Cu doped Bi2Te3 nanotubes with a length of 1 μm and a diameter of 40 nm were synthesized through a simple and fast solution process by using ultrathin Te nanowires as sacrificial templates. The synthesized nanotubes were investigated with HR-TEM, XRD, FT-IR spectroscopy, SEM-EDS, TGA analysis. Nanostructured bulk materials were prepared by sintering of Bi2Te3 and Cu doped Bi2Te3 nanotubes using spark plasma sintering. The densification behavior, microstructure, and phase formation of sintered samples were characterized. The electrical conductivity, Seebeck coefficient, and thermal conductivity were investigated and the resulting thermoelectric figure of merit was determined. Unlike pure Bi2Te3, Cu doped Bi2Te3 showed a highly reduced thermal conductivity. The maximum thermoelectric figure of merit ZT ~ 0.68 was obtained at 418 K, which is one of the highest among the reported values of n-type nanostructured materials based on chemically synthesized nanoparticles.

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Synthesis of bismuth nanoparticles with controlled morphology and size

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Bismuth nanoparticles were prepared by reducing Bi3+ with oleylamine in the presence of 1-dodecanethiol. It was found that the sizes and morphologies of bismuth nanoparticles could be tuned by changing the relative ratio of 1-dodecanethiol to oleylamine, reaction temperature and reaction time. The as-prepared nanoparticles are characterized by X-ray diffraction, scanning electron microscope, and high-resolution transmission electron microscope using an energy dispersive spectroscopy. The average particle size of bismuth nanoparticles was found to increase with the relative ratio of 1-dodecanethiol to oleylamine. While these bismuth nanoparticles were synthesized at 60℃, we obtained 200 nm length bismuth nanoplates with reaction temperature over 100℃.

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A simple structure of semiconducting copolymer for Organic Thin Film Transistors

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A simple copolymer was synthesized by stille coupling. The copolymer has good solubility in chlorobenzene, and dichlorobenzene while it was soluble chloroform, toluene, tetrahydrofuran with heating condition. The organic semiconductor's soluble system was realizable as bulky alkyl group. The polymer achieve high organic semiconductor field effect mobilities by fused aromatic ring. The material was confirmed by FT-IR and 1H-NMR spectra, and the molecular weight was measured by GPC in THF. The copolymer was characterized by UV, CV, DSC, and TGA.

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Synthesis and Photoluminescence Properties of Green Phosphors CaWO4:Tb3+

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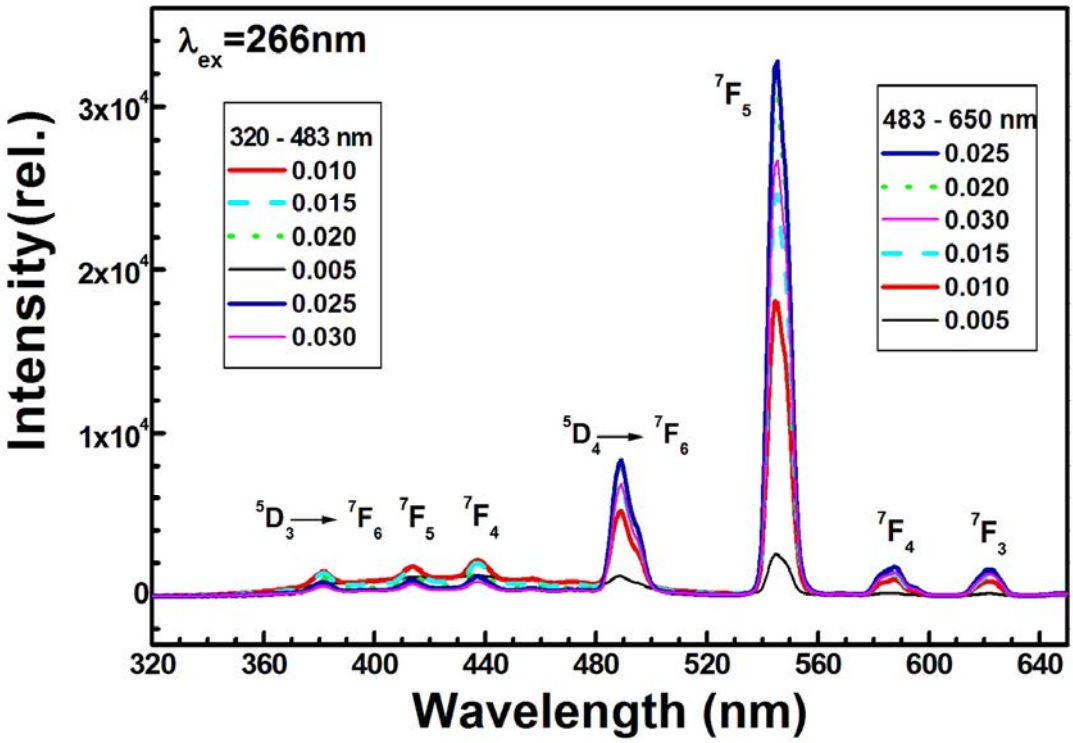
신라대 신소재공학과

Green phosphors Ca1-1.5xWO4:Tbx3+ were synthesized with different concentrations of Tb3+ ions by using a solid-state reaction method. The crystal structure of the green phosphors were found to be a tetragonal system. X-ray diffraction (XRD) results showed the (112) main diffraction peak centered at 2=28.72°. The excitation spectra of all the phosphors were composed of a strong broad band centered at 266 nm in the range of 220-320 nm due to O2-?W6+ and 4f-5d transitions of Tb3+. In the case of emission spectrum (Fig 1), all the phosphor powders, irrespective of Tb3+ ion concentrations, indicated a strong green emission peaked around 550 nm due to the 5D4?7F5 transition, with other 4f-4f transitions of Tb3+. The highest green emission intensity occurred at x=0.025 of Tb3+ ion concentration. The dependence on the Tb3+ concentration in the Ca1-1.5xWO4:Tbx3+ photoluminescence shows very effective use of energy in the range of 320-480 nm, with cross-relaxations of Tb3+, and finally yields it as a strong emission of green light.



THE KOREAN CHEMICAL SOCIETY

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Development of polymeric adhesion layer for nanotransfer molding

이기석 이린 성명모

한양대 화학과

We studied an effect of the polymeric adhesion layer, eg. PVP, PMMA, PVA, PAA, between organic nanowires and a Si substrate when the nanowires are transferred by liquid-bridge-mediated nanotransfer molding method(LB-nTM).Their structural stability was examined by optical microscopy, scanning electron microscopy as multiple transfer molding and washing process. Field-effect transistors were fabricated with organic semiconductor nanowires on a polymeric adhesion layer and their electrical properties showed no significant difference as the one without the adhesion layer.

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Two-Dimensional Large-Area Graphitic Structure Driven from Hyperbranched Polymer and Electrical Performance

배서윤

울산과학기술대 친환경에너지

Graphene, two-dimensional (2D) single layer of carbon atoms, is a promising material having remarkable properties such as zero band-gab, ambipolar electric field effect, Quantum Hall effect and so on. Currently, many researchers focus on obtaining low-cost and high-quality graphene via chemical vapor deposition (CVD), oxidation of graphite, electrochemical exfoliation of graphite. Here, we report a new method for the formation of large-area graphitic film from hyperbranched polymer, which is prepared from the polymerization of 4-ethylbenzoic acid (EBA). The resultant hyperbranched polymer displayed 2D crystalline structure. As a result, 2D graphitic structure, which was observed by transmission electron microscope (TEM) and atomic force microscopy (AFM), could be prepared by a simple solution casting and subsequent thermal annealing. The electrical properties of large-area graphitic film were studied by using field effect transistors (FET).

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Structural, magnetic and infrared studies of La0.8SrxCa0.2-xMnO3 (0 ? x ? 0.2)

장수진 손세민

동국대 화학과

Abstract. We report the results of magnetic, X-ray powder diffraction and infrared Spectroscopic studies on the La0.8SrxCa0.2-xMnO3 (0 ? x ? 0.2) manganite. The structure refinement by using the Rietveld method indicates that the partial substitution of strontium by calcium (for x ≥ 0.15) modifies the orthorhombic structure of the CaMnO3 perovskite towards a rhombohedral phase. Magnetic measurement confirms increase in the Curie tempearature from 182 K for La0.8Ca0.2MnO3 to 307 K for La0.8Sr0.2MnO3, respectively. It is argued that the substitution with the larger with Sr2+ ion strengthens the double-exchange interaction and gives rise to the observed increase of transition temperatures. All manganites show two active IR vibrational modes around 400 and 600 cm?1. Moreover, when x ? 0.1, the absorption band around 400 cm?1 splits into two peaks and the results were well explained by the electronic delocalization.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The study of spinel $Li_4Ti_5O_{12}$ enhanced rate-capability as an anode material in lithium ion batteries

김경옥 류광선

울산대 화학과

$Li_4Ti_5O_{12}$ can accommodate Li with a theoretical capacity of 175mAh/g. And it has very flat charge and discharge curves and the potential for Li-insertion is about 1.55V vs. Li/Li+, which is above the potential range where most electrolytes or solvents are reduced. Unfortunately, $Li_4Ti_5O_{12}$ exhibits poor electronic conductivities, thereby limiting its rate-capability. To overcome a disadvantage, we study doped-$Li_4Ti_5O_{12}$ and carbon-coated $Li_4Ti_5O_{12}$. These materials can reduce the damage of electrode and improve rate-capability and cyclic performance. Synthesis was conducted solution combustion method. As a result, these experiments affect to improve rate-capability and electrical conductivity rather than pristine $Li_4Ti_5O_{12}$ at high current density.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Solution processed wide band-gap $CuInGaS_2$ thin film for solar cell applications

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고려대 화공생명공학과 [1]KIST 청정에너지연구센터

A wide band-gap (1.55 eV) $CuInGaS_2$ thin film was prepared by a precursor solution based coating method. In order to eliminate carbon residue derived from organic binder and solvent, air annealing was applied. Subsequently, sulfurization was carried out for the formation of the $CuInGaS_2$ alloy. The film was characterized by various analysis techniques including XRD, SEM, EPMA and AES. As a result, the film revealed two distinct morphologies: a densely packed bulk layer and a rough surface layer. We found that the rough surface is caused by the formation of Ga deficient $CuInGaS_2$ crystallites. Although two distinct morphologies existed simultaneously on the surface, the film showed good device performance. Due to the wide band-gap optical property of the $CuInGaS_2$ absorber film, a solar cell device with this film showed a relatively high open circuit voltage (~787 mV) with a power conversion efficiency of 8.28 % under standard irradiation conditions.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of Cu_2ZnSnS_4 thin film for solar cells using paste

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Cu_2ZnSnS_4(CZTS) is a very promising materials in the use of absorber layers of solar cells. CZTS contains earth-abundant elements of zinc and tin, a high optimal absorption coefficient and ideal band gap for photovoltaic applications. The CZTS thin films in Ethanol was successfully prepared via precursor solution method. The solution was spin coated on molybdenium substrates and dried at 350 °C. The coated substrate were sulfurized by annealing at 500 °C in a hydrogen sulfide-containing atmosphere. The characterization of its structure, composition, morphology and absorption spectra were done using X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM) and UV-vis absorption spectra. The solar cells with a structure of glass/Mo/CZTS/CdS/ZnO/i-ZnO/Al and a result of the investigations, the best solar cell showed an open circuit voltage of 556 mV, a short current density of 13.5 mA/cm2, a fill factor of 40.3 % and a conversion efficiency of 3.02 %.

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Bifacial CuInGaS2 thin film solar cells by a low cost paste coating method

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Solution processed chalcopyrite compound film (CuInGaS2, CIGS) was synthesized on transparent conducting oxide substrates (tin-doped indium oxide, ITO) aiming at fabrication of bifacial inorganic thin film solar cells by a low cost and printable method. According to the solar cell performance of the CIGS solar cell devices with the CIGS thin films of three different thickness (400, 800, and 1200 nm) the solar cell device with the thickest film (1200 nm) resulted in the highest power conversion efficiency for front side illumination (5.61%) while the 800 nm thick film revealed the best solar to electricity conversion performance for rear side illumination (1.01%). Compared to the simple sum of the efficiencies of the front and rear side illumination only, the bifacial illumination resulted in an extra increase of the apparent power conversion efficiency in the range of 0.1?0.5 %, depending on the CIGS film thickness. We also confirmed that this extra output power acquisition due to bifacial irradiation was not apparently influenced by the light intensity of the rear side illumination, implying that reflected light from the ground (weak light) can be efficiently utilized for improving the overall solar cell efficiency of bifacial devices. This was further confirmed by power conversion efficiency measurement in an outdoor test. The details will be discussed in the presentation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and charicterization of CMK-3 with various shape and size

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고려대 소재화학과 [1]고려대 신소재화학과

Well-ordered two-dimensional hexagonal mesopore silica structure (SBA-15) material (space group p6mm) with rodlike morphologies were controlled by adjusting hydrochloric acid concentration in the range 0.1-5.0 M. But, Synthesis of convensional SBA-15 with under 1 aspect ratio (ratio of length vs. diameter) is not possible. A novel synthesis route for preparing highly ordered plate-like SBA-15 silica with short mesochannels (150 ? 350 nm), which have about 0.2 aspect ratio and large pore diameters up to 12 nm has been developed for the past. In this work, a small amount of Zr(IV) ions and trimethylbenzene (TMB) as the pore swelling agent were added to the conventional SBA-15 (SBA-15-c) synthesis method to prepare platelet SBA-15 (SBA-15-p) materials with expended pores. The fast self-assembly rate of P123 micelles and tetraethyl orthosilicate (TEOS) was accelerated by the Zr(IV) ions in the synthesis solution, producing thin plate-like hexagonal thin SBA-15.Highly ordered mesoporous carbon, denoted CMK-3 was synthesized by using mesoporous silicates, SBA-15 as the starting templating materials and phenol as the carbon source. This CMK-3 with various shape and size can be tuned for specific applications such as fuel cell, lithium-ion battery, capacitor, etc.

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Europium (III) Complex-Clay Nanohybrids for Latent Fingerprint Detection

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서울대 화학부 [1]동국대 화학과 [2]국립과학수사연구원

Complex of europium (III) with 1, 10-phenanthroline was intercalated into Na+-montmorillonite and Na+-hectorite clay minerals by ion exchange reaction. The guest lanthanide complex was obtained by simple complex reaction between europium chloride (EuCl3?6H2O) and 1, 10-phenanthroline (phen) as 1:2 molar ratio of Eu3+ ion to ligand molecule. The precursor complex was characterized by powder X-ray diffraction and elemental analysis. After intercalation reaction, nanohybrids display interlayer distances and stoichiometries in agreement with the ion exchange capacity and the interlayer space available in the clays.The obtained samples were characterized by elemental analysis, thermal analysis (TG-DTA), X-ray powder diffraction measurements, Fourier transform infrared, UV-vis, and fluorescence spectra, and their properties and structure were determined. The intercalated complex exhibits luminescence where both ‘‘antenna’’ effect of the 1, 10-phenanathroline and the intensity maxima (a characteristic red 5D0-7F2 emission) are comparable to the free complex suggesting that these products promising for the latent fingerprint detection.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal structural and surface change of ZnO nanoparticles in controlled pH system

곽경현 최진호[1] 오제민

연세대 화학및의화학과 [1]이화여대 화학.나노과학과

We have studied the crystal structural and surface change of ZnO nanoparticles which have two different sizes (20 and 70nm) and three types of surface chemistries (pristine, positively and negatively coated). The pH of dispersing media was controlled as 7.4, 1.2 and 6.8 which simulate the pH condition of saliva, stomach and intestine. The change of crystal structure of ZnO nanoparticles was measured by the X-ray diffraction and then analyzed by Rietveld refinement in detail. We observed a phase transition from zinc oxide (Wurtzite) to zinc hydroxide (hydrozincite) at time points after 10 h in the XRD patterns. However, the crystal structure of ZnO analyzed with the Rietveld refinement showed no significant change in occupancy. All the zinc ions in the crystal structure remain in the place with little vibration, on the other hand, oxygen atoms showed notable change of equivalent isotropic thermal parameter value. In order to verify the change in particle shape and surface with respect to the pH of dispersing media, scanning electron microscopic images were obtained. As a result, their shape, size and surface were remained regardless of the original surface charge and colloidal pH condition.

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Conductive zinc oxide thin films deposited by atomic layer deposition with UV irradiation

양다솜 김홍범 성명모

한양대 화학과

Zinc oxide(ZnO) is semiconductor with a wide band gap(3.35eV) and transparent in the visible region(400~800nm). ZnO can be deposited with various methods, such as metal organic chemical vapour deposition, magnetron sputtering and pulsed laser ablation deposition. . Atomic layer deposition(ALD) is based on the sequential, saturating surface reaction, which are accomplished by alternative dosing the gaseous precursors. Due to its self-limiting growth mechanism, ALD is useful to deposit conformal and precise thin films.In this experiment, ZnO thin films was deposited by UV-enhanced atomic layer deposition(ALD) using diethyl zinc(DEZ) and D.I. water(H2O) as precursors with UV irradiation. When H2O is dosing, the UV light is exposed to the substrate or the additional exposure is done after H2O dosing. The main wavelength of UV light is 365nm. As varying the UV exposure time, the conductivity changed. It was very effective to improve the conductivity of ZnO thin films. The thickness is measured by the ellipsometry and the transmittance of thin film is measured by the UV-visible spectroscope. The resistivity of ZnO thin films is investigated by the four-point probe. From these result, it is expected to be applied to electronic or photonic devices as electrode (for example, field effect transistors, memories and so on.) and especially, the transparent conductive oxide in solar cells or organic light emitting diode.

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전기영동 디스플레이 적용을 위한 카본 블랙입자의 표면 개질

김주연 서경수[1]

ETRI 전자종이연구팀 [1]한국전자통신연구원 전자종이연구팀

비발광형 디스플레이 소자에 속하는 전기 영동 디스플레이는 기존의 종이 위에 표시되던 정보를 대체 할 수있으며, 인간의 눈에 미치는 피로도가 낮은 장치로, 전자 종이용 디스플레이 기술 가운데 현재 상용화가 되어있다. 전기 영동 디스플레이는 전기 영동 방식을 기반으로 하며, 전기 영동은 전기 이동의 다른 말로 전하를 띤 입자가 유체내에 분산된 상태에서 인가된 전압에 의해 생성되는 전기장에 의해 이동하는 현상을 말한다.예를 들어, 흑백의 모노톤인 경우에는 일정한 크기를 가지는 구나 셀내에 흑백의 나노 입자를 넣어 인가된전압에 따라 양극이나 음극으로 움직이며, 이로 인해 회부에 정보를 표시하는 것이다.본 연구에서는, 흑색을 나타내기 위하여 카본블랙을 도입하였으며, 도입된 카본 블랙의 오일상에서의 분산 안정성을 높이기 위하여 입자 크기 조절 및 표면 개질을 하였다. 또한, 카본 블랙 입자의 전하 이동도와 전하량에 영향을 미치는 charge control agent 양에 따른 특성을 측정 및 최적화하고자 하였다. 이렇게 얻어진 카본 블랙 입자를 화이트 잉크와 배합하여, 인가되는 전압에 따른 전기 영동 이미지 특성을 확인 할 수 있었다.

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Band Gap Tuning of the Ordered Mesoporous $Cd_{0.5}Zn_{0.5}Se$ Compound Semiconductors through Framework Size Control

이윤연 김지만[1]

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II-VI compound semiconductors, such as ZnE and CdE (E = S, Se, 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. However, only a few examples of the ordered mesoporous compound semiconductors that consist of II, III, V and VI group elements were reported up to now.The band gap tunability of the semiconducting material has a considerable impact on their applications in photovoltaics or LEDs. And the efficiency of the organic-inorganic hybrid solar cell is mainly affected by exciton diffusion from organics to interface of organic-inorganic junction. According to the Marcus theory, the efficiency and speed of exciton diffusion are affected by the energy difference of conduction band of organics and that of inorganics. Due to the band gap change is mainly related to the conduction band shift rather than valence band shift, the band gap tunability of the inorganics in hybrid solar cell might be plays an important role for improving the efficiency.Herein, we report on the band gap tunability of the ordered mesoporous $Cd_{0.5}Zn_{0.5}Se$ materials through the framework size control which could be synthesized using the mesopore size controlled 3-D cubic Ia3d structured KIT-6 as hard-templates via nano-replication. The synthesized materials were investigated by X-ray diffraction, N_2-sorption isotherms, electron microscopy, and diffuse reflectance UV-visible spectroscopy.

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Study for durability and antibacterial activity enhancement of Silver/PMMA nanocomposite films

김효섭 성소희 이승윤 김재호

아주대 분자과학기술학과

나노 소재는 기존의 물질과는 다른 다양한 물리, 화학, 광학적인 성질을 나타내며 나노 소재만이 갖는 넓은 비표면적을 이용한 연구가 활발히 진행되고 있다. 특히 은 나노 제품은 최근 항균 및 자정기술에서 주목받고 하고 있다. 그러나 산업적 응용이 활발히 이루어지고 있지만, 환경 유해성 우려를 해결하기 위해 내구성 향상 기술이 필요하다. 본 연구에서는 항균성과 내구성 모두가 요구되는 항균용 Silver/PMMA Nanocomposite Films 의 PMMA 분자량 조절을 통하여 분산특성과 용출특성 및 항균특성을 평가하는 것에 목적이 있다. PMMA 분자량 3 종(120 KDa, 350 KDa, 996 KDa)을 사용하여 Silver/PMMA Nanocomposite Films 을 제조하였다. 제조된 film 들은 UV-Vis 분광기와 PSA, TEM 장비를 이용하여 Silver/PMMA Nanocomposite Films 의 흡광도 및 AgNPs 의 입자크기와 분산특성을 확인하였다. ICP 분석을 통해 분자량에 따른 Silver 의 용출특성을 관찰하였으며 제조된 film 들은 E.coli Test 을 통하여 항균성 평가를 하였다. UV-Vis. 분광기와 TEM 이미지를 통해 분산 특성을 평가하였다. 그 결과 분자량 120 KDa 과 350 KDa 은 분산 특성이 우수하였으나, 996 KDa 은 분산 특성이 다소 떨어지는 것으로 관찰되었다. ICP 분석을 통한 용출특성 결과 분자량 350 KDa 과 996 KDa 에서 보다 120 KDa 에서 10 배나 많은 양의 Silver 입자가 용출되었다. 항균특성은 Silver 입자의 농도 3,140 ppm 에서 분자량 3 종 모두 우수하게 나타났다.

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Synthesis and characterization of spinel-type lithium adsorbent $LiM_{0.5}Mn_{1.5}O_4$ (M=Co, Ni, Cu) using flux methods

배봉문

충남대 화학과

Spinel-type lithium manganese oxides have received considerable attention as lithium selective adsorbents. Among them, $Li_{1.6}Mn_{1.6}O_4$ consisted of the absolute Mn(Ⅳ) has sufficiently high chemical stability. Its theoretical Li^+ ion exchange capacity may be markedly larger than other lithium manganese oxides. However, Li^+ ion exchange capacity is expected to be improved when transition metal substituted, $LiM_{0.5}Mn_{1.5}O_4$, are prepared with divalent ions (Co, Ni, Cu, etc.). $LiM_{0.5}Mn_{1.5}O_4$ with M(Ⅱ) ordering on the 16d sites is expected to have the optimized structure for the Li^+ selective adsorbents because all Li^+ locate on 8a sites in the structure. In this study, we are quite successful in preparing homogeneous $LiM_{0.5}Mn_{1.5}O_4$ (M=Co, Ni, Cu) using lithium-containing flux at relatively low temperature. Their Li^+ exchange capacity is measured and compared with the unsubstituted ones. The characterization of $LiM_{0.5}Mn_{1.5}O_4$ is performed X-ray powder diffraction (XRD), inductively coupled plasma-atomic emission spectroscopy (ICP-AES), BET method and scanning electron microscope (SEM).

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Structural changes according to the composition and synthesis of nanoparticels, Sn, SnS, and SnSe using pulsed laser.

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고려대 미세소자공학협동/마이크로소자공학 [1]고려대 소재화학과

Nanoparticles were synthesized by the pulsed laser and mixture of TMT (tetramethyltin), H2S (hydrogen sulfide), and DMS(dimethyl selenide) of gas phase. We studied the crystal structure variety form of Sn(tin), SnS(tinsulfide), and SnSe(tinselenide) NPs, tetragonal, orthorhombic, hexagonal, respectively. And the results of differents NPs Tin has type two from of oxidation number, Sn(Ⅱ, Ⅳ) and each compound has different structure of tetragonal(SnS, SnSe), and hexagonal(SnS2, SnSe2) phase. Also, we was syntesis NPs of SnSxSe1-x using control of gas phase.The structure of NPs were analyzed using XRD(X-ray diffraction), HR-TEM(high-resolution transmission electron microscopy).To adjust the pressure of the gas through various substances, and changes the composition of the band gap of the material characteristics can be controlled.

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Metal-Nanodiamond Hybrid Photocatalysts for Hydrogen Generation from Water

장동명 임형순[1] 백승혁 명윤 조용재 김한성 이치우[2] 박정희 이민영[3] 차은희[4]

고려대 소재화학과 [1]고려대 미세소자공학협동/마이크로소자공학 [2]고려대 신소재화학과 [3]이화여대 화학나노과학부 [4]호서대 그린에너지 공학과 대학원

Nanodiamonds (ND) were found to generate hydrogen (H2) from water via multi-photon absorption of Nd-YAG laser pulses (266~1064 nm) at a remarkable rate. The rate of H2 generation increased proportionally with the higher pH, which suggests the H2 oxidation (H2+2H2O→2H3O++2e-) as a main hole scavenging reaction. The ND served as an excellent photocatalyst for the synthesis of various metal nanoparticles such as Au, Ag, Pt, Pd, and Cu, from aqueous precursor solution. All the nanoparticles on the ND were found to increase the rate of H2 generation and specifically, Au was found to be most efficient amongst other nanoparticles with an order of Au > Pt = Pd > Ag. The observed result had a good correlation with standard reduction potential. The Au-ND hybrid on the reduced graphene oxide sheets produced a greater photocurrent than the ND upon irradiation with 514 nm argon ion laser. Both the results proposed an efficient photoelectron transfer from the Au NP to the ND, which was supported by X-ray photoelectron spectroscopy. This simple yet efficient photocatalyst system is expected to contribute toward the development of improved solar energy conversion systems.

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Controlled packing of metal-organic polyhedra by changing peripheral organic substituent

고낙은 김태민[1] 양지은 김자헌

숭실대 화학과 [1]숭실대

Two metal-organic polyhedral (MOP) were prepared through solvothermal reactions between copper ions and 5-hydroxyisophthalate derivatives as bridging linkers. The organic linkers were synthesized by coupling 5-hydroxyisophthalate with benzyl bromide and biphenyl bromide, respectively. Crystal structures indicate that two MOPs termed MOP-1Bz and MOP-1Ph have the same molecular skeleton as that of MOP-1, exhibiting cuboctahedron geometry. Both MOPs are packed through extensive pi-pi interactions among the peripheral benzyl or phenyl groups. MOP-1Ph shows a larger void space in the lattice because the MOP cores were separated far from themselves due to the protruding long phenyl groups.

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Carbon dioxide absorbing behavior of 1-dimethyl-2-methylaminoethanol and its carbamate structure

조은희 전영호 노영수 김자헌

숭실대 화학과

Monoethanolamine (MEA) is the most popular absorbent for removing CO_2 from flue gas streams, but its stripping process requires a large energy cost. To develop more cost-effective alkanolamine than MEA, 1-dimethyl-2-methylaminoethnaol (DMAE) was prepared by an alkylation reaction of methylamine and 1-chloro-2-methyl-2-propanol. After purification in a Kugelrohr apparatus, the product was characterized by FAB-MS, IR, ^{1}H-NMR, and ^{13}C-NMR analyses. The CO_2 absorption capability of DMAE was compared with those of MEA and methylaminoethanol (MAE) in their 30wt% aqueous solutions by measuring the ^{1}H-NMR spectra and solution weight changes of the solutions. In addition, the crystal structure of the carbamate form of DMAE was determined to confirm its reaction with CO_2.

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Electrical Properties of Oxygen-Induced Self-Polymerized Polydopamine Thin Film

차준호 남혜진[1] 정덕영[2]

성균관대 화학 [1]성균관대 기초과학연구소 [2]성균관대 화학과

Polydopamine (PDA) thin film was formed on glass and indium tin oxide substrates by spontaneous self-polymerization of dopamine (DA) using dip-coating in basic buffer solution. Polymerization of DA using dip-coating under various reaction conditions such as O_2 bubbling, UV irradiation and solution temperature control was attempted and O_2 bubbling exhibited the best synthetic result on film surface and thickness. From I-V characteristics analysis, it revealed that the PDA showed diode characteristics and light-induced photocurrent, in which the average resistance was 2.4×10^{10} Ω and the photocurrent increased as a light intensity increased. Hall effect measurement demonstrated that the prepared PDA thin film had amorphous p-type semiconducting property with a carrier concentration of 3.6×10^{13} cm^{-3} and mobility of 36 cm^2/Vs, in good agreement with that of silicon. The electrical resistivity measured by transmission line model (TLM) pattern was 1.5×10^3 Ω·cm, indicating potential applications in photovoltaics, optoelectronic devices and chemical sensors as a photoconductor.

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Cu-Sn Intermetallic Nanoparticles by Borohydride ReductionFor fabrication on Cu_2ZnSnS_4 solar cells

이한경 이연수 차지현 정덕영

성균관대 화학과

Cu_2ZnSnS_4(CZTS) thin films are one of the most viable materials for low-cost, thin film solar cells. In order to reduce the cost of producing CZTS thin films, it is necessary to use a non-vacuum process. We synthesized Cu-Sn alloy metallic precursor by chemical reduction. Cu-Sn alloy synthesized by reduction method using $NaBH_4$ as reductant. Cu-Sn Alloy materials were synthesized by reacting $CuCl_2$ and $SnCl_2$ in glycol at room temperature. The stoichiometric ratios of the copper and tin were 2 to 1 respectively. The CZS thin films were obtained by using sulfurization in Ar atmosphere. The characteristics of Cu-Sn nanoparticles were analyzed with powder X-ray diffraction, scanning electron microscopy, inductively coupled plasma atomic emission spectroscopy.

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Sonochemical synthesis of $CuGaS_2$ Nanoparticles

박승욱 차지현 정덕영

성균관대 화학과

Ⅰ-Ⅲ-$Ⅵ_2$ ternary chalcopyrite semiconductors are materials having potential applications for electro-optical devices and infrared-radiation generation and detection. $CuGaS_2$ is a chalcopyrite semiconductor with a large direct energy of 2.46eV. We synthesized $CuGaS_2$ nanoparticles for application of solar cell by employing a sonochemical process under ambient conditions. Metal precursor used to synthesize $CuGaS_2$ included copper chloride, gallium nitrate and sulfur powder. These materials were dissolved glycol and triethylenetetramine. Gallium nitrate and sulfur powder were mixed and supplied ultrasound in liquid media at 110 ℃. After copper chloride was added in the mixture, the samples were washed with distilled water and ethanol, dried. The X-ray diffraction pattern indicated that the products are Chalcopyrite structure $CuGaS_2$ and X-ray fluorescence, Inductively coupled plasma(ICP) data indicates that this product's ratio is $CuGaS_2$

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Characterization of Co_2Al-Layered Double Hydroxide Nanosheets Containing Platinum Nanoparticles

김보미 김하나 정덕영

성균관대 화학과

Platinum nanoparticles (Pt-NPs) immobilized on Co_2Al - layered double hydroxide nanosheets (LDH NS) were successfully synthesized. LDH-NS were incorporated with the black colloids of Pt-NPs with 3-4 nm average size distribution, synthesized by a typical methanol/citrate method with H_2PtCl_6.This electrostatic assembly of high density Pt-NPs on the exfoliated LDH-NS which can be applied as a hybrid supporter for Pt-NPs catalysts was characterized by high resolution - transmission electron microscopy (HR-TEM), scanning electron microscopy (SEM) and X-ray diffraction (XRD) pattern. The HR-TEM images show clearly that platinum nanoparticles were deposited on the surface of LDH-NS with homogeneous distribution and without any aggregated form of Pt-NPs. These LDH-Pt nanocomposites are expected to provide ‘new flat form’ for the development of heterogeneous nanocatalysts.

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Sonochemical Synthesis of Zinc-blend $Cu(In_x,Ga_{1-x})Se_2$ (CIGSe) Nanoparticles for use in low-cost photovoltaics

차지현 노세진 박승욱 정덕영

성균관대 화학과

Metastable zinc-blend structure$Cu(In_x,Ga_{1-x})Se_2$ (CIGSe) nanoparticles have been synthesized by sonochemical process. Depending on the solvent condition and reactants ratio in reaction mixture, chemical composition of CIGSe nanoparticles could be controlled over the entire composition range(x) = 0 to 1. Upon thermal treatments, zinc-blend CIGSe nanoparticles converted into well-crystallized pure quaternary chalcopryite polycrytals. Colloidal suspensions of nanoparticles are attractive for use as ink for nonvacuum process of thin film solar cell by various coating methods. The compounds were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray fluorescence (XRF), and raman spectroscopy.

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High-Performance *n*-Type Organic Transistor with a Solution-Processed and Exfoliation-Transferred Two-Dimensional Crystalline Layered Film

박상규 안병관[1] 박수영

서울대 재료공학부 [1]가톨릭대 화학과

We report herein that high-performance *n*-type organic field-effect transistors (OFETs) based on 2-dimensional crystalline layered films of the novel dicyanodistyrylbenzene (DCS) derivative (2Z,2'Z)-3,3'-(1,4-phenylene)bis(2-(3,5-bis(trifluoromethyl)phenyl)acrylonitrile) (CN-TFPA) were fabricated using a simple solution process. The CN-TFPA molecule was elaborately designed to satisfy both solubility and dense molecular packing state, utilizing twist elasticity behavior of DCS based organic semiconductors. We also present here on characteristic behavior of laterally aligned cyano (-CN) units which not only lead to appropriate LUMO level for *n*-type carrier transport but also induce strong intermolecular hydrogen bonding interaction for dense packed 2D crystal formation. The OFETs showed electron mobilities of up to 0.55 $cm^2V^{-1}s^{-1}$, which was attributed to the appropriate electron affinity and dense molecular packing in the well-ordered 2D terrace structure. Due to the easy exfoliation capabilities of the CN-TFPA 2D crystalline layers, 2-10 CN-TFPA molecular monolayers could be successfully transferred onto the substrates, enabling the fabrication of ultra-thin OFET devices with an active layer thickness of ~30 nm.

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Synthesis and Characterization of High-Performance *n*-Type Organic Semiconductor: Novel Dicyanodistyrylbenzene Derivative Forming Large 2D Single Crystal

김진홍 박상규 박수영

서울대 재료공학부

We have been intensively involved in the development of highly crystalline *n*-channel organic semiconductors based on a push-pull Pi-conjugated frameworks, and recently reported that a specific dicyanodistilbene (DCS) derivative with multiple electron-withdrawing units, HEX-4-TFPTA, exhibits an excellent n-type field-effect electron mobility up to 2.14 $cm^2V^{?1}s^{?1}$. On the basis of our previous observation that a stabilized energy level and outstanding 2D molecular stacking from specific units favorably enhance electrical properties, we designed and synthesized a new DCS derivative, (2E,2'E)-3,3'-(2,5-dimethoxy-1,4-phenylene)bis(2-(5-(4-(trifluoromethyl)phenyl)thiophen-2-yl)acrylonitrile) (ME-4-TFPTA), which shows sufficiently lowered energy level and secures good solubility. Solution-grown millimeter sized 2D single crystalline ribbon exhibited an electron mobility up to 2.12 $cm^2V^{?1}s^{?1}$ and on/off ratio of 10^6.

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New thermo- and pH-sensitive polymers with amine functional groups based on N-isopropyl acrylamide and 4-vinylaniline

서재원 신원상[1]

단국대 WCU [1]단국대 나노바이오의과학

A series of thermosensitive polymers with amine functional groups were synthesized by free-radical polymerization in methanol, using N-isopropyl acrylamide (NIPAAm) and 4-vinylaniline (VAn). The copolymers, N-Isopropylacrylamide-co-VAn, with a range of compositions were designed to have the lower critical solution temperature (LCST) around physiological temperature. The copolymers were characterized for their molecular weight, LCSTs, and rate of response to a change in temperature, using MALDI-TOF, DSC, and concentrated dispersion & emulsion stability analysis. The binding possibility of plasmid DNA and this copolymers was studied in batch method. The optimum pH for the binding of plasmid DNA by phase transition from homogeneous to heterogeneous solution was 6. The suitable binding time was 10 min about 60 ℃. The maximum sorption capacity of plasma in the polymer solution(100μg/50μl) was about 1.64μg. These results demonstrated that the developed thermosensitive polymers with amine functional groups have great potential for use in temperature- and pH-activated DNA binding, gene and drug delivery, and hydrogel preparation for tissue engineering.

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Fabrication of Graphene Layer for Oxidation Protective Coating on IF Steel by Chemical Vapor Deposition

박재현 김태훈 박종래

서울대 재료공학부

Due to the chemical reactivity of the refined metals, US industries spend more than $200 billion annually on the protective coatings on metals. For the protective coatings, various approaches are conducted including coating of an inert metal, conductive polymers, organic layers, paints, oxide layers etc. However, most conventional methods have their limitations. The addition of protective coating usually changes physical and optical properties of the metals. As a result, an ultrathin protective coating is required for the minimal changes of properties of metals. Graphene is a single atomic monolayer of graphite and one of the most ideal materials for this purpose because of chemical inertness, thermal stability and transparency. Furthermore, growth of graphene on several metal substrates including Fe, Ni, Cu, etc. by chemical vapor deposition (CVD) has been successfully researched from many researchers. Recently, ability of graphene coating for protecting metals from corrosion has been researched on Ni and Cu in some research groups. In this research, for the first time, we researched about the oxidation protecting ability of the graphene coating on Fe. We grew graphene layers on IF (Interstitial Free) steel by CVD process. We put IF steel into the furnace and supplied acetylene gas with hydrogen in high temperature (800℃) and atmospheric condition. Properties of graphene layers are examined by Raman spectroscopy, SEM, and TEM. To observe the protection ability of graphene coating on IF steel, we compared the Raman and XPS results of coated and non-coated IF steel which are exposed to the highly oxidative environment. Also, in this research, mechanical and structural property changes of IF steel after CVD process were measured by tensile strength test and XRD.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and photocatalytic activity of magnetic core-shell particles with various sizes

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강릉원주대 화학과 [1]강릉원주대 화학신소재

Multifunctional Fe3O4@TiO2 core-shell particles were fabricated by sol-gel process with various sizes. Sol-gel process induces the magnetic particles to be coated with a TiO2 shell. Multifunctional core-shell particles are characterized by field emission scanning electron microscopy(FE-SEM), transmission electron microscopy(TEM), energy dispersive x-ray spectroscopy(EDS). Photocatalytic experiment is demonstrated by utilizing the oxidation reaction of rhodamine B with the photofunctional magnetic core-shell particles. Photocatalytic experiment is shown that small size particle is more effective than large size particle.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of YAG:Ce micro-cube phosphor as scatter-free phosphor for white light-emitting diodes

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국민대 생명나노화학과 [1]국민대 화학과

A transparent $Y_3Al_5O_{12}:Ce^{3+}$ (YAG:Ce) micro-size cube phosphor (MCP) with diameters of ~100 μm was designed and prepared in order to enhance the low conversion efficiency (CE) and to reduce scattering and reflection loss of YAG:Ce micro-size powder phosphors (MPPs) used for white phosphor-converted light-emitting diodes (pc-LEDs). The transparent MCPs (100 x 100 x 100 μm) were fabricated by dicing a 100 μm thick YAG:Ce ceramic plate phosphor (CPP) into 100 μm squares using a diamond wheel. To fabricate the newly designed micro-size cube-based white pc-LEDs, the prepared MCPs were dispersed in silicone binder and then directly coated onto a blue InGaN LED chip as a function of the phosphor concentration in the silicone binder. The structural, morphological and optical properties of transparent YAG:Ce MCPs were investigated by performing scanning electron microscopy (SEM), atomic force microscopy (AFM) and photoluminescence (PL) measurements.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of anatase TiO_2 nanowires using a solvothermal method

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Titanium dioxide (TiO_2), especially anatase TiO_2, is the one of most important metal oxide semiconductor material because it can be used in many fields, such as solar cells, photocatalysis, and lithium-ion batteris. The enhanced performances of the TiO_2 nanowires, nanorods, and nanobelts have been reported in many researches due to their anisotropic structure. The anatase TiO_2 nanowires were directly synthesized by a solvothermal method containing N,N-dimethylformamide (DMF), acetic acid (AA) with lithium acetate (LiAc), and titanium (lV) butoxide (TB) as a TiO_2 precursor, in order to enhance the surface area and charge transport in dye-sensitized solar cells. The morphology and structure of the anatase TiO_2 nanowires are characterized by field-emission scanning electron microscopy (FE-SEM) and X-ray diffraction (XRD) analysis.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

PL Origin of Cubic Spinel $AgIn_5S_8$ nanocrystal: Donor-Acceptor Pair Recombination

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Cubic spinel $AgIn_5S_8$ (c-$AgIn_5S_8$) nanocrystals (NCs) were successfully synthesized at a stoichiometric molar ratio of [In]/[Ag] = 5. X-ray diffraction (XRD) patterns and transmission electron microscopy (TEM) images show that obtained c-$AgIn_5S_8$ NCs are well-crystallized cubic spinel structures and single crystals. In this study, we investigate the photoluminescence (PL) origin of c-$AgIn_5S_8$ NCs. Broad PL bands and large Stokes shifts indicate that PL behaviors of c-$AgIn_5S_8$ NCs can be attributed to donor-acceptor (D-A) pair recombinations. The PL peak energy shifts and PL intensity changes depending on the excitation intensity and temperature confirm that the PL mechanisms of c-$AgIn_5S_8$ NCs comply with D-A pair transitions. Furthermore, the PL decay profiles of c-$AgIn_5S_8$ NCs measured at various emission energy peaks in the PL bands, which are strongly dependent on the distance of D-A pairs. This investigation of PL origin of c-$AgIn_5S_8$ NCs provides the possibility of application in solar cells.

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발표코드: **MAT.P-1360**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

In-Situ Growth of ZnO Nanorods in P3HT Matrix to Improve Performance of Hybrid Solar Cells

누구웬 비치푸옹 김태훈 박종래

서울대 재료공학부

The power conversion efficiency (PCE) of hybrid solar cells composed of polymer and metal oxide critically depends on both morphology of the active layer and interface of two materials. Bulk heterojunction structure based on polymer and nanocrystals (NCs) of metal oxide is known to show the best performance in hybrid solar cells. Surfactants that control the size and shape of the metal oxide are, on the other hand, insulating materials which block the electron transfer from donor to acceptor. In this work, ZnO NCs grow directly in the conjugated polymer poly(3-hexylthiophene) (P3HT) to avoid use of surfactant and/or ligand. Role of the P3HT is a molecular template for the ZnO NCs as well as an electron donor material. In addition, aspect ratio of ZnO NCs is easily increased by control of cosolvent ratio, which formed charge transport pathway in the individual components to each electrode effectively. An improved PL quenching and PCE show improved intimacy of interface and efficient charge transportation achieved from the high aspect ratio of ZnO NCs, respectively.

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발표코드: **MAT.P-1361**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Effect of aspect ratios on "Dot-in-a-Rod" CdSe/CdS Quantum Rods

김민채 홍성표[1] 도영락[2]

국민대 화학과 [1]국민대 생명나노화학 [2]국민대 생명나노화학과

We successfully synthesized the "dot-in-a-rod" core/shell structured CdSe/CdS quantum rods (QRs) and obtained CdSe/CdS QRs with various length-to-diameter ratios. The CdSe/CdS QRs were prepared by a two-step method using different reactivity between octadecylphosphonic acid (ODPA) and hexylphosphonic acid (HPA). Here, the length-to- diameter ratios can be tuned easily via variation of the rod growth times. The obtained CdSe/CdS QR samples showed a high photoluminescence (PL) quantum yields (QYs) and their optical properties were varied with the length-to-diameter ratios of CdSe/CdS QRs. The "dot-in-a-rod" core/shell structured CdSe/CdS QRs were characterized by UV-vis spectroscopy, PL spectroscopy, X-ray diffraction (XRD) and transmission electron microscopy (TEM).

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장소: 부산BEXCO

발표코드: **MAT.P-1362**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Electrically Tunable Quasi-Amorphous Photonic Dyes Working in Low Dielectric Media

현진호 이성민

한양대 화학과

Electrically tunable quasi-amorphous photonic band gap (PBG) materials based on nanoparticles have been developed for an active component of displays. Despite considerable advance, the intrinsic drawbacks including the poor stability of cell in polar solvents hamper their practical applications. Herein, we report quasi-amorphous colloidal structures with high refractive index particles (TiO2 NPs) which can be dispersed in nonpolar organic solvents. Our system is effective for stabilizing surface charge of nanoparticles in low dielectric media, and accordingly increasing cell stability.

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장소: 부산BEXCO

발표코드: **MAT.P-1363**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of highly transparent films capable of multicolor luminescence

배정수 변송호

경희대 화학과

Transparent luminescent thin films, which have multicolor tunability, were fabricated by a layer-by-layer (LbL) assembly of activator doped-layered gadolinium hydroxide (LGdH:RE, RE = Eu and Tb) nanosheets and spherical SiO_2 nanoparticles on a quartz glass substrate. As primary color components to implement multicolors, Eu and Tb were selected as activator cations for red and green displays in LGdH host matrix. Spherical SiO_2 nanoparticles were used to induce a porosity of film surface, led to high transmittance in visible range. The emission color of films can be simply controlled by adjusting the mixing ratio of LGdH:Eu and LGdH:Tb colloidal solutions used in LbL deposition. This film coating enabled us to display a uniform and efficient multicolor luminescence without significant loss of transparency compared with bare quartz substrate.

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장소: 부산BEXCO

발표코드: **MAT.P-1364**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Recovery behavior of calcined layered gadolinium hydroxychloride

이병일 변송호

경희대 화학과

Layered rare-earth hydroxides (LRHs), composed of positively charged rare-earth layers and exchageable inorganic/organic anions in interlayer, are structurally similar to layered double hydroxides (LDHs). Particularly, the recovery ability of LDHs after annealing (from mixed oxide to essentially layered structure), called 'memory effect', have an advantage for loading more molecules into interlayer space. In this study, we have investigated recovery behavior of calcined layered gadolinium hydroxychloride, which is different from those of LDHs under specific conditions. By rehydration and rehyroxylation in aqueous solution containing organic and inorganic anions, the intralayer structure of LGdHs calcined up to 600°C can be reconstructed to recover the intercalation ability. This calcinations temperature capable of after-reconstruction is quite high compared to those of classical LDHs. High thermal stability and reconstructability would provide the LRH family, including LGdH, with many advantages for high temperature applications.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Directional assembly of layered rare-earth hydroxocation nanosheets and paradodecatungstate anions

정희진 변송호

경희대 화학과

The layered rare-earth hydroxides (LRHs) can be readily exfoliated to provide positively-charged nanosheets and the resulting nanosheets can be reconstructed with anionic molecules to form hierarchical superstructures. In this study, paradodecatungstate anions ($H_2W_{12}O_{42}^{10-}$) of high charge density were used as anionic linker for hydroxocation nanosheets. The direction of self-assembly depends on the structure of parent layered rare-earth hydroxide, ultimately resulting in micro-sized superstructures with different morphology. Thus, the assembly of $[Eu_2(OH)_5 \cdot nH_2O]^+$ and $[Tb_2(OH)_5 \cdot nH_2O]^+$nanosheets with $[H_2W_{12}O_{42}]^{10-}$ produced hybrid structure with rectangular and quasi-hexagonal shape, respectively. These hybrids exhibit efficient energy transfer from the oxygen to metal charge transfer (OMCT, $O^{2-} \rightarrow W^{6+}$) band to rare-earth ions in the hydroxide layers as well as highly enhanced f → f transitions. Because direct intercalation of polyanions into the interlayer galleries is difficult, this assembly approach will provide many opportunities to design and build more complicated (LRH nanosheet/POM) systems with new functions.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid Preparation of Reduced Graphite Oxide with Controlled Dispersion Property under Ambient Condition

정해솔 양승재[1] 박종래

서울대 재료공학부 [1]서울대 공과대학/재료공학부

Graphene - a honeycomb-like single layer consisting of sp^2 hybridized carbons - has outstanding mechanical, thermal, and electrical properties as well as lightness. In order to exploit these potentials into practical applications, preparation of high-quality graphene on a large scale is an essential prerequisite. Among various strategies, chemical reduction of graphite oxide (GO) is commonly used for mass production of graphene, and numerous studies have been expended to exploring effective reduction methods by adopting many different kinds of reducing agents such as hydrazine,[1] sodium borohydride,[2] sulfuric acid,[3] and so on. However, those early reported reducing agents require stringent reduction conditions (high temperature and long time). Furthermore, insufficient affinity of reduced graphite oxide (r-GO) with various solvents especially water, hindered various application of resultant r-GO. In this presentation, we report a new reduction method where GO was readily converted to r-GO in extremely short time (less than 10 min) under ambient conditions. Besides, dispersibility and stability of r-GO are significantly improved and easily controlled without any further processes.[1]. Stankovich, S.; Dikin, D. A.; Piner, R. D.; Kohlhaas, K. A.; Kleinhammes, A.; Jia, Y.; Wu, Y.; Nguyen, S. T.; Ruoff, R. S., Synthesis of Graphene-Based Nanosheets Via Chemical Reduction of Exfoliated Graphite Oxide. Carbon 2007, 45, 1558-1565.[2]. Gao, W.; Alemany, L. B.; Ci, L. J.; Ajayan, P. M., New Insights into the Structure and Reduction of Graphite Oxide. Nat. Chem. 2009, 1, 403-408.[3]. Kim, D.; Yang, S. J.; Kim, Y. S.; Jung, H.; Park, C. R., Simple and Cost-Effective Reduction of Graphite Oxide by Sulfuric Acid. Carbon.

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발표코드: **MAT.P-1367**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

의료기기 내 수은 대체물질 및 대체기기 현황 조사

이승규 신승원[1] 박현수[2]

(주)티오이십일 화학전략팀 [1](주)티오이십일 컨설팅본부 [2](주)티오이십일 사장실

수은(Mercury; 80Hg)은 체내에 흡수되면 쉽게 배출되지 않으며, 미나마타병과 같은 중추신경계에 이상을 야기 시켜 UNEP 를 비롯한 국제사회에서는 그 사용을 규제하고 있다. 국내에서도 수은 사용 규제를 위한 저감대책이 시행되고 있으며, 관련 연구조사가 진행되어 왔지만 의료기기에 함유된 수은에 대해서는 충분한 조사가 진행되지 않아 본 조사를 통해 수은 대체물질 및 대체제품 현황을 알아보고자 하였다. 유관기관 협조를 통해 국내 병원을 대상으로 수은함유 의료기기 사용량 및 대체제품 사용여부를 확인하였다. 제조 및 수입 현황의 경우, 국내 유통되는 수은함유 체온계 및 혈압계는 전량 일본, 중국 등에서 수입되고 있었다. 체온계는 종합병원급에서 대체기기로 전환이 빠르게 진행되어 사용량이 꾸준히 감소하고 있었으나 병원급에서는 일정 사용량을 유지하고 있어 충분한 전환이 이루어지지 않은 것으로 추정하였다. 혈압계의 경우, 대체기기 측정값에 대한 의료진의 불신으로 모든 조사대상 병원에서 일정 사용량이 유지되고 있었다. 하지만 수은 대체물질로 Alcohol, Gallium 등이 가능하다는 많은 연구 자료들이 있으며, 주요 국가들에서는 이들 물질이 함유된 대체제품의 성능비교, 국가인증 및 교환프로그램 등을 통해 빠르게 전환하고 있어 대조적인 양상을 보였다. 이에 국내에서도 대체제품 사용 확대를 위한 대책 마련이 필요한 것으로 판단된다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanocomposites of layered double hydroxides and EVA polymer with the enhanced thermal stability

zhang wei 양재훈 최진호

이화여대 화학.나노과학과

Layered double hydroxides (LDHs) are a new class of promising materials as a potential additive which improve the physicochemical properties of the polymer. In this work, we prepared nanocomposites of ethylene-vinyl acetate copolymer (EVA) with LDHs via solution blending method. However, intact LDHs are not compatible with the hydrophobic polymer matrix due to their hydrophilic property. At first, we synthesized various kinds of organo-LDHs through the conventional co-precipitation method by changing the divalent metal ions in LDHs (Mg ,Zn ,Ca), the kinds of organic surfactants such as dodecyl sulfate (DS) and dodecylbenzene sulfonate (DBS), and the metal ratios of divalent metal to trivalent one. According to the x-ray diffraction analysis, the basal spacing of LDHs was expanded to 2.4 - 2.9 nm for the DS and DBS intercalated LDH compared to that of nitrate form LDH (0.86 nm), indicating that DBS or DS molecules were successfully intercalated into LDH to form interdigitated bilayer structure with perpendicular orientation to the basal plane of LDH. From the FT-IR spectra, we found that the anionic surfactants are present in the interlayers of the LDHs due to the electrostatic interaction based on the characteristic bands of $-SO_3^-$ along with aromatic and alphatic C-H and C-C stretching vibrations. The nanocomposites of EVA with varying amounts of organo-LDHs were prepared by solution blending method. According to the XRD analysis, LDHs were exfoliated and partially exfoliated/intercalated in the EVA matrix depending on the LDH loading content. Thermogravimetric analysis shows that thermal stability of the nanocomposites is improved compared to the pristine EVA.

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Broadband Antireflection Coating Based on Nanoporosity-controlled Silica Thin Films Prepared with Si-containing Block Copolymer

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KAIST(KAIST) 신소재공학과 [1]KAIST 신소재공학과

Light reflection from an interface can cause a glare in flat panel displays. Thus, the reduction of reflection is very important for the accomplishment of high contrast and brightness of various display devices, which requires superior antireflection (AR) coatings with low reflectance and high durability. Here, we demonstrate that excellent AR performances in the visible wavelength range can be achieved by using double-layered poly (styrene-b-dimethylsiloxane) (PS-PDMS) block copolymer (BCP) thin films. The Si-containing PS-PDMS BCPs were spin-coated on a glass substrate and treated with CF4 and O2 plasma to obtain highly porous silica films. The refractive indices of the porous silica films can be systematically controlled by adjusting the volume fraction of PDMS in the BCPs. Nanoporous double-layered films show a maximum transmittance of 99.3% (wavelength = 420 nm) for double-side coated samples. This AR coating exhibited a broadband and omnidirectional antireflection phenomena and superior thermal and chemical stability stemming from the inorganic nature of the nanoporous thin film. Furthermore, anti-fogging can also be attained via the good wettability of water droplets, achieving a significantly improved transmittance in highly humid atmosphere. The facile fabrication process, excellent AR characteristics and good durability make the porous silica thin films very practical for many optoelectronic devices such as flat panel displays or solar cells.

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발표코드: **MAT.P-1370**

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The Synthesis and structures of $CsPdPS_4$

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In the middle of searching for new soluble inorganic polymers using the reactive halide-flux technique, we have found two new phases with same chemical formula, $CsPdPS_4$ but with different crystal structures depending on the synthetic condition. The crystal structures and composition of the compounds were determined by single-crystal X-ray diffraction. Two different kinds of one-dimensional $^1_\infty[PdPS_4]$ chains were found. The $^1_\infty[PdPS_4]$ chain found in the monoclinic system is composed of alternating square planar PdS_4 and tetrahedral PS_4 and this chain can be found in the previously reported $AMPS_4$ phases (A=Na, K, and Rb; M=Ni, Pd). In the orthorhombic $CsPdPS_4$, the square planar PdS_4 units are linked by sharing a S atom and the tetrahedral PS_4 unit is bridging these PdS_4 units. In both phases, the one-dimensional $^1_\infty[PdPS_4]$ chains are separated by the Cs^+ ions. The classical charge balance of the both compounds can be represented as $[Cs^+][Pd^{2+}]\,[P^{5+}]\,[S^{2-}]_4$.

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장소: 부산BEXCO

발표코드: **MAT.P-1371**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

The uptake of deoxyribonucleotide strands on layered double hydroxide depending on particle size

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연세대 화학과 [1]연세대 화학및의화학과

The uptake of deoxyribonucleotide (DNA) strands on layered double hydroxides (LDH) nanoparticles was investigated with respect to the particle size of LDHs. The size and morphology controlled LDH nanoparticles ($Mg_2Al(OH)_6(CO_3)_{1/2}6H_2O$) were prepared as follows; 0.6 M Mg/Al metal solution with ratio 2:1 was coprecipiated with alkaline solution gave rise to small particles and the hydrothermal treatment followed by urea hydrolysis on metal solution resulted in larger particles. The electronic microscopic study revealed that the two LDH samples have average particle size and morphology of 20 nm with spherical morphology and ~ 2,500 nm with hexagonal lamellar morphology, respectively. In order to examine the uptake of DNA, both different sized LDHs were dispersed in nucleotide solution with various concentrations. Thus obtained nucleotide adsorption isotherms exhibited that the DNA strands were taken up by both LDHs in concentration-dependent manner and the adsorption behaviors well correspond to the Freundlich kinetics. According to the agarose gel electrophoresis assay for the supernatant of DNA-LDH uptake mixture, it was obviously shown that the there is a correlation between the length of taken-up DNA strands and the particle size of LDH.

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발표코드: **MAT.P-1372**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Intercalation of folic acids into hydrocalumite-like layered structures through exfoliation-reassembly

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We successfully intercalated folic acid, vitamin B_9, molecules into hydrocalumite-like layered materials. Two different types of hydrocalumites, $Ca_2Al(OH)_6(NO_3)mH_2O$ and $Ca_2Fe(OH)_6(NO_3)mH_2O$ were prepared through conventional coprecipitation route and their structures were verified with X-ray diffraction and X-ray absorption spectroscopies. For the intercalation of folic acid, the pristine hydrocalumite layers were treated with formamide and delaminated into several nanosheets. The transmission electron microscopy and selected area electron diffraction patterns revealed that the nanosheets of hundreds-nanometers width were exfoliated into several layers having low crystallinity. Then the colloid containing exfoliated sheets were mixed with folic acid solution resulting in solid precipitates. The powder X-ray diffraction patterns of folic acid intercalated hydrocalumites have d-spacing of 1.60 and 1.46 nm for CaAl- and CaFe-hydrocalumite intercalates, respectively, showing the tilted arrangement of folic acid in the interlayer space. According to the fourrier transform infrared (FT-IR) spectra and thermogravimetry (TG), we could also confirm that the folic acid molecules were chemically stabilized in the hydrocalumite structures through exfoliation-reassembly reaction.

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장소: 부산BEXCO

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of Two-Dimensional GaS and GaSe Nanomaterials

정찬수 백승혁 조용재 박정희

고려대 소재화학과

Layer-structured semiconductor materials such as group Ⅲ monochalcogenides have highly anisotropic electrical, optical, and mechanical properties, which result from the strong intralayer covalent bonding and the weak interlayer van der Waals interaction.Hexagonal GaS and GaSe crystallizes in layered structure with double layer of nonmetal atoms, consisting of S(Se)-Ga-Ga-S(Se) sheets, stacking along c axis, is structurally similar to graphite.We controlled synthesis and characterization of layer-structured GaS and GaSe nanosheets via a catalyst-assisted vapor-liquid-solid (VLS) growth mechanism during GaS or GaSe powder evaporation. And their Cu doping was achieved by gas-phase and solution-phase cation exchange reaction.

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장소: 부산BEXCO

발표코드: **MAT.P-1374**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High-Yield Gas-Phase Laser Photolysis Synthesis of Germanium Nanocrystals for High-Performance Photodetectors and Lithium Ion Batteries

김창현 조용재 명윤 장동명 정찬수 김한성 임형순[1] 박정희 차은희[2]

고려대 소재화학과 [1]고려대 미세소자공학협동/마이크로소자공학 [2]호서대 그린에너지 공학과 대학원

We developed a new high-yield synthesis method of free-standing germanium nanocrystals (Ge NCs) by means of the gas-phase photolysis of tetramethyl germanium in a closed reactor using an Nd-YAG pulsed laser. Size control (5-100 nm) can be simply achieved using a quenching gas. The Ge1-xSix NCs were synthesized by the photolysis of a tetramethyl silicon gas mixture and their composition was controlled by the partial pressure of precursors. The as-grown NCs are sheathed with thin (1-2 nm) carbon layers, and well dispersed to form a stable colloidal solution. The hybrid nanostructures of Ge NC and reduced graphene oxide (RGO) became transparent flexible photodetectors that respond sensitively over the UV-visible-NIR wavelength range. Both Ge NC and Ge-RGO hybrids exhibit excellent cycling performance and high capacity of the lithium ion battery (800 and 1100 mA h/g after 50 cycles, respectively) as promising anode materials for the development of high-performance lithium batteries. This novel synthesis method of Ge NCs is expected to contribute to expand their applications in high-performance energy conversion systems.

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발표코드: **MAT.P-1375**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Antioxidant activity evaluation for *Angelica Gigas* extract encapsulatied with inorganic nanoparticles

김형준 김태현 최진호[1] 오제민

연세대 화학및의화학과 [1]이화여대 화학.나노과학과

Angelica gigas nakai extract, which is known to have antioxidant activity, was successfully incorporated into the inorganic nanoparticles, layered double hydroxide (LDH), through dehydration-rehydration method. The X-ray diffraction (XRD) patterns, fourier transform infrared (FT-IR) spectra and scanning electron microscopy (SEM) study indicated that the extract was well encapsulated with LDH layers forming house-of-cards like structure. Since the antioxidant component in the extract, can be negatively affected by the external strong stimuli, the encapsulation with inorganic nanoparticles is considered to preserve the antioxidant activity of the extract under harsh conditions. A well-known assay, 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging was utilized for the antioxidant evaluation. The DPPH radical scavenging occurs in two steps producing DPPH hydrazine (DPPH-H) and DPPH anion ($DPPH^-$). Usually in DPPH assay, only the increase of DPPH-H is measured with UV-spectrometer, however, in this study, there produced significant amount of $DPPH^-$ as the LDH has strong positive charge. In order to reduce the errors coming from the unspecific light absorption of DPPH-H and $DPPH^-$ together in UV-spectrometer, we utilized high performance liquid chromatography (HPLC) to quantitatively analyze the amount of DPPH only. Therefore, we could accurately evaluate the antioxidant activity of *Angelica gigas* extract in inorganic nanoparticle encapsulated system.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

morphology control of $Cu_2O@SiO_2$ core-shell structures and fabrication of hollow SiO_2 Particles.

양희승

연세대 신소재공학과

This study demonstrates an environment-friendly one-pot process to obtain hollow SiO_2 particles. The preparation of $Cu_2O@SiO_2$ particles via the well-known sol-gel process was presented for the first time. Silica coating on the Cu_2O particles has been considered not appropriate due to the easy etching of Cu_2O in an NH_4OH solution. We found that diluted concentration of NH_4OH delayed the etching of the Cu_2O particles in the sol-gel process and allowed thick coating of silica. With the as-synthesized core-shell particles, time-dependent etching of the Cu_2O core generated yolk/shell particles and finally produced the hollow SiO_2 particles. The etched Cu solution was recycled to produce Cu_2O particles again.

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장소: 부산BEXCO

발표코드: **MAT.P-1377**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Perfect Lattice-Engraftment of Au@Fe3O4 Core-Shell Nanowire Arrays for Magnetoplasmonics

김시인 이효반 김봉수

KAIST 화학과

The multicomponent nanosystem by the marriage of two or more different materials may improve the overall performance through the close interaction between different components, and generate novel synergetic properties that are unachievable in the individual components. Au and Fe3O4 are representative materials showing excellent plasmonic and magnetic property at room temperature, respectively. For this reason, many research groups are attracted to hybrid nanomaterials made of Au and Fe3O4, but most research is focused on magnetic core(Fe3O4)/plasmonic shell(Au) nanoparticles(NPs). We introduced iron chloride as a Fe precursor and fabricated epitaxial thin film on as-synthesized single-crystalline Au nanowires(NWs) by simple chemical vapor deposition(CVD) method. Epitaxial growth of NPs have been reported due to perfect lattice matching between two materials, but it is for the first report on the growth of core-shell NWs entirely covered with Fe3O4 layer. Fe3O4 thin film was formed by combining multi-seeds epitaxially-grown on the Au surface because of atomic-level flatness and defect-free crystallinity of Au NWs. We observed that Au@Fe3O4 NW arrays have ferrimagnetic properties at room temperature due to Fe3O4 material, and individual Au@Fe3O4 NW shows the negative MR property at 2 K. Such diverse properties demonstrate that the hybrid nanostructure of Au@Fe3O4 could be utilized for magnetoplasmonic application.

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장소: 부산BEXCO

발표코드: **MAT.P-1378**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Spherical Meso-macroporous Silica Particles from Emulsion Droplets

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한국기계연구원 부설 재료연구소 기능재료연구본부 [1]성균관대 고분자시스템공학과 [2]재료연구소 표면기술연구본부

We report the bulk synthesis of spherical meso-macroporous ceramic particles by emulsion templating process with hierarchical pore structures. Polystyrene (PS) beads were employed as templates for macroppores and structure directing agents such as triblock copolymer were used for mesopores, and assembled simultaneously inside emulsion with tetraalkoxysilane as silica source, which formed composite structured particles during the evaporation of droplets. Then, by burning out PS beads and the structure directing agents, spherical meso-macroporous silica particles were produced as powder form. The size of macropores could be controlled by changing the diameter of PS beads. The formation of the hierarchically porous particles led to the drastic increase of the specific surface area as 360 % compared to that of simple macroporous particles, implying that our meso-macroporous particles are potentially applicable to various fields which requires extremely porous materials such as catalytic supports, adsorbents, or drug carriers.Acknowledgment: This subject is supported by Korea Ministry of Environment as “The Eco-Innovation Project”, the grant from ‘Creative Research Program (PNK3060) in Korea Institute of Materials Science (KIMS), and Korea CCS 2020 Project.

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발표코드: **MAT.P-1379**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

microRNA sensing platform inside living cells based on nanomaterials

유수윤 민달희

서울대 화학과

MicroRNAs (miRNAs) are a class of small-sizes (10~25nt) and non-coding RNA molecules that play an important regulatory role in the expression of diverse genes. Interestingly, miRNAs as the attractive biomolecule have been paid great attentions in a wide range of biological processes like development and metabolism and pathological progresses of disease/ disorders. Here, we fabricated the microRNA analytical platform for rapid, simple, and sensitive detection using nano-sized graphene derivatives and detection probe antisense oligonucleotide for this study. We evaluated that 1) the probe-graphene derivative complex can work as microRNA sensing platform with efficient fluorescence quenching and recovery ability, 2) nanomaterials can serve as a delivery carrier of detection probe into live cells for real-time monitoring and quantitative analysis of microRNA and 3) the nanomaterials provide the stable loading platform in the complex biological solutions and samples.

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발표코드: **MAT.P-1380**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Dye-Sensitized Solar Cells (DSSCs) with [(dcbpy)M(dmit)] (M=Ni (II), Pd (II), Pt (II)) Organometallic Complexes

정혜인 장연임 박수나 안병관

가톨릭대 화학과

Dye-sensitized solar cells (DSSCs) based on a novel series of d^8 transition metal?based organometallic dye complexes with a dithiolato ligand, (dcbpy)Ni(dmit), (dcbpy)Pd(dmit) and (dcbpy)Pt(dmit) [dcbpy = 4,4’-dicarboxy-2,2’-bipyridine; dmit = 2-thioxo-1,3-dithiole-4,5-dithiolate] were fabricated, and their photovoltaic properties were investigated and compared to those of DSSCs based on Ru(4,4'-dicarboxylic acid-2,2'-bipyridine)$_2$(NCS)$_2$ (N3).

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장소: 부산BEXCO

발표코드: **MAT.P-1381**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Urea intercalation route for graphitic carbon nitride single layer between layered silicate

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이화여대 화학.나노과학과

A single layer of graphitic carbon nitride was synthesized in the gallery of layered silicates via solid state intercalation and pyrolysis. At first, urea was intercalated into layered silicates via solid state reaction at 150 ℃ for 3 hours. Thus prepared urea-layered silicates nanohybrid was calcinated at 200 ℃ - 550 ℃ for 4 hours in order to polymerize urea in the interlayer of layered silicates. According to the x-ray diffraction analysis, the basal spacing of urea-layered silicates nanohybrid was expanded to 1.86 nm, compared to that of Na^+ intercalated layered aluminosilicates (0.96 nm), indicating that urea was successfully intercalated into layered silicates. The basal spacing of the nanohybrid calcined at 550 ℃ was decreased to 1.28 nm, indicating that the urea complexes in the interlayer of silicates were polymerized to form a single sheet of graphitic carbon nitride through the melamine and melem(tri-s-triazine). UV-visible spectra demonstrated that the absorption edge of the calcined nanohybrid was red-shifted and the color was changed from white to pale yellow with increasing the calcination temperature. The nanohybrid calcined at 550 ℃ has bandgap energy of 2.8 eV, which is similar to that of the bulk graphitic carbon nitride. From the FT-IR spectra, we also confirmed that the graphitic carbon nitride was successfully synthesized from the finger print of the aromatic C=N vibration band and the disappearance of C=O vibration bands depending on calcination temperature.

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장소: 부산BEXCO

발표코드: **MAT.P-1382**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Intercalation of nicotinamide into the layered aluminosilicates for the controlled release

류현주 양재훈 최진호

이화여대 화학.나노과학과

Nicotinamide, a part of the water soluble vitamin B group, has a variety of pharmaceutical and dermatological functions such as effective skin whitening, anti-inflammatory, and anti-axiety properties, etc.. However, high dose nicotinamide is considered as a toxic drug. Therefore, in order to add slow and sustained release property to nicotinamide, we have incorporated nicotinamide into layered aluminosilicates (montmorillonite) by intercalative ion-exchange reaction at 80 ^{o}C by using protonated montmorillonite. According to the x-ray diffraction analysis, the basal spacing of nicotinamide-montmorillonite nanohybrid was determined to be 1.5 nm compared to that of Na^{+} intercalated montmorillonite (0.96 nm), indicating that nicotinamide was successfully intercalated into the interlayer space of montmorillonite. From the thermogravimetric analysis, the content of nicotinamide stabilized in the montmorillonite lattice was estimated as ~ 15 wt%. In the present study, an attempt has been made to control the release behavior of nicotinamide out of montmorillonite lattice by coating the nanohybrid with polymer. The release behavior of nicotinamide from the nanohybrids was investigated in the phosphate buffer solution of pH 7.

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발표코드: **MAT.P-1383**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic Semiconductor Based on Asymmetric Naphthalene-Thiophene Molecule for Organic Thin Film Transistor

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경상대 고분자공학과 [1]경상대 화학과 [2]경상대 나노신소재공학부

The technological interest of organic thin film transistors(OTFT) resides in their potential to promote low-cost, large areas, and flexible electronic circuitry. The most important criteria for a commercial application of OTFTs are high charge carrier mobility and high on-off current ratio. Among the rest, the facts important for obtaining high mobilities are the use of organic molecules with high structural order and an extended π system as active layer. The new asymmetric semiconductor 5-(6-decylnaphthalen-2-yl)-5'-(naphthalene-2-yl)-2,2'-bithiophene (NBTND) was synthesized by Suzuki coupling reaction and designed for an organic thin film transistor (OTFT) material. This asymmetric molecule was characterized by H-NMR, HRMS, UV-visible spectroscopy, cyclovoltammetry, thermogravimetric analysis, differential scanning calorimetry. The thin film transistor using new asymmetric semiconductor exhibited the field effect mobility of 2.68 x 10-2 cm2V-1s-1.

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장소: 부산BEXCO

발표코드: **MAT.P-1384**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Benzo[1,2-b:4,5-b']dithiophene Derivative with Deep HOMO level and High Fill Factor: Application for Organic Photovoltaic Cells and Organic Semiconductors

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We have used stille coupling polymerization to synthesize a series of new crystalline deep HOMO level polymers PhBDT-TPD, PhBDT-BT and PhBDT-DTBT constituting mainly electron-withdrawing thieno[3,4-c]pyrrole-4,6-dione (TPD), 4,7-dibromobenzo [c] [1,2,5] thiadiazole(BT), 4,7-bis(5-bromothiophen -2-yl)benzo[c][1,2,5]thiadiazole (DTBT) units in conjugation with electron-rich 4,8-bis(2-octyldodecyloxyphenyl)-benzo-[1,2-b:4,5-b']dithiophene (PhBDT) moieties. All of these polymers exhibited low-lying highest occupied molecular orbital (HOMO, -5.43 ~ -5.66 eV) for high open circuit voltage(Voc) and Band gaps of PhBDT-TPD, PhBDT-BT and PhBDT-DTBT were tuned from 1.86, 1.72 and 1.69 eV, respectively. As a result, bulk heterojunction photovoltaic devices derived from these polymers and fullerenes provided open-circuit voltages (Voc) as high as 0.73 ~ 1.02 V. In particular, the photovoltaic device comprising the PhBDT-DTBT / PC70BM (1:2) blend system exhibited excellent performance with a value of Voc of 0.73 V, a short-circuit current density (Jsc) of 7.06 mA/cm2, a fill factor (FF) of 0.67, and a promising power conversion efficiency (PCE) of 3.5%. In addition, OTFT device also exhibited performance with value of hole mobility 4.7 × 10-2 cm2 V-1s-1. These results are proved by XRD and AFM. PhBDT-DTBT of the thiophene bridge provides enough space for the bulky alkoxyphenyl side chains interdigitation and increases the planarity with enhanced π-π stacking, so, It showed good performances when applied in organic photovoltaic and semiconductor.

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발표분야: 재료화학

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Graphene Oxide based DNAzyme Delivery for Hepatitis C Virus Gene Knockdown

김성찬 민달희[1]

서울대 화학부 [1]서울대 화학과

Down-regulation of viral genes via oligonucleotide-based gene therapy is a potential strategy for the treatment of virus infection such as hepatitis C. One of the potential therapeutic strategies for hepatitis C is to cleave HCV RNA genome with proper antisense nucleic acids, which inhibit virus replication. Deoxyribozymes (DNAzyme, Dz) is known as a RNA-cleaving antisense oligodeoxyribozyme and an attractive therapeutic oligonucleotide candidate which enables cleavage of mRNA in a sequence-specific manner, thus silencing target gene. Graphene oxide (GO) displays many advantageous characteristics to be used as a biosensing platform and drug carrier owing to their excellent capabilities for direct wiring with biomolecules, the quenching capabilities, and the possibility to be processed in solution. Here, we report an efficient DNAzyme delivery system based on nano-sized graphene oxide (nGO). Our research demonstrates that DNAzyme-nGO complex can serve as potential gene silencing therapeutics for viral diseases such as hepatitis C virus.

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장소: 부산BEXCO

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Layered Metal Hydroxides/Polymer Composites Enabling X-ray Visibility on Biodegradable Polymer Fixation Plates

김명훈 양재훈[1] 최진호[1]

서울대 바이오엔지니어링 협동과정 [1]이화여대 화학.나노과학과

Biodegradable polymer plates can be clinically used as an alternative to metal plates (e.g., titanium) for internal fixation, which, however, are not visible with X-ray for post-operative diagnostics. In this study, therefore, we prepared biodegradable plates with X-ray visibility by physically mixing radiopaque inorganic metal hydroxides materials such as MgAl-LDH, ZnAl-LDH, CaFe-LDH, and Zinc basic salts (ZBS) with a biodegradable binder material, poly (lactic-co-glycolic acid) (PLGA). The radiopacity increases with the attenuation coefficients of metals composed of inorganic layered materials. The radiopacity also increases as the thickness of biodegradable fixation plate increases from 1.0 mm to 2.0 mm. When the fixation plate was applied to the simulated body fluid solution, the radiopacity gradually decreases due to the decreased density of layered materials in the fixation plate by swelling and degradation of PLGA regardless of the chemical composition of inorganic layered materials and thickness of layer. According to the in-vitro biodegradation test, a discernible image of the radiopaque plate could be obtained by X-ray for up to around 2 months. Therefore, the biodegradable radiopaque fixation plate, prepared in this work, have a high potential as a fixation device with X-ray visibility

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mesoporous silica nanoparticles with large pores as a potential delivery carrier for drug delivery system

함슬범 민달희[1]

서울대 화학부 [1]서울대 화학과

The fundamental purpose of drug delivery is to deliver the potential drugs with their therapeutic activity to the target organs for the treatments of specific disease in living organisms. Therefore, various functional nanomaterials have been actively developed with appropriate surface functionalizations to provide biocompatibility, bio-imaging, targeting ability and long-term circulation. Among various nanocarriers as drug delivery carriers, mesoporous silica nanoparticles (MSNPs) have been considered as an attractive candidate for drug delivery systems, due to their tunable pore and particle size, high surface area, large pore volume, and biocompatibility.Here, we report the MSNPs mediated protein delivery as a potential carrier for drug delivery system. MSNPs were synthesized by a simple procedure and the pores of MSNP (~2 nm) were further expanded to (~25 nm) by trimethylbenzene treatment. The pore expanded MSNPs were successfully harnessed as a delivery carrier of model proteins such as β-galactosidase and FITC-BSA to HeLa cells while maintaining their own functions. We believe that the present MSNPs based protein delivery system will be a useful and general tool for protein therapy.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A Colorimetric ATP Sensing Platform based on Mesoporous Silica Nanospheres

박민경 민달희

서울대 화학과

Adenosine 5′-triphosphate (ATP), a chemical energy currency within cells for metabolism, functions as an intracellular or extracellular signaling molecule in many biological processes including biosynthetic reactions, motility and organ development. Therefore, measuring ATP-level change is of utmost importance to understand how the concentration of ATP and other intracellular metabolites are regulated in cells. There have been previous studies for measurements of ATP in cells, where the concentration of ATP in the cell extract has been analyzed by various off-line methods such as HPLC. Herein, we developed a sensitive ATP sensing colorimetric platform, based on mesoporous silica nanospheres (MSN) with the expanded pores to be capable of loading β-galactosidases. In the absence of ATP, the each of the MSN pores was capped with ATP-aptamer grafted gold nanoparticles by combining with adenosines modified to the outside of the MSNs, which can effectively prevent the loaded β-galactosidases from hydrolyzing ortho-Nitrophenyl-β-galactoside (ONPG) into galactose and ortho-nitrophenol. By a competitive displacement reaction, the gold nanoparticles were released in the presence of ATP molecule, resulted in amplification of the ATP-triggered signal through an increase intensity of the color at 420 nm wavelength produced by the exposed β-galactosidase activity. Our results suggested that this platform could be used to detect ATP change more efficiently in vitro. We expect that this system could be applicable to cellular ATP assays.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of alucone-Al_2O_3 superlattice films for OLED gas diffusion barrier determined by Ca test

윤관혁

한양대 화학과

We fabricated alucone-Al_2O_3 superlattice films using molecular layer deposition (MLD) and UV-assisted atomic layer deposition (ALD). The MLD relies on a self-terminating surface reaction of organic precursor like to atomic layer deposition (ALD) which results in the formation of a monolayer in each sequence. In the MLD process, Alucone layers were grown by repeated sequential surface reactions of trimethylaluminum (TMA) and ethylene glycol at substrate temperature of 80°C. In addition, we developed UV-assisted Al_2O_3 with film quality better than thermal Al_2O_3. The UV light was effective to obtain high quality, defect-free, more dense Al_2O_3 thin film which is determined by water vapor transmission rate (WVTR). Composition of the alucone films was confirmed by infrared (IR) spectroscopy. Ellipsometry analysis showed a self-limiting surface reaction process and linear growth of each alucone, Al_2O_3 film. Ultra-violet (UV) spectroscopy was employed to measure transparency of the alucone-Al_2O_3 superlattice films. WVTR is calculated by Ca test. The alucone-Al_2O_3 superlattice film using UV-assisted Al_2O_3 and alucone have possible use in gas diffusion barrier for OLED.

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장소: 부산BEXCO

발표코드: **ELEC.P-1390**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Countercation-sensitive cobalt Prussian blue analogues films for color tuning of Prussian blue analogue electrochromic devices

정영희 곽준영 김영일

부경대 화학과

Cobalt hexacyanoferrate(Co-PBA) is a Prussian Blue analogue which is unique electrochromic material. The redox behavior and color of Co-PBA are dependant on the redox potential and the nature of an intercalated hydrated countercations. When the Na+ and Li+ ions are used as countercation, It's color is changed between green(reduction) and purple-brown(oxidation). But the Co-PBA color is changed between olive-brown(reduction) and purple-brown(oxidation) in K+ and Cs+ ions. We synthesized Na2CoⅡFeⅡ(CN)6(Na-Co-PBA) and K2CoⅡFeⅡ(CN)6 (K-Co-PBA) nano particles by simple precipitation and characterized by XRD, TGA, TEM, FE-SEM, and EDS.The flexible Co-PBA films were prepared on ITO/PEN substrate by bar-coating and the flexible electrochromic film devices were assembled by the combination of the PB and Co-PBA electrodes with a polymer-gel electrolyte. PB/Na-Co-PBA and PB/K-Co-PBA devices(ITO/PEN, 10cm2) showed electrochromic color change between greenish blue and light pink or blue and light yellow color.

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장소: 부산BEXCO

발표코드: **ELEC.P-1391**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Performance of Silica-$LiNi_{0.5}Mn_{1.5}O_4$ Core-Shell Structure Cathodes

홍순기 여인형[1] 모선일

아주대 에너지시스템학부 화학 [1]동국대 화학과

The spinel $LiNi_{0.5}Mn_{1.5}O_4$ can provide high operating voltage at 4.7 V versus Li^+/Li and specific energy of ~689 Wh/kg for high power applications. In addition, the nickel substituted $LiNi_{0.5}Mn_{1.5}O_4$ spinel has a good cycling performances and good thermal stability compared to spinel $LiMn_2O_4$. In the case of $LiMn_2O_4$, the cathodes suffer from poor cycling efficiency at high temperature. The capacity fading was caused by the structural instability and the dissolution of manganese ions. These main causes of the capacity fading a little occur at $LiNi_{0.5}Mn_{1.5}O_4$ also. The SiO_2-$LiNi_{0.5}Mn_{1.5}O_4$ composite with core-shell structure can improve cycle performance, because the silica has a structural stability role in composite. The morphology plays a key role in its electrochemical performance as the intrinsic properties of the cathode material. The morphology controlled $LiNi_{0.5}Mn_{1.5}O_4$ can have different structure, surface composition and diffusion lengths for the lithium ion. In this work, SiO_2@$LiNi_{0.5}Mn_{1.5}O_4$ was prepared by combination of precipitation and heat treatment method. The lithium batteries were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled galvanostatically in a potential range of 3.5 ? 5.0 V at various C rates, using multichannel battery test mode. Crystalline structures were analysed by both X-ray diffraction (RigakuD/max 2700V/VP) and neutron diffraction, in order to identify the positions and the ordering/disordering of transition metal ions and Li-ion. The morphology was characterized by using a scanning electron microscope (JEOL JSM-6380). The comparing of morphologies, structure and electrochemical properties will be discussed in detail.

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

Rod-shape Li_2MnO_3 Cathodes Prepared from γ-MnOOH or β-MnO_2 Precursors

유다연 여인형[1] 모선일

아주대 에너지시스템학부 화학 [1]동국대 화학과

Monoclinic-layered Li_2MnO_3 has been extensively studied as a cathode material for rechargeable lithium ion batteries because of the relatively lower cost, less toxicity, environment-friendly property, and high theoretical capacity. Especially, Li_2MnO_3 has higher theoretical capacity than other layered materials. However, it has disadvantages such as severe capacity fading in comparison to the other layered structure materials. Structure of layered Li_2MnO_3 was partially changed into spinel structure during charge/discharge. It makes the manganese redox reaction to be possible and allows doing electrochemical activation. The oxidation state of Mn in Li_2MnO_3 is fixed at 4^+, so that Li_2MnO_3 does not show any electrochemical reaction, because Mn^{4+} ions are very difficult to be oxidized to the Mn^{5+} state. The morphology plays a key role in its electrochemical performance as the intrinsic properties of the cathode material.In this work, Li_2MnO_3 powders were synthesized by using the solid-state reaction with different Mn sources, Li sources, and experimental conditions such as temperature and time for heat treatment. From various experimental conditions, morphology controlled- Li_2MnO_3 can be shown improved cycling performances.The characteristics of Li_2MnO_3 as a cathode have been investigated by scanning electron microcopy (SEM), X-ray powder diffraction (XRD), and battery performance with multichannel battery test mode.

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

Increasing Conductivity of $LiMnPO_4$ Cathodes by Pyrolyzing Sucrose on the Surface

Hung-Cuong Dinh 여인형[1] 모선일

아주대 에너지시스템학부 화학 [1]동국대 화학과

$LiMnPO_4$ olivine structure has received much attention as a promising cathode material for Li-ion batteries because of its moderate theoretical capacity (171 $mAhg^{-1}$), low cost, reversibility, thermal stability, environmental friendliness, and an increased level of safety. The $LiMnPO_4$ offers greater energy density owing to its Mn^{2+}/Mn^{3+} redox potential of about 4.1V vs. Li/Li^+, which is practicable and safe operational voltage with common electrolytes being used. In order to increase the conductivity, much effort has been made such as controlling particle size (nano-scale) and coating various conductive materials on the surface of $LiMnPO_4$ particles. Various synthesis routes to prepare nano-shaped crystals of the $LiMnPO_4$ have been developed, which include a solid-state reaction, the sol-gel synthesis, the polyol process, and hydrothermal method. In this work, well-defined $LiMnPO_4$ crystals with various morphologies were prepared by hydrothermal method using LiOH, $MnSO_4.H_2O$, H_3PO_4 and ascorbic acid as starting materials with adding various surfactants. In order to improve battery performance of $LiMnPO_4$ crystals materials, the conductive carbon was coated on the $LiMnPO_4$ surfaces by pyrolysing sucrose; The $LiMnPO_4$ particles were well dispersed in sucrose solution, dried in vacuum, and heated at an elevated temperatures. The structure, morphology, carbon coating amount and electrochemical properties were analyzed by the X-ray powder diffraction (Rigaku D/max 2700V/VP), scanning electron microscopic (JEOL JSM-6380) images, Fourier transform infrared spectroscopy (Nicolet iS10), Raman spectrometer (Nicolet Almega XR Dispersive Raman spectrometer), thermal gravimetric analyzer (Scinco TGA N-1000), electrochemical impedance spectroscopic (EIS) data, and battery performance data (Maccor 4000).

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

C-coated Nano-crystalline Li_2FeSiO_4 Cathodes for Li-ion Battery

이정진 Hung-Cuong Dinh 여인형[1] 모선일

아주대 에너지시스템학부 화학 [1]동국대 화학과

Li_2FeSiO_4 orthosilicate has become of great interest as a cathode material for rechargeable Li-ion batteries (LIB), due to high theoretical capacity (~332 $mAhg^{-1}$, it can be extracted more than one Li^+ ion per formula unit), cost effectiveness, high thermal through strong Si-O bonding, safety. The Li_2FeSiO_4 was as well as eco-friendly close to $LiFePO_4$ properties. However, the poor ionic conductivity restricts the possibility of using orthosilicates in practical cells. To improve electrochemical characteristic of Li_2FeSiO_4, optimizing particle size to nano-scale is necessary owing to its high specific surface area, short diffusion lengths for Li-ion and increased electronic conductivity by using conductive materials as carbon, polymers, etc. In this work, nano-crystalline Li_2FeSiO_4 particles were prepared by a hydrothermal method using different of Li^+, Fe^{+2}, Si-ion sources. In order to improve conductivity of Li_2FeSiO_4 crystals materials, the conductive carbon was coated on particles surface by pyrolyzing glucose; The Li_2FeSiO_4 particles were well dispersed in glucose solution, dry in vacuum, and heated in N_2 atmosphere. The structure, morphology, and carbon coated amount were analyzed by the X-ray powder diffraction (XRD) patterns, scanning electron microscopic (SEM) images and thermal gravimetric analyzer (TGA). The lithium batteries with the C-coated Li_2FeSiO_4 nanoparticles cathode were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled galvanostatically a potential range of 1.5-4.4 V using a multichannel battery test mode.

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장소: 부산BEXCO

발표코드: **ELEC.P-1395**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Spinel $Li_{1.07}Mn_2O_4$ Cathodes Synthesized from Various Manganese Oxide Precursors

이종문 모선일 여인형[1]

아주대 에너지시스템학부 화학 [1]동국대 화학과

Spinel $LiMn_2O_4$ has many intrinsic advantages with structural stability, high voltage capability, low material cost, and environmentally safety for electrochemical performance. For these reason, $LiMn_2O_4$ became one of the most promising material for rechargeable Li-ion batteries. $LiMn_2O_4$ has shown capacity fading because of electrochemical reaction with electrolyte at high voltage, Mn-dissolution, and jahn-teller effect of Mn^{3+} in electrolyte. Mn-dissolution occurs due to disproportion reaction at the particle surface. From the control morphology and crystalline size, battery performance can be improved.In this study, spinel $LiMn_2O_4$ with various morphology and crystalline size were prepared. The morphology and size controlled-$LiMn_2O_4$ were synthesized from manganese oxide precursors such as α MnO_2, ß MnO_2, γ MnO_2, Mn_3O_4 and amorphous MnO_2. These precursors were made by using hydrothermal and precipitation method. And then $LiMn_2O_4$ were synthesized by using solid-state reaction with Mn precursor and LiOH. The crystallinity and morphology of the material were examined by X-Ray diffraction and SEM image. We were analysis of $LiMn_2O_4$ structure by using rietveld analysis method with Fullprof program. To compare electrochemical performance of $LiMn_2O_4$ with various morphology, made coin-type (CR2032) Li-ion rechargeable and tested their electrochemical performance by using Maccor 4300K.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic activity of platinum nanostructures electrodeposited on ITO surfaces

최강희 김종원

충북대 화학과

본 연구에서는 indium tin oxide(ITO) 표면에 전기화학적 석출을 통해 형성한 백금 나노구조체 전극의 전기화학적 촉매 현상을 관찰하였다. 직접 메탄올 연료 전지(DMFC) 에서 백금은 일반적으로 메탄올 산화반응의 촉매적 활성이 높기 때문에 산화전극으로 사용된다. 또한 백금은 산소 환원반응에서 뛰어난 촉매적 활성을 가지기 때문에 환원 전극으로도 사용된다. 백금은 나노입자의 크기와 구조에 의해 촉매적 활성이 달라지고, 따라서 촉매 활성이 가장 큰 구조를 찾는 것이 중요하다. 본 연구에서는 메탄올 산화반응과 산소 환원반응에 촉매적 활성이 좋은 백금 구조를 전기화학적 석출을 통해 형성하는 연구를 수행하였다. K2PtCl4 시약을 사용하여 -0.2V 로 석출하는 과정에서, 전하량을 조절하여 다양한 백금 구조를 형성하고 이에 따른 전기화학적 메탄올 산화 반응과 산소 환원 반응의 전기화학적 촉매 활성을 관찰하였다. 메탄올 산화반응에서는 전류의 변화를 살펴보았으며, 산소 환원 반응에서는 봉우리 전위의 변화를 살펴보았다. 두 가지 반응 모두 일정 전하량까지 촉매활성의 변화를 보였고 그 이후의 전하량에서는 변화가 거의 없었다. 이러한 현상을 설명하기 위해 전자 주사 현미경(SEM) 을 통하여 구조적인 특성을 알아보았으며, X-선 회절 분석기(XRD) 통한 결정 구조의 규명을 통하여 촉매활성과의 상관관계를 살펴보았다. [본 연구는 지역혁신 인력양성사업의 지원으로 수행되었음.]

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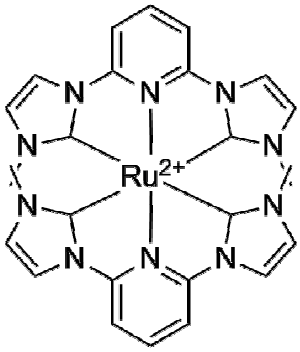
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Color-Tunable Electrogenerated Chemiluminescence of Ruthenium N-Heterocyclic Carbene Complexes

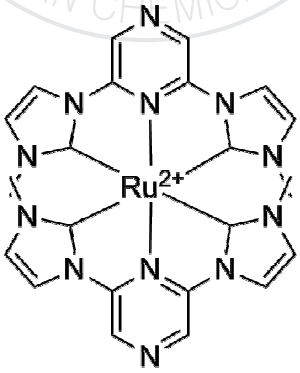
박희준 유상욱[1] 신익수 김주훈[1] 정영근

서울대 화학부 [1]경희대 화학과

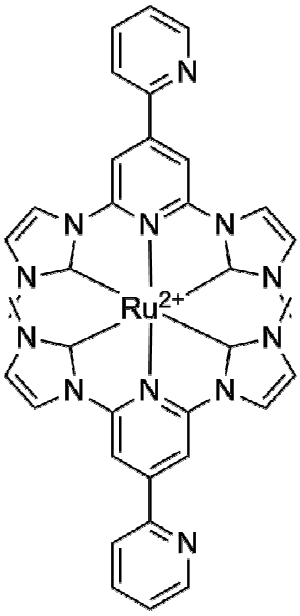
Ru(II) complexes 1-3 bearing various N-heterocyclic carbene (NHC) ligands were synthesized, and their photophysical, electrochemical, and ECL properties were discussed to evaluate the possibility of their use as multicolor ECL labels. Interestingly, complex 1 produced green ECL via a coreactant process using TPrA in nonaqueous and mixed aqueous solutions.



1



2



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일시: 2012년 10월 17~19일(수~금) 3일간

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발표코드: **ELEC.P-1398**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical behavior of aqueous SeO2 solutions on FTO

문나은 이덕연 이치우

고려대 세종캠퍼스 신소재화학과

최근까지 Au(111) 표면에서의 SeO2 의 CV(cycloltammetry), UPD(underpotential deposition), bulk deposition 에 대한 많은 연구들이 진행되었다. 이에 본 연구에서는 Se 이 FTO 전극에서 어떠한 전기화학적 특성을 보이며 어느 정도 두께까지 양질의 electrodeposited Sample 을 얻어낼 수 있는지 알아보기 위한 실험을 수행하였다.FTO 표면에서 SeO2 용액의 CV(cyclic voltammetry)를 측정 하였고, 이를 통해 적절한 potential(E/V vs. Ag/AgCl/sat. KCl)을 선택하여, CA(chrono amperometry)로 시간 차이별로 FTO 에 Selenium 을 electrodeposition 시켜보았다. 얻어낸 Sample 들이 시간에 따라 어떠한 특성을 보이는지 SEM, EDS, XRD, ASV 를 사용하여 알아보았다.

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발표코드: **ELEC.P-1399**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and characterization of nanostructured Pd with high electrocatalytic activity

최수희 최강희 김종원

충북대 화학과

A simple electrodeposition method was used to fabricate palladium nanostructures on gold electrodes. Triangular Pd structures of 70 nm size were characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD). The electrocatalytic activities of triangular Pd structures were examined for oxygen reduction, formic acid oxidation, and methanol oxidation reactions. In addition Surface-enhanced Raman scattering (SERS) activity was investigated using 4-aminothiolphenol as a probe molecule. The electrocatalytic activity of the triangular Pd structures was similar to bare platinum electrode for oxygen reduction reaction. The oxidation peak current is greater than bare Pd electrode in methanol oxidation reaction. While the oxidation wave of formic acid was not observed at bare Pd surfaces, triangular Pd structures exhibited enhanced electrocatalytic activity. The triangular Pd structures provide electrocatalytic activities and efficient SERS activities. [This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation]

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장소: 부산BEXCO

발표코드: **ELEC.P-1400**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Heterogeneous electrochemical immunoassay based on the anion polymer film-modified electrode

최영봉 오인돈 김혁한

단국대 화학과

Recent progress of technology facilitates immunoassay simpler and faster using small quantity of sample, and several chip-based immunoassay systems have been proposed. Electrochemical detection method is one of the most attractive systems for simple designed signal generation of immunosensors. The electrochemical immunoassays are divided into homogeneous and heterogeneous immunoassays. Although heterogeneous assays are more complicated due to the washing steps and immobilization steps at solid surface, most of the reported electrochemical immunoassays are the heterogeneous methods because they usually provide higher sensitivity and show less interference. In this paper, we report a heterogeneous electrochemical immunosensor for the detection of small antigen, hippuric acid (HA). Anion polymers, poly(sodium 4-styrenesulfonate (PSS), were immobilized with the physical absorption onto the Indium tin oxide (ITO) electrode. The anion poymer-functionalized surface was used to bind *anti*-HA monoclonal antibodies (*anti*-HA) and then applied metal-antigen complex, ($Fe(CN)_5$-aminomethyl pyridine-HA), using antibody-antigen reactions. The electrical signals were measured by voltammetry technique. Good sensitivity and reproducibility were obtained by the proposed immunosensor. Moreover, the proposed heterogeneous electrochemical immunoassay method can be extended to the applications to detect a wide range of different antigens in the health care area.

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발표코드: **ELEC.P-1401**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High sensitive electrochemical immunoassay for detecting hippuric acid using the ethylenediamine-modified multiwall carbon nanotubes electrode.

김남혁 이성규[1] 최영봉[1] 김혁한[1]

단국대 첨단과학대학 화학과 [1]단국대 화학과

A nanostructured immunosensor based on the ethylemediamine-modified multiwall carbon nanotubes electrode was developed for detection of hippuric acid (HA). Urinary hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring of exposure to toluene is very important in occupational health care, and a hydrogel-based electrochemical immunoassay for rapid and quantitative detection of HA. Carboxylated multiwall carbon nanotubes were covalently bound to the ethylenediamine and then functionalized nanostructured surface was used to bind hippuric acid(HA) antigen. The HA antigen functionalized surface was used to bind anti-HA monoclonal antibodies using antibody-antigen reactions. Stepwise modification of the electrode was characterized by cyclic voltammogram of $Fe(CN)_6^{3-/4-}$. The electrical signals were proportional to analyte hippuric acid (HA) in the range of 0.01-10 mg/mL which is enough range to be used for the point-of-care.

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장소: 부산BEXCO

발표코드: **ELEC.P-1402**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimization of Redox Polymer for High Power Biofuel Cells.

이정민 박햇님 최영봉 김혁한

단국대 화학과

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 lifetime. Previously polymer complexed with $[Os(dichlo\text{-}bipyridine)_2]^{2+/3+}$ has been used as a cathode. But we introduced a new cathode, poly(acrylicacdi-bipyridine-4-vinylpyridine-acrylamide) complexed with $[Os(dicarboxylicacid\text{-}bipyridine)_2]^{2+/3+}$, appeared greatly superb performance. So we report the electroreduction of O_2 to water under several conditions controlled pH, temperature, enzyme loading rate. The immobilized electrocatalyst enabling the reduction is the electrostatic adduct of bilirubin oxidase from Myrothecium verrucaria, and redox poly-Os complex, cross-linked on the screen printed carbon electrodes. We have investigated the condition that the high potential to achieve higher current densities, longer stability and less precipitation in the electrodes.

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장소: 부산BEXCO

발표코드: **ELEC.P-1403**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic activity of nanoporous gold surfaces fabricated by cathodic anodization

복영웅 김종원

충북대 화학과

본 연구에서는 양극 산화반응을 통해 nanoporous black gold (이하 NPBG)를 형성하여 표면결정구조에 따른 전기화학적 촉매활성을 관찰하였다. Nanoporous gold (NPG) 구조의 특징은 큰 표면적을 가지고 있다는 것이다. 이런 특징으로 NPG 는 연료전지부터 전기화학적 센서 등 많은 분야에 걸쳐 연구가 진행되고 있다. NPG 를 만드는 방법에는 몇 가지 방법이 존재하는데 그중 하나인 양극 산화반응을 통해서 nanoporous black gold (NPBG)를 형성하였다. 본 연구에서는 양극 산화반응 시간을 조절하여 표면적의 변화를 주었으며, 이 표면적의 변화를 통해 산소, 메탄올, 그리고 글루코오스의 산화/환원반응으로 NPBG 의 촉매적 활성을 살펴보았다. 표면적은 양극 산화반응 시간이 길어짐에 따라 선형적으로 증가하는 것을 확인할 수 있었다. 촉매적 활성을 살펴보기 위해 산소, 글루코오스 그리고 메탄올을 이용하였다. 산소와 글루코오스의 경우 표면적이 증가함에 따라 봉우리 전위는 변하였지만, 봉우리 전류는 큰 변화가 없는 것을 확인할 수 있었다. 메탄올의 경우 동일한 농도에서는 표면적이 증가함에 따라 봉우리 전위는 변하지 않지만, 봉우리 전류는 증가하는 것을 보였다. 또 동일한 표면적일 땐 메탄올의 농도가 증가함에 따라 봉우리 전위가 변하는 것을 확인하였다. 이와 같은 현상을 설명하기 위해 UPD 를 이용하여 NPBG 표면 결정구조를 확인 하였으며, 확인된 표면 결정구조의 비율을 통해 전기화학적 촉매 활성을 설명하였다.
[본 연구는 지역혁신 인력양성사업의 지원으로 수행되었음.]

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장소: 부산BEXCO

발표코드: **ELEC.P-1404**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Phosphorus-Doped Ordered Mesoporous Carbons with Different Lengths as Efficient Metal-Free Electrocatalysts for Oxygen Reduction Reaction

양대수 송민영 박진솔 김민식 김정호 박현열 유종성

고려대 신소재화학과

Energy is one of the biggest challenges for twenty first century. There has been an ever increasing demand for environmentally friendly high power energy sources. Fuel cells are envisioned as one best possible solution due to their high energy density, high efficiency and negligible emission of harmful gases. The foremost limitation in low temperature FCs is the kinetically sluggish oxygen reduction reaction at the cathode, which necessitates the use of a substantial amount of catalyst. Recently, heteroatom-doped carbon has been reported as efficient cathode material for oxygen reduction reaction (ORR) in fuel cell. Since hetero atom is usually covalently bonded with carbon framework, its effect will not fade even for long time operation. In fact, N-doped carbon materials have shown better durability than that of commercial Pt/VC catalyst. These properties encouraged researchers to explore doping of carbon materials with other hetero atoms such as boron, phosphorus and iodine. Here, we developed a phosphorus-doped ordered mesoporous carbons (POMCs) with different lengths using a metal-free nanocasting method of SBA-15 mesoporous silica with different sizes as template and triphenylphosphine and phenol as phosphorus and carbon sources, respectively. The resultant POMC is demonstrated as a metal-free electrode with excellent electrocatalytic activity for ORR, coupled with much enhanced stability and alcohol tolerance compared to those of the state of the art Pt catalyst via four-electron pathway in alkaline medium. Interestingly, the POMC with short channel length is found to have superior electrochemical performances compared to those with longer sizes.

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장소: 부산BEXCO

발표코드: **ELEC.P-1405**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Improved Rate and Cycle Performances of Sandwiched $LiNi_{0.5}Mn_{1.5}O_4$-Graphene for High Voltage Applications

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Particle aggregation and high rate of electrolyte decomposition lead to a passive solid electrolyte interface (SEI) formation on the surface of nano-material cathode subjected to high voltages in Lithium Ion Battery. In this respect, development of protocols by simple techniques to enhance the electronic conductivity and suppress electrolyte decomposition (suppression of SEI) on high voltage electrodes (e.g., $LiNi_{0.5}Mn_{1.5}O_4$(LNMO)) remains attractive and critical. In this work an optimized LNMO-graphene composite is described in which graphene behaves as an excellent conducting network, exhibiting suppression of SEI and thereby, contributing to the improvement of rate capability and capacity retention of LNMO. The interaction between the LNMO particles and the residual oxygen functionalities on the basal plane of graphene spontaneously produce LNMO particles sandwiched by graphene in a solution. The sandwiched structure exhibits better rate performance at high C-rates with less polarization and higher coulombic efficiency (thereby, excellent capacity retention), especially at high voltages. HR-TEM, SAED, XRD, XPS, and electrochemical techniques were used to characterize and compare crystallinity, extent of SEI growth, and electrochemical behavior of the LNMO-graphene composite with the pristine material. A $LiMn_2O_4$/graphene composite prepared in the same procedure or a simple mixture of LNMO and graphene showed no significant improvement in electrochemical performances, unlike graphene-sandwiched LNMO.

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장소: 부산BEXCO

발표코드: **ELEC.P-1406**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic Properties of RuO_2 Nanorods Modified Carbon Fiber Microelectrode

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Single crystalline RuO_2 nanorods (NRs) on carbon fiber (CF) were successfully synthesized by using a simple thermal annealing. Morphology and crystalline structure of RuO_2-NRs decorated on a single CF were characterized by FE-SEM, HR-TEM, XRD, and Raman spectroscopy. Cyclic voltammetry (CV) experiments at various potential scan rates in background electrolyte solution were performed to estimate relative real surface area (RSA) enhancement of RuO_2 NR-CF by measuring nonfaradaic capacitive current difference. CV and amperometric experiments were also performed to show that RuO_2 NR-CF reveals favorable electron-transfer kinetics of $[Fe(CN_6)]^{4-/3-}$ and higher electrocatalytic activity for H_2O_2 oxidation compared to a bare CF. Moreover, RuO_2 NR-CF exhibits a superior resistance to Cl- poisoning on the elctrocatalyst surface compared to commercial Pt/C loaded on CF (Pt/C-CF) in H_2O_2 oxidation.

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장소: 부산BEXCO

발표코드: **ELEC.P-1407**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Single Crystalline IrO_2 Nanowires on Au Microelectrode for pH Sensing

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Highly single crystalline IrO_2 nanowires (NWs) were grown on an Au (diameter=25 μm) microwire by using a simple vapor phase transport method. Surface of Au microwire acted as a good nuclear center for gaseous IrO_3 precursors to grow IrO_2 NWs on Au microwire without hard condition. IrO_2 NWs on Au microwire (IrO_2-Au) were characterized with FE-SEM, HR-TEM, XRD, and Raman spectroscopy. In view of electrochemical activity, IrO_2-Au represents better electron transfer kinetics of $[Fe(CN)_6]^{4-/3-}$ and $Ru(NH_3)_6^{3+/2+}$ than a single Au microwire without IrO_2. Moreover, it shows a possibility of using as miniaturized pH sensor by exhibiting super-Nernstian behavior with a larger slope of potential/pH than a glass pH electrode. In conclusion, hierarchical 1-D nanostructures IrO_2 NWs show useful electrochemical applications.

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장소: 부산BEXCO

발표코드: **ELEC.P-1408**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Thermal Treatment on the Electrocatalytic Activities and Surface Roughness of ITO Electrodes

최문정 조경민 양해식

부산대 화학과

The electrocatalytic activities and surface roughness of indium-tin-oxide (ITO) electrodes have been investigated after thermal treatment at 100, 150, or 200 ℃ for 30 min, 2 h, or 8 h. To check electrocatalytic activities, the electrochemical behavior of four electroactive species (p-hydroquinone, $Ru(NH_3)_6^{3+}$, ferrocenemethanol, and $Fe(CN)_6^{4?}$) has been measured. The electron transfer rate for p-hydroquinone oxidation and ferrocenemethanol oxidation increases with increasing the incubation temperature and the incubation period of time, but the rate for $Ru(NH_3)_6^{3+}$ is similar irrespective of the incubation temperature and period because $Ru(NH_3)_6^{3+}$ undergoes an outer-sphere reaction. Overall, the electrocatalytic activities of ITO electrodes increase with increasing the incubation temperature and period. The surface roughness of ITO electrodes increases with increasing the incubation temperature, and the thermal treatment generates many towering pillars as high as several tens of nanometer.

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장소: 부산BEXCO

발표코드: **ELEC.P-1409**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Time-Dependent Decrease in the Enhanced Electrocatalytic Activities Observed after Three Different Pretreatments of Gold Electrodes

Dutta Gorachand 양해식

부산대 화학과

This study reports how the electrocatalytic activities of gold (Au) electrodes change with aging under ambient conditions. The enhanced electrocatalytic activities of Au electrodes observed after piranha treatment, mechanical polishing, or $NaBH_4$ treatment decrease with aging. The enhanced electrocatalytic activities toward *p*-benzoquinone reduction and glucose oxidation decrease 7 days after the treatments, even though the change in surface contamination during aging is not significant. The surface roughness of the Au electrodes is maintained during the $NaBH_4$ treatment, whereas it changes substantially during the piranha treatment and mechanical polishing.

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장소: 부산BEXCO

발표코드: **ELEC.P-1410**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Cholesterol Biosensor Using Pt nanoparticle embedded carbon ink

김경태 천경주[1] 장승철[2] 박덕수[3]

부산대 바이오센서연구소/분자과학기술 [1]부산대 분자과학기술협동과정 [2]부산대 바이오피지오센서연구소 [3]부산대 바이오피지오연구소

A new electrochemical biosensor has been developed based on screen-printed carbon electrodes (SPCEs) for the detection of cholesterol. The working electrodes of the SPCEs were printed by using Pt nanoparticle embedded carbon ink which was manufactured by using an 'in-house' procedure and electrodes' tracks, reference and counter electrodes were printed by using a commercial Ag/AgCl ink onto a PVC substrate film. An enzyme, cholesterol oxidase (ChOx), was immobilized by simple drop-coating of the enzyme solution which was prepared in a cellulose matrix. An enzymatic reaction of the immobilized ChOx produces hydrogen peroxide and the peroxide produced can be electrochemically detected at -150mV vs. Ag/AgCl by the Pt-modified SPCEs. The two-step fabrication process of the SPCEs could be indicated a new approach to simple, sensitive and rapid detection of cholesterol in real clinical samples. The detailed characteristics for the SPCEs developed were investigated by cyclic voltammetric and amperometric techniques. The mode of operation and full analytical performance of the system will be described in this experiment.

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장소: 부산BEXCO

발표코드: **ELEC.P-1411**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile decrease in the electron-transfer rate and surface roughness of gold by ultrasonic treatment

조경민 Dutta Gorachand 양해식

부산대 화학과

The development of simple and reliable methods for tuning the heterogeneous electron-transfer rate is one of the most important issues in electrochemistry. Especially, reduction of the electron-transfer rate at an electrode without surface modification is more challenging than its enhancement. Importantly, Nowicka, Scholz, and co-workers recently showed that the electron-transfer rate at Au electrodes can be rapidly and significantly reduced *via* treatment with Fenton's reagent. Ultrasonic irradiation is commonly employed to clean electrode surfaces after electrode polishing. This presentation reports that 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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발표코드: **ELEC.P-1412**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Flame Synthesis of Maghemite (γ-Fe2O3) polyhedral nanocrystals, their Crystal Growth Mechanism and Li-ion battery applications

INAMDAR SHAUKATALI 최혁수[1] 김민식[2] 유종성[2]

korea university material chemistry [1]고려대 소재화학과 [2]고려대 신소재화학과

Ferrocene, when burned using simple alcohol lamp in high concentrations by dissolving in various solvents, produced highly crystalline iron oxide polyhedrons. Through the flame pyrolysis method the obtained iron oxide was found to have solely maghemite (γ-Fe2O3) phase. Systematic investigations showed that solvent plays an important role in the formation and development of the polyhedral maghemite nanocrystals. Methanol, ethanol and DMF yielded polyhedrons while isopropanol, butanol, acetone and THF yielded smaller nanoparticles encapsulated in carbon matrix. The maghemite polyhedrons were characterized by XRD, TEM and HR-SEM analyses in details and on the basis of these the crystal growth mechanism is proposed. The maghemite nanocrystals were found to have well-developed truncated cuboctahedron morphology with 26 facets grown via 14 faceted truncated octahedrons by flame pyrolysis method. The faces of polyhedrons were assigned as six octagons {100}, eight hexagons {111} and twelve squares {110} in the 26 faceted truncated cuboctahedron. The flame pyrolysis method has many advantages such as time and cost effective, and can deliver bare oxide nanoparticles in the form of dry powders in gram scale. The as obtained γ-Fe2O3@C products were directly used as anode material for Li ion battery without any processing or purification steps. The maghemite-carbon composite showed superior storage performance when tested for Li-ion battery applications.

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발표코드: **ELEC.P-1413**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium Nanostructures Grown on Vulcan Carbon

김지언 심준호[1] 이종목[2] 이영미

이화여대 화학나노과학과 [1]대구대 화학·응용화학과 [2]이화여대 화학과

Development of nanoscale-devices toward their applications for ultra sensitive, selective and reliable sensing systems for chemical or biological species have been one of the most fascinating research directions in our life science. In particular, the sensing devices for biological applications need a low detection limit, high stability, and good sensitivity. In this presentation, we demonstrate nanostructured palladium directly grown on Vulcan carbon (nPd/VC), which has large specific surface area and shows favorable electronic property desired for sensing of glucose and dihydronicotinamide adenine dinucleotide (NADH) without the aid of enzymes.The nPd/VC is very simply synthesized via chemical vapor deposition (CVD) and shows possible applicability for electrochemical biosensors, enabling the efficient, ultrasensitive detection of biologically important molecules. The structure, morphology and electrocatalytic activity of the nPd/VC is characterized by scanning electron microscopy (SEM) and electrochemical analyzer. This research was also supported by the General R/D Program of the Daegu Gyeongbuk Institute of Science and Technology (DGIST), funded by Ministry of Education, Science and Technology (MEST) of the Republic of Korea.

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발표코드: **ELEC.P-1414**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Core-shell Nanocomposites Based on Silver Nanowires: Synthesis and Electrocatalytic Activity for Oxygen Reduction

김수진 심준호[1] 이종목[2] 이영미

이화여대 화학나노과학과 [1]대구대 화학·응용화학과 [2]이화여대 화학과

Oxygen reduction reaction (ORR) is of interest in the areas of amperometric oxygen sensing, fuel cell, and etc. Since the ORR is a sluggish reaction requiring a high overpotential, relevant electrocatalysts are employed. Pt and its alloys are still the best electrocatalysts for ORR, but the high cost and limited supply of Pt are the problem. Metal nanowires have been studied extensively because of their potential use as active components of interconnects in fabricating electronic, photonic, and sensing devices. Meanwhile silver exhibits the highest electrical and thermal conductivities.Therefore, this presentation demonstrates the synthesis and characterization of one dimensional nanocomposites composed of AgCl or AgBr (denoted as Ag/AgCl, Ag/AgBr) The Ag/AgCl core-shell nanowires and Ag/AgBr core-shell nanowires are prepared by galvanic replacement reaction between Ag nanowires and $FeCl_3$ or $FeBr_3$. The structures, morphologies and electrocatalytic activities of these nanomaterials are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV?vis absorption spectroscopy, and scanning TEM and rotating disk electrode (RDE).This work was supported by Mid-career Researcher Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No.2012-0005422)

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

Electrochemical Dual Microsensor for Simultaneous O_2/pH Measurements

하예진 심준호[1] 이영미

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To obtain improved information contents, sensing tools capable of simultaneously monitoring inter-related two different analytes in biological systems are advantageous. In this presentation, we demonstrate the development and characterization of an electrochemical dual microsensor to detect oxygen (O_2) and pH simultaneously. O_2 is essential for sustaining the lives of most living organisms and pH is critical to maintain the activities of biological systems. The developed sensor consists of a working electrode possessing two Pt microdisks (10 μm in diameter) along with two Ag/AgCl reference/counter electrodes. Each Pt microdisk of the working electrode is modified independently. One (WE1) is electrodeposited with porous Pt layer and then covered with a fluorine-containing hydrophobic polymer membrane for the selectivity to O_2 gas. The Pt on the other disk (WE2) is etched to form a micropore-shaped electrode and then electrodeposited with iridium oxide layer sensitive to pH change. At the WE1 and WE2 of the working electrode, O_2 and pH changes are measured in amperometry and potentiometry, respectively. The O_2/pH dual microsensor is also examined for its feature as a tip electrode in scanning electrochemical microscopy (SECM). In fact, O_2 and pH changes are measured simultaneously while the sensor is being scanned over a rat kidney surface using SECM. 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 (2012-0003779).

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발표코드: **ELEC.P-1416**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic Activity of Carbon Supported Gold Nanoparticles Improved by Electrochemical Pretreatment

고아라 심준호[1] 이종목[2] 이영미

이화여대 화학나노과학과 [1]대구대 화학·응용화학과 [2]이화여대 화학과

β-Nicotinamide adenine dinucleotide (NADH) is a coenzyme made from Vitamin B_2 or niacin. It is present in all living cells. As a coenzyme, NADH serves an important role in helping enzymes to function. The importance of the study of NADH/NAD^+ lies in that NADH/NAD^+ is a cofactor for over 300 dehydrogenase enzymes, which may be helpful to understand the parameters that may control the redox activity of biological coenzymes. However, the direct oxidation of NADH at conventional electrode materials is usually encountered by low sensitivity and the fouling of the electrode surface by its oxidation products. Then, we prepared NADH sensor using carbon supported gold nanoparticles improved by electrochemical pretreatment. Carbon supported gold nanoparticles were pretreated by repetitive potential cycling between -0.2 and +1.0 V (vs SCE). Carbon supported gold nanoparticles improved by electrochemical pretreatment show enhanced sensitivity to the electrocatalytic oxidation of NADH at low potential. This work was supported by Mid-career Researcher Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No.2012-0005422).

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발표코드: **ELEC.P-1417**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Measurements of Location-Dependent Nitric Oxide Levels on Skin Surface in Relation to Acupuncture Point

김미선 하예진[1] 나지선[1] 이영미[1]

이화여대 화학나노과학부 [1]이화여대 화학나노과학과

Acupuncture is one of traditional eastern medical treatments. Recently, western countries also accepted it as an alternative therapy method. Even though the acupuncture has been widely practiced, the lack of scientific evidence supporting the rationality of the meridian theory, there is a debate on the real effect of the acupuncture.In previous studies, higher nitric oxide (NO) synthase enzyme and oxygen (O_2) level were observed around acupuncture point and meridians than nonacupuncture area. NO is a representative signaling gas in body mediates vasodilation and therefore relates to oxygen transport. From these results, we inferred that NO concentration on skin surface could be higher around acupuncture point than the other area. The distribution of partial nitric oxide pressure (pNO) is analyzed for the back of the hand and the anterior wrist of the left hand with an amperometric nitric oxide microsensor composed of a small planar Pt disk-sensing area. The pNO levels are different depending on the location over the skin, and they are measured in the analysis for two spots on the back of the hand. Additional measurements were carried out for both one-dimensional single line (along the wrist transverse crease) and two-dimensional square area of the wrist region. Relatively higher pNO values are measured at certain area in near position of acupuncture points with statistical significance, supporting relationship between NO and acupuncture.
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(2012-0003779).

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장소: 부산BEXCO

발표코드: **ELEC.P-1418**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Charged Carbon nanotube-modified electrodes for the simultaneous determination of dopamine and ascorbic acid

윤여운 김태현

순천향대 화학과

Through various modifications of multi-walled carbon nanotubes (MWCNTs), charged molecules were selectively coated to the nanotube. The negatively and positively charged MWCNT-modified electrodes were prepared by coating the MWCNTs with a layer of negatively charged citrate anion (CA) or positively charged polyethyleneimine (PEI) onto glassy carbon electrode through drop casting method. The functionalization of MWCNT with CA or PEI was confirmed by FT-IR, Zeta potential and contact angle analyses. The modified electrodes resulted in a favourable voltammetric resolution of dopamine in the presence of excess ascorbic acid, and the anodic potential difference (ΔEpa) in differential pulse voltammetry (DPV) was 230 mV in pH 7.4 phosphate buffer.

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장소: 부산BEXCO

발표코드: **ELEC.P-1419**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

AuPd Nanoparticle-Reduced Graphene Oxide Nanohybrid as Electrocatalyst

손정우 김수진[1] 김지언[1] 이종목[2] 이영미[1] 심준호

대구대 화학·응용화학과 [1]이화여대 화학나노과학과 [2]이화여대 화학과

In this presentation, we demonstrate the synthesis and characterization of non-platinum bimetallic AuPd nanoparticles supported on reduced graphene oxide (AuPd/RGO). AuPd/RGO catalysts were prepared by a simple synthetic method of RGO-supported Pd-coated Au nanoparticles via a spontaneous reduction of Pd(II) to Pd(0) on a Au nanoparticle surface without a treatment with any additional reducing agent. The prepared AuPd/RGO catalysts were characterized by field emission scanning electron microscope (FE-SEM), X-ray diffraction (XRD), UV-vis spectroscopy to examine the structural features. SEM images show that the AuPd particles are uniformly distributed on RGO sheets. The electrocatalytic activity and stability of the AuPd/RGO for oxygen reduction reaction in alkaline media was measured by rotating disk electrode (RDE) polarization experiments.

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장소: 부산BEXCO

발표코드: **ELEC.P-1420**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Functionalization of Single-Walled Carbon Nanotube with Amine-terminated dendrimers on flexible substrate

이유진 김주훈[1] 김태현

순천향대 화학과 [1]경희대 화학과

Single-walled carbon nanotube (swCNT) was functionalized with amine-terminated polyamidoamine (PAMAM) dendrimers on flexible substrate via electrochemical oxidation of the terminal amine groups of dendrimers. The electrochemical functionalization of swCNT film with dendrimers was confirmed by cyclic voltammetry (CV), contact angle analysis and fluorescence microscope. The immobilized dendrimer films were robust and behaved as charge-selective electrochemical gates for oppositely charged redox molecules. The immobilization approach was applied to assemble Pt dendrimer-encapsulated nanoparticles (Pt DENs) on flexible swCNT film and the resulting Pt DEN / swCNT films showed electrocatalytic activity to H_2O_2 oxidation and low detection limit of 1 $\mu mol L^{-1}$.

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발표코드: **ELEC.P-1421**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-step Synthesis of Graphene-Pt Composite Film by Pulsed Electrodeposition

우승희 김하석[1] 정택동 박원철[2]

서울대 화학부 [1]대구경북과학기술원 에너지시스템학과 [2]서울대 융합과학기술대학원 나노융합학과

Graphene has recently attracted great attention due to its unique electrical, optical, and mechanical properties as well as its potential use in various field, such as electronics, supercapacitors, sensors, and composite materials. However, the practical applications of graphene are challenged by its irreversible agglomeration both in the drying state and in common solvents, which significantly reduces its effectiveness. Graphene-metal nanocomposites have been prepared by chemical or thermal reduction of mixtures of graphene (or graphene oxide) and metallic precursors. These methods involve highly toxic chemical such as hydrazine or high temperature. Recently, electrochemical reduction of graphene oxide by cyclic voltammetry or chronoamperometry has been developed. It is attractive for graphene synthesis due to its simple, fast, and green nature. In this study, we demonstrate the co-electrodeposition synthesis of graphene-Pt composite by pulsed electrodeposition. The resulting electrodes were characterized by electrochemical methods and electron microscopy. The graphene layers were regularly spaced by layers of Pt nanoparticles. As a result, the electrochemical surface area of the graphene-Pt composite film significantly improved compared to the pure graphene film.

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장소: 부산BEXCO

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a triggerable composite electrode for voltammetric pH sensing using a dyad molecule

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건국대 생명공학과 [1]건국대 특성화학부 [2]건국대 화학과 [3]건국대 특성화학부생명공학과

We synthesized a dyad molecule that contained ferrocene and methoxyphenol moieties and used it as a voltammetric pH sensor based on the formal potential difference between these moieties. Unlike ordinary voltammetric pH sensors that have sensing layers on the electrode surface, we developed a composite electrode where the whole electrode body could be used as an electrode. Simple grinding the surface can expose a fresh surface. The composite electrode was made by mixing dyad-adsorbed carbon powder with styrene and divinylbenzene, and then polymerizing it with AIBN. One of characteristics of this electrode is that electro-triggering step is needed to exposed pH-sensitive quinone moiety through demethoxylation. We employed differential pulse voltammetric technique to precisely locate the potential. It was proved that anodic peak potential difference between hydroquinone and ferrecene groups gave a linear response over a wide pH range.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Non-enzymatic glucose detection using single-crystalline Au nanowire and AuM (M=Cu, Ag) bimetallic alloy nanowires.

김지환 엄가영 강미정[1] 김시인[1] 김봉수[1]

KAIST(KAIST) 화학과 [1]KAIST 화학과

Because of rapid detection with high sensitivity and selectivity, electrochemical glucose sensors are widely used in blood sugar monitoring. Especially, the researches on non-enzymatic glucose sensors with great sensitivity have risen at a considerable rate over the past decade since irreproducible bioactivity and stability of enzyme used in enzymatic glucose sensors can be excluded. Direct electrooxidation of glucose occurs at the electrode surface on which glucose is adsorbed first and then oxidized. Electrocatalytic activity of electrode varies considerably depending on the electrode material used. Au electrode has the great electroactivity to glucose oxidation and the small chemisorption of other electroactive species. We developed nonenzymatic glucose sensor using single crystalline Au nanowires (NWs). Well-defined surface with atomical smoothness of Au NWs resulted in particular cyclic voltammogram for the electrooxidation of glucose. In order to enhance the selectivity of the glucose sensor against interfering species such as ascorbic acid, we employed Au-Cu and Au-Ag alloy nanowire electrodes. The introduction of foreign metal to Au NWs shifted the oxidation potential of glucose effectively while that of ascorbic acid remained constant. This indicates that by applying the potential corresponding to the newly generated glucose oxidation due to the added foreign metal, glucose can be selectively detected without being interfered by ascorbic acid.

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발표코드: **ELEC.P-1424**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

정전기적 탈이온(CDI) 담수공정 성능향상을 위한 탄소나노튜브의 화학적 표면 개질

강한빛 이재영[1]

광주과학기술원(GIST) 환경공학과 [1]광주과학기술원 환경공학과

정전기적 탈이온(CDI)기술은 친환경적이고 에너지 소모량이 낮아 수처리 분야 중에서 최근 주목 받고 있는 기술 중 하나이다. CDI 성능 향상을 위한 많은 탄소소재의 전극 중에서, 탄소나노튜브(CNT)는 전기전도도가 매우 뛰어나고 높은 비표면적을 가지고 있어 CDI 공정에 새로운 소재로 부각되고 있다. 하지만 튜브와 튜브간의 강한 반데르발스 상호작용으로 수용액상에서 분산이 어려운 문제가 있어 CDI 공정의 응용에 약점으로 작용된다. 따라서 본 연구에서는 수용액상에서 CNT 를 잘 분산시키기 위해 화학적 산처리 방법으로 CNT 표면에 산소/탄소 비를 최적화하였고, 산처리된 CNT 가 CDI 의 전극으로서 사용될 때 성능향상 메커니즘을 연구하였다. CNT 표면에 생성된 산소 작용기는 전해질과의 접촉성을 최대화시키고, 그 결과 double layer capacitance 가 9.4 F/g 에서 21.3 F/g 로 두 배 이상 증가하였고, CDI 공정에 응용하였을 때 처리되지 않은 CNT 보다 더 좋은 흡착능력을 나타냈다.

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발표코드: **ELEC.P-1425**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Pt?Ru?Co?W quaternary anode electrocatalysts for methanol electrooxidation

권선영 김정호 유종성

고려대 신소재화학과

Direct methanol fuel cell (DMFC) is one of the most promising technologies for energy generation, which directly converts chemical energy of the fuel, (CH3OH and O2) into electrical energy. Supported Pt/Ru alloys are so far considered the best anodic materials for DMFC. It is well known that the oxidation of methanol on platinum catalysts generates CO as intermediate, which is a poison that adsorbs on the active sites of the catalyst. Ru forms oxygenated species at lower potentials than Pt and its presence in the catalyst promotes the oxidation of CO to CO2. Commercially available state-of-art Pt-Ru/C anode catalysts have optimal Pt:Ru ratio between 1:1 to 2:1, which still possesses very high Pt ratio and thus practically hinders the commercialization of the fuel cell. In this work, in addition to Ru, third and fourth metals such as Co and W are considered to be added to Pt to form multi-component electrocatalysts. Particularly, Co and W are known as highly active redox catalysts and thus seem to be a good addition to PtRu binary component system. Some active PtRuCoW quaternary electrocatalysts are explored as anode catalyst for DMFC using a robotic dispenser and combinatorial optical screening method. The newly developed alloy catalysts were synthesized by several different synthesis methods such as impregnation-NaBH4 reduction method, microwave-assisted polyol processes and urea-assisted homogeneous deposition (HD) and ethylene glycol (EG) reduction method. Urea-assisted HD-EG method was found to be most effective way of synthesizing Pt-Ru-Co-W quaternary alloy system, showing homogenous dispersion of the alloy catalyst nanoparticles with small particle size and thus, revealing the best electrocatalyitc activity for methanol oxidation. The enhancement of catalytic activity for methanol oxidation in the new quaternary catalyst could be explained by electronic effect, redox process and cooperative synergic effects of added Co and W metals.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Increased Pt oxygen reduction reaction activity with a hollow core-mesoporous shell (HCMSC) carbon catalyst support

송민영 양대수 김정호 박현열[1] 유종성

고려대 신소재화학과 [1]고려대 세종캠퍼스 신소재화학과

The hollow core-mesoporous shell (HCMS) carbon has been explored to support platinum (Pt) cathode catalyst with high metal loading in proton exchange membrane fuel cell (PEMFC). In this strategy, Pt nanoparticles (NPs) were deposited with high metal loading homogeneously on the HCSMC support through a urea-assisted homogeneous deposition (HD) method by using ethylene glycol (EG) as the precursor of a reducing agent. The HCMS carbon consisting of discrete spherical particles possesses unique structural characteristics including large specific surface area and mesopore volume and well-developed interconnected void structure, which are highly desired for a catalyst support in low temperature fuel cells. The Pt NPs deposited on HCMS carbon by the HD-EG strategy show smaller size with more uniform dispersion, resulting in higher Pt utilization efficiency and considerably improved Pt catalyst activity for the oxygen reduction reaction (ORR) compared with the Pt NPs/HCMSC prepared by conventional sodium borohydride reduction approach. We find the for the ORR compared with carbon black Vulcan XC-72 supported ones

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발표코드: **ELEC.P-1427**

발표분야: 전기화학

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Diamine-induced graphene oxide framework for anodes in sodium ion batteries

이빛나 표명호[1]

순천대 인쇄전자공학부 [1]순천대 화학과

Li ion battery (LIB)는 소형 전자기기 및 전기자동차 (EV)의 전원으로 활발히 적용되고 있으나, Li 의 소모량 및 현 EV 의 시장 점유율 등을 고려할 때 대용량 energy storage system (ESS) 에 적용할 경우, Li 매장량 한계 등으로 많은 문제점이 발생할 것으로 예측되고 있다. 이에 따라 Li 대신 Na 를 적용한 이차전지로 ESS 를 개발하려는 연구가 활발히 진행되고 있다. 그러나, 비록 작동원리 상 sodium ion battery (SIB)가 LIB 와 유사하다하더라도 이온 크기의 차이로 동일 소재를 그대로 적용할 수 없으며 음극의 경우 이런 현상이 더욱 뚜렷해진다. Graphene oxide 는 sp^2 결합을 이루는 탄소들이 벌집형태로 구성되어 있는 single-atom-thick sheet 로 넓은 표면적과 우수한 전도성, mechanical flexibility 가 뛰어난 SIB 의 음극재료로 유망한 소재이다. Graphene oxide 는 surface 와 edge 에 많은 oxygen-containing group 을 가지고 있기 때문에, 이를 수용액 상에서 diamine 과 혼합하면 아민이 protonation 되어 생성하는 -NH_3^+와 GO 가장자리에 존재하는 carboxylic acid group (-CO_2^-) 과의 electrostatic interaction 및 surface oxide 와 amine 사이의 수소결합으로 framwork 을 자발적으로 형성된다. 본 연구에서는 diamine 으로 수용성인 ethylene diamine (EDA), hexamethylene diamine (HDA), decamethylene diamine (DDA) 을 사용하여 graphene oxide framework 의 형성 하였으며, framework 생성에 따른 구조변화를 XRD, SEM 및 다양한 spectroscopy 법으로 확인하였다. 최종적으로, 이들 소재를 SIB 의 음극으로 사용하여, 전지의 capacity 및 cyclability 등을 확인하였다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1428**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of hollow carbon capsules from thioether-bridged organosilica for high electrical charge storage

김정호 송민영 양대수 박현열[1] 유종성

고려대 신소재화학과 [1]고려대 세종캠퍼스 신소재화학과

The in situ novel synthesis strategy of spherical thioether-bridged organosilica (TBOS) through the hydrolysis, self-assembly and co-condensation of bis-[3-(triethoxysilyl)propyl]disulfide (TESPDS) and octadecyltrimethoxysilane (C18TMS) generates hollow carbon capsules (HCCs) with hierarchical nanoarchitecture after calcination in N2 followed by soaking in HF to remove silica framework. Through initial hydrolysis and self-assembly of C18TMS and subsequent further co-condensation with C18TMS and TESPDS, a macroscaled core can be produced with formation of extended C18TMS-derived siloxane linkage (?Si?O?Si?) framework, while relatively carbon-rich organosilica shell can be formed through self-assembly of organic octadecyl bonds and ?(CH2)3?S2?(CH2)3? moieties on the C18TMS-derived silica-rich core. The as-prepared TBOS is then calcined in N2 flow at an elevated temperature and soaked in HF to produce the silica-free HCC. Our present synthesis approach greatly simplifies the fabrication process of so-called hollow core-mesopore shell type carbon, namely HCC here and can be expected to provide further insight into the facile synthesis of hierarchical nanostructured materials with a macroporous core?mesoporous shell. Due to its unique hierarchical nanostructure composed of hollow macroporous core and meso/microporous shell, which facilitates fast mass transport, along with large surface area for electrical charge storage, the HCC for the first time exhibits ultrahigh specific capacitance, good cycling performance and rate capability.

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장소: 부산BEXCO

발표코드: **ELEC.P-1429**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

FeF_3/Ordered Mesoporous Carbon (OMC) Nanocomposites and Their Enhanced Electrochemical Performance as a Cathode Material of Lithium Ion Batteries

정혜윤 신지현 김종식

동아대 화학과

FeF_3 is of great interest as a potential candidate of cathode materials because of their low cost, safety and environmental friendliness. FeF_3 has theoretical capacities of 712.52 mAh/g at 1.5 - 4.5 V range and 237.51 mAh/g at 2.0 - 4.5 V, respectively, which are higher than that of $LiCoO_2$ (≈273 mAh/g). However, FeF_3 has a low intrinsic electrical conductivity, slow diffusion of lithium ions, and poor cycle stability. These issues of FeF_3 should be improved to be applied in lithium ion battery systems. In this study, pristine FeF_3 showed an initial discharge capacity of 149 mAh/g at 0.1C (23.7 mA/g) with voltage range of 2.0 - 4.5 V at room temperature with poor cyclability. The electrochemical performance of FeF_3 was successfully improved via forming FeF_3/ordered mesoporous carbon (OMC) nanocomposites, e.g. higher capacity, capacity retention, and rate performance.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1430**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

전기화학적 에칭으로 제조된 다공성 실리콘 음극의 방전 특성

김소은 박동원[1] 이재영[2]

광주과학기술원(GIST) 환경공학부 [1]광주과학기술원 솔라에너지연구소 [2]광주과학기술원 환경공학과

기존 화석연료의 제한된 매장량과 환경문제 그리고 더 많은 에너지 수요를 충족시키기 위한 친환경 배터리 시스템에 대한 관심이 집중되고 있다. 특히, 전기자동차의 기술이 발전함에 따라 항속거리를 연장하기 위한 이차전지의 고성능화 기술이 요구되고 있으며, 현재 가장 유망한 기술로는 가격이 비교적 저렴하고 출력밀도가 높은 금속-공기전지가 주목 받고 있다. 본 연구에서는 수산화칼륨 전해질 기반의 다공성 실리콘 금속 음극을 이용하여 실리콘-공기전지의 에너지 효율향상에 대한 연구를 수행하였다. 불산 수용액의 농도와 에칭 시간 등의 인자 제어을 통해 다공성 실리콘의 모포로지를 조절하였고, 음극의 모포로지에 따른 방전율을 비교하였다. 이를 통해 실리콘-공기전지의 효율을 향상시킬 수 있는 다공성 실리콘 음극의 최적 형성조건을 확인하였다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1431**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

pH and glucose sensors based on a conducting polymer coated-Pt oxide dendrite probe

정지영 이영경[1] 이은정[1] 김덕수[2] 심윤보[1]

제주대 화학과 [1]부산대 화학과 [2]제주대 화학과

We report the development of pH and glucose sensors using the conducting polymer coated-pt oxide dendrite probe. Scanning Electron Microscopy (SEM), X-ray photoelectron spectroscopy (XPS) were used to investigate the structural and morphological features of electrodeposited dendrite layer. The conductive polymer coated pH sensor was designed to work in the range of pH 3~13. The calibration curve in buffer solutions exhibited a Nernst behavior (slope 59.2 mV/pH). Additionally, the potentiometric analysis of glucose through monitoring pH change was performed, which was enzymatically generated on the sensor at the range from 0.5 mM to 10 mM with a sensitivity of 5.839 mV/mM. The proposed glucose microbiosensor was examined for monitoring of glucose in a real blood sample.

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장소: 부산BEXCO

발표코드: **ELEC.P-1432**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Sensitive Detection of Esophageal Carcinoma Using a Nano Structured Collagen-AuNP-Hydrazine Bioconjugate

Ramjee Pallela Pranjal Chandra 김동민 심윤보

부산대 화학과

A nano-structured collagen-AuNP-hydrazine nanobioconjugate was prepared and applied for the amperometric detection of squamous cell carcinoma of the esophagus (ESCC). The sensor probe was developed by the immobilization of epithelial cell adhesion molecule antibody (EpCAM Ab) onto the AuNP-poly?(2,2':5',2"-terthiophene-3'-(p-benzoic acid)) (pTTBA) composite to form GCE/AuNP/pTTBA/EpCAM-Ab surface. The developed sensor probe and the nanobioconjugate were characterized by XPS, QCM, AFM and TEM. The amperometric response of the immunoreaction was monitored through the catalytic activity of H2O2 by the conjugate. The experimental parameters affecting the analytical performance were optimized, and the detection limit of the ESCC cells was determined. The interaction between the sensor probe and the number of cancer cells was determined with electrochemical impedance spectroscopy.

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장소: 부산BEXCO

발표코드: **ELEC.P-1433**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic activity of Cu2O/Au microcrystals for aerobic alcohol oxidation in water.

K.Sudhakara Prasad S.subba reddy Eswarreddy 심윤보

부산대 화학과

Cu2O/Au microcrystals were synthesized by using simple microwave assisted technique and the produced catalyst was characterized by various techniques such as UV?Visible spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, transmission electron microscopy, and scanning electron microscope energy dispersive spectroscopy (STEM-EDS). The studied catalyst exhibited good activity in aerobic oxidation of benzyl alcohol by using molecular oxygen and universal solvent water. The catalyst could easily be recovered after the reaction for repeated use.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1434**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A superoxide biosensor using Iron oxide containing cytochrome c bonded on the conducting polymer layer

이영경 RAJENDRA N GOYAL 심윤보

부산대 화학과

For the development of the superoxide biosensor, Fe2O3 as a long-distance electron transfer conduit was deposited at a Cytochorme C bonded on the Au nanoparticles composited- conducting polymer layer. A radical detection was performed using the biosensor, where probe materials including cyt c, lipids, Fe2O3 and conductive polymer was assembled on a screen-printed carbon electrode. The characteristics of the biomimetic layers were investigated employing cyclic voltammetry, SEM, and XPS. The optimum experimental conditions for the analysis were investigated and a calibration plot for super oxide detection revealed the dynamic range between 4.6 X10-6 M and 8.0X10-8 M.

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장소: 부산BEXCO

발표코드: **ELEC.P-1435**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Density functional theory calculation of redox potentials of M(acac)3 (M=V, Cr, Mn, Fe, Co)

이상연

경북대 응용화학과

The oxidation and reduction potentials of M(acac)3 (M=V, Cr, Mn, Fe, Co) in acetonitrile have been calculated using the Solvation Model Density(SMD) and the Conductor-like Polarizable Continuum Model(CPCM) for salvation modeling. The results will be presented and discussed.

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1436**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Density functional theory calculation of redox potentials of 1,4-benzoquinone and its derivatives

이상연

경북대 응용화학과

The reduction potentials of 1,4-benzoquinone and its derivatives in acetonitrile have been calculated using the Solvation Model Density(SMD) and the Conductor-like Polarizable Continuum Model(CPCM) for salvation modeling. The results will be presented and discussed.

대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1437**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Impedimetric quantitative analysis of metal ion on electrode surfaces

고현준 김세진 김규원

인천대 화학과

In this presentation, we demonstrate distance-dependent quantitative analysis on the DNA-modified electrode surfaces which permitted highly sensitive detection of Hg2+. Thiol-functionalized aptamer-oligonucleotide including poly-T sequence was immobilized on a gold electrode surface, and the resulting surface was used as a platform for sensing Hg2+. After the sensor surface was exposed to the solution of Hg2+ we monitored the insertion of Hg2+ between T-T mismatches to form a T-Hg2+-T bond using electrochemical impedance spectroscopy. The results showed that the charge transfer resistance on the surface increased with increasing Hg2+ concentration, which indicates the higher Hg2+ concentration the closer distance between the aptmer part and electrode surface.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1438**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Covalent functionalization of platinum to graphene sheet with the assistance of sulfur atom for electrochemical oxygen reduction

Mohammad Shamsuddin 한형순 정해상 전승원

전남대 화학과

A covalently bonded thiolated graphene sheet-supported platinum electrocatalyst (GO?S?Pt) has synthesized for electrochemical oxygen reduction reaction (ORR) in neutral media. The catalyst's structural features are characterized by transmission electron microscopy (TEM), energy dispersive X-ray (EDX), and X-ray photoelectron spectroscopy (XPS). Its activity towards the ORR has investigated by using cyclic voltammetry (CV), rotating disk electrode (RDE), and rotating ring disk electrode (RRDE) in 0.1 mol L^{-1} phosphate buffer solution (PBS) at pH 7, which is also used to assess the catalyst's kinetic parameters. Kinetic analysis in comparison to unbonded GOS/Pt and bulk Pt, a significant enhancement for the covalently bonded GO?S?Pt has found. On a glassy carbon electrode (GCE), the catalyst shows a significant catalytic activity, with its electrocatalysis of O2 reduction occurring via four-electron transfer reduction to H2O with minimal generation of H2O2.

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장소: 부산BEXCO

발표코드: **ELEC.P-1439**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Platinum nanoparticles graphited to thiolated graphene for improved electrocatalytic alcohol oxidation

김민수 전승원

전남대 화학과

We have studied Pt nanoparticles monodispersed on thiol graphene oxide (t-GO) surface and were successfully synthesis by the chemical reaction between K2PtCl6 and t-GO. As-prepared catalysts were characterized by SEM, TEM, XPS and FT-IR. The t-GO-Pt nanoparticles in H2O were ultrasonically dispersed and loading onto glassy carbon electrode (GCE) for alcohol oxidation, have been investigated using cyclic voltammetry (CV) and chronoamperometry (CA) methods. For measurement of methanol and ethanol electrooxidation reaction activities, CV and CA was performed in a solution containing respective 2.0 M CH3OH in 1.0 M H2SO4 , 1.0 M C2H5OH in 1.0 M H2SO4 at 25℃. This experiment data show that the t-GO-Pt catalyst loaded on GCE exhibits high electro-catalytic activity, superior tolerance towards reaction intermediates and unusually high stability towards alcohol electrochemical oxidation. This simple and straight forward method is of significance for the facile preparation metal-carbon nanocatalyst with high catalytic activity on proper supporting materials. The proposed catalyst could be used in DAFCs successfully.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1440**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical detection of thrombin using graphene oxide

최동철 박혜진 황신재 김규원

인천대 화학과

In this presentation, we report an electrochemical detection for thrombin using grarphene oxide. Graphene oxide, an insulating and disordered analog of highly conducting graphene has been used in various biosensor applications. Thiolated thrombin aptamer- modified electrode surface was employed as a platform for the thrombin detection. The changes in the interfacial properties of the electrode surface before and after its exposure to a solution of thrombin and graphene oxide were monitored using electrochemical impedance spectroscopy and cyclic voltammetry. We demonstrate that our method using graphene oxide permitted simple and sensitive detection of thrombin.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1441**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of non-enzymatic superoxide anion radical sensor by GCE modified with MWCNTs-Pt

김슬기 전승원

전남대 화학과

We developed a non-enzymatic superoxide anion biosensor using glassy carbon electrode (GCE) modified with Pt nanoparticles covalently bonded to the multi-walled carbon nanotubes (MWCNTs-Pt) and polydiallyldimethylammonium chloride (PDDA). The MWCNTs-Pt composite was characterized by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and electrochemical method. PDDA/MWCNTs-Pt/GCE showed irreversible diffusion-controlled electrode process for the mechanism of the reduction of superoxide anion. In the obtained cyclic voltammetry (CV) and chronoamperometry reponse, it has good sensitivity, wide linear range of detection, low detection limit, good reproducibility, and excellent storage stability for the electrocatalytic reduction of superoxide anion. PDDA/MWCNTs-Pt/GCE displayed better electrocatalytic activity than the previously reported enzyme electrodes enzyme toward the dismutation of superoxide.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1442**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel determination of hydrogen peroxide by electrochemically reduced graphene oxide grafted with aminothiophenol-Pd nanoparticles

유정민 전승원

전남대 화학과

Graphene oxide (GO) functionalized with aminothiophenol (ATP) by N,N'-dicyclohexyl carbodiimide (DCC)-activated amidation was used as a coupling agent. The GO-ATP formations of thiolated linkage were covalently bonded to palladium (Pd) nanoparticles (NPs). The GO-ATP-Pd was electrochemically reduced to graphene oxide (ERGO) at a potential range of 0 ~ -1.5 V and used in electrochemical biosensing for hydrogen peroxide (H_2O_2). The ERGO-ATP-Pd-modified electrode showed the advantages of excellent electrocatalytic activity toward H_2O_2 in PBS solution. The ERGO-ATP-Pd was characterized by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS) and electrochemical impedance spectroscopy (EIS). Cyclic voltammetry (CV) and chronoamperometry (CA) were used to characterize the biosensors' performance. The proposed H_2O_2biosensor exhibited a wide linear range from 0.1 μM to 10 mM and a low detection limit of 0.016 μM (S/N=3), with a fast response time within 10s. The biosensor therefore demonstrated excellent capability as a candidate for H_2O_2 analysis.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1443**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of poly(L-lactide) grafted MWCNT and application to electrochemical sensing of Hydrogen peroxide.

한형순 전승원 정해상

전남대 화학과

In this study, chemically synthesized poly(lactic acid) grafted Multi Wall Carbon Nano Tube (MWCNT-g-PLA)was used as electrocatalysts and their electrochemical properties were systematically characterized. Methylene diphenyl diisocyanate (MDI) was used to create the anchor sites on MWCNT. The synthesized MWCNT-g-PLA was characterized by the FT-IR, 1H-NMR, XPS and RAMAN spectroscopy methods. Again the composition and melt crystallization behavior was investigated by the TGA and DSC. The surface morphologies of MWCNT-g-PLA were evaluated using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The possibilities of employing MWCNTs for the electrochemical detection of H2O2, were studied. Electrocatalytic activities were verified from cyclic voltammetry (CV)

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1444**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A selective electrochemical sensor for ascorbic acid detection using the aminopyrimidyl fuctionlized-conductive polymer

Adel A. Abdelwhab 김동민 심윤보

부산대 화학과

A simple and selective detection method for ascorbic acid (AA) has been developed using a novel conducting polymer (poly-3'-(2-aminopyrimidyl)-2,2':5',2''-terthiophene (pAPTT)). The pAPTT was successfully formed on the electrode surface via electropolymerization of the APTT monomer, which was newly synthesized, in a 0.1 M TBAP/acetonitrile solution. The pAPTT layer on the sensor was characterized employing scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV). The pAPTT electrode showed an excellent selectivity in facilitating the electron transfer of AA and blocked the interferences of cationic species, which was due to the positively charged pAPTT film. The dynamic range of AA detection was from 10 to 200 ?M, and the detection limit was 1.4 ± 0.06 ?M. The reliability of the proposed sensor was evaluated using the real sample.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1445**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Amperometric Perchlorate Anion Selective Sensors with microhole array-water/organic Gel Interface

이상혁 이혜진

경북대 화학과

In this poster, we describe an amperometric perchlorate selective sensor based on the assisted transfer reaction of perchlorate ions by the perchlorate selective ligand namely, bis(dibenzoylmethanato)Co(II) ($Co(DBM)_2$) and bis(dibenzoylmethanato)Ni(II) ($Ni(DBM)_2$) across a microhole array interface between the polyvinylchloride - 2-nitrophenyloctylether (PVC - NPOE) gel and water phase. The current response associated with the facilitated transfer of perchlorate anion by either $Co(DBM)_2$ or $Ni(DBM)_2$ across the micro-water/gel interface versus the perchlorate concentration was linearly increased as a function of the perchlorate anion concentration. It was found that the use of differential pulse stripping voltammetry could enhance the sensitivity of our perchlorate sensing down to 0.1 μM via preconcentrating perchlorate anions in the gel layer by means of holding the ion transfer potential at 0 mV for 30 s followed by stripping the complexed perchlorate ion with the ligand. The effect of interfering anions such as Br^-, NO_2^-, CH_3COO^-, SO_4^{2-}, SCN^-, I^-, and CN^-, when using the perchlorate selective ion sensor was also investigated and both ligands showed an excellent selectivity towards Br^-, NO_2^-, CH_3COO^-, SO_4^{2-} ions.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1446**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Amperometric detection of phenol using tyrosinase immobilized polypyrrole modified carbon paper electrodes

Karim Md. Nurul 이혜진

경북대 화학과

In this poster, we demonstrate an amperometric phenol biosensor based on the immobilization of the tyrosinase onto a carbon paper electrode modified with electrodeposited polypyrrole films. Electropolymerization of pyrrole was first carried out in an aqueous solution containing 0.2 M pyrrole and 0.2 M KCl by cyclic voltammetry between 0 V and +0.70 V for 10 cycles at a scan rate of 20 mV/s. Tyrosinase, which previously reported as a good electrochemical catalyst for phenol detection [1], was then immobilized onto the polypyrrole modified carbon paper electrode. The immobilized tyrosinase assisted the hydroxylation of the phenol to form catechol molecules which was then oxidized to produce quinone. Finally, an amperometric signal upon the subsequent reduction of quinone was measured which increased linearly as a function of the phenol concentration. The determination of phenol in water samples using our phenol biosensors is underway.References: [1] J. Ren, T.-F. Kang, R.Xue, C.-N. Ge and S.-Y. Cheng, Microchim Acta (2011) 174, 303?309

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1447**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Use of degraded benzenediazonium-grafted organic layers to develop sensitive electrochemical immunosensor on ITO electrode surfaces

Al-Monsur Jiaul Haque 김규원

인천대 화학과

We describe use of degraded benzenediazonium-grafted organic layers to develop sensitive electrochemical immunosensor on indium-tin-oxide (ITO) electrode surfaces. Aldehyde-functionalized benzenediazonium cations (ABD) were electrochemically reduced to form the organic layers on the ITO electrode surfaces. The ABD-grafted organic layers were degraded by treating with phosphate buffer saline containing 0.05% Tween 20 (PBST). The modified ITO surfaces were characterized by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), and X-ray photoelectron spectroscopy (XPS). An electrochemical immunosensor was developed on the degraded ABD-grafted ITO surface through a sandwich-type enzyme-linked immunosorbent assay (ELISA) followed by electrochemical reduction of an enzyme-catalyzed reaction product, benzoquinone (BQ), at the sensor surface. The developed electrochemical immunosensor could detect an antigen mouse IgG at concentration as low as 10 pg/mL with high signal-to-noise ratio.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1448**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical detection of tyrosine at poly (thionine) modified anodized glassy carbon electrode

나스린쉬라즈로파 **Md.Mahbubur Rahman**[1] 이재준[2]

건국대 동물산업응용화학과 [1]건국대 신기술융합학과 [2]건국대 응용화학과

We developed a poly (thionine) [PTH] modified electrode on the anodized glassy carbon (GC) substrate, PTH/GC, for electrochemical detection of tyrosine. Cyclic voltammetry (CV) for the tyrosine showed a well-defined oxidation peak on PTH/GC at ca. 0.64V. CV results demonstrated that, the maximum sensitivity for tyrosine oxidation was observed at the 15 cycles electrochemically deposited PTH layer at pH 7.0. Differential pulse voiltammetric (DPV) measurements showed that the PTH/GC electrode could detect tyrosine in the linear range of 0.05mM to 1mM with a sensitivity of 0.028 mA/cm2/mM. This approach provides a simple and easy method to detect tyrosine selectively without interferences from dopamine (DA), ascorbic acid (AA), uric acid (UA), and epinephrine (EP).

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장소: 부산BEXCO

발표코드: **ELEC.P-1449**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic Efficiency of TiO_2Thin Film Prepared by Electrochemical Oxidation

이종호 김현우 윤오영 이용혁 장소희 오한준[1]

한서대 화학과 [1]한서대 신소재공학과

Titanium dioxide (TiO_2) is one of the most promising photocatalysts due to its excellent chemical stability and high efficiency for degradation of organic pollutants, good stability and nontoxicity. Thus, the titania catalyst has been attracted in environmental applications suh as waste water purification. In the present research, in order to improve the photocatalytic efficiency and photoresponse in visible light region, the TiO2 films as photocatalyst were synthesized using anodizing process which is based on the electrochemical oxidation of Ti substrate.The surface properties of synthesized titania film was characterized by SEM, XRD, XPS and UV-vis spectrophotometry. To evaluate the photocatalytic efficiency of titania film, dye decomposition test under exposure to Hg lamp radition was carried out. From the photocatalytic results, the titania film synthesized by anodizing process exhibited the high efficiency of dye decomposition.

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장소: 부산BEXCO

발표코드: **ELEC.P-1450**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Real-time detection of nitric oxide generated from snail's ganglia using a perfluorinated xerogel-derived amperometric microsensor

서보찬 Rebecca Hunter[1] 김승기 Mark H. Schoenfisch[1] 신재호

광운대 화학과 [1]University of North Carolina at Chapel Hill, U.S.A.

Endogenously produced nitric oxide (NO) has been studied broadly because it is distributed all over the body as a powerful signaling molecule. Nitric oxide takes a role to deliver the specific functions as a neurotransmitter and regulates the activity of the vascular endothelial and neuronal cells. Ganglia, a part of the peripheral nervous system provides intermediary connections between different neurological structures. Therefore, the detection of NO generated from ganglia may be essential to elucidate NO's neuronal functions. An electrochemical NO gas sensor possesses several advantages, including fast response time, high sensitivity, and easy miniaturization for in vivo measurements. These characteristics are suitable for spatial and temporal detection of NO in biological milieu. However, the electrooxidation of NO requires a relatively high working potential (+0.8 V vs. Ag/AgCl); thus, other readily oxidizable biological species may interfere selective detection of NO. The electrode surface has been modified with a xerogel membrane to improve the sensor's selectivity. It is well-known that amorphous and hydrophobic perfluoropolymers are highly permeable to various gaseous species including NO. In our previous work, applying a perfluorinated xerogel-derived gas permeable membrane allow us to improve selectivity of amperometric sensors while remaining high sensitivity towards NO. Herein we evaluate the perfluorinated xerogel-modified NO microsensor for the real-time detection of NO generated from snail's ganglia under stimulated and inhibited conditions. The potassium ion and 7-nitroindazole (7-NI) will be employed as a stimulator and an inhibitor for NO generation, respectively.

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장소: 부산BEXCO

발표코드: **ELEC.P-1451**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Power generation in a scaled-up microbial fuel cell

전용원 김형주[1] 김성현[2]

건국대 생명공학과 [1]건국대 미생물공학과 [2]건국대 특성화학부생명공학과

Wastewater treatments have great importance because direct wastewater discharge pollutes environment, significantly accelerating eutrophication in natural water body. Microbial fuel cell (MFC) technologies are promising to solve water-related environmental problems. Current MFC studies, however, have been limited to a laboratory scale. In this study, we constructed a large volume MFC in liter scale to pursue the possibility to apply in a real world, for example, to wastewater treatment as it requires large size MFCs. We have developed a hexagonal prism-shaped MFC of a 1.285 L using carbon fiber as anode material. Effects of temperature and substrate concentration on the performance have been examined. When operated in batch mode, maximum power density of 8.4 W/m^3 was obtained at temperature of 40 ℃ and 3 g/L acetate.

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장소: 부산BEXCO

발표코드: **ELEC.P-1452**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication and surface characterization of TiO2 Nanotube Arrays Prepared by Using Anodic Oxidation and Its Photocatalyst activity

백성림 정의덕[1] 정옥상 강영비[1]

부산대 화학과 [1]한국기초과학지원연구원 부산센터

TiO_2 nanotube array thin films (TiO_2 NTs) using both HF and NH_4 F electrolyte, anodic oxidation method has been processed. Comparisons were made ??with two kinds of electrolytes TiO_2 NTs. Prepared TiO_2 NTs photocatalytic characteristics were studied X-ray differaction(XRD) and Scanning electron microscopy(SEM) were used to investigate the morphology and thickness. Secondary ion spectroscopy(SIMS) analysis was used to investigate the surface atom image and depth profile analysis of TiO_2 NTs. Photocatalytic activities of TiO_2 NTs was evaluated by using UV-VIS Spectrophotometer(UV/Vis).

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장소: 부산BEXCO

발표코드: **ELEC.P-1453**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

전해질 조성에 따른 고압용 양극 화성박의 전기화학적 특성 분석

Electrochemical Properties of High Voltage Anodized Foil on Composition of Electrolyte

최형선 김현철

삼영전자공업(주) 박개발실

최근 전자 기기의 소형화, 높은 구동전압 및 용량이 요구됨에 따라 에너지 저장장치의 소형화 및 대 용량화에 대한 연구가 활발히 진행 중이다. 높은 파워밀도, 높은 구동전압 그리고 반 영구적인 수명을 갖고 있는 커패시터역시 소형화에 대한 연구가 활발 히 진행중에 있는데 그 중 적층형 커패시터는 양극으로 알루미늄박을 사용하고 유전체로써 양극산화피막을 사용하며 대극으로써 Ni 도금층을 전극으로 활용함으로써 전해액과 음극박을 사용하지 않아 기존의 커패시터보다 슬림하고 직・병렬 연결이 용이하여 높은 전압과 대용량을 구현할 수 있다. 반면 전해액을 사용하지 않게 되면서 피막의 자가회복력이 없어지고 피막의 안정성이 떨어지게 되어 기존의 구조보다 낮은 내전압을 갖는 문제점이 제시되고 있다.본 연구에서는 이러한 적층형 콘덴서의 양극산화피막의 문제점을 보안하기 위해 몇몇의 유기산 전해액을 통하여 양극산화피막을 형성시키고 각각의 피막이 가지는 특성을 FE-SEM, BDV, tanδ, impedance 분석을 통하여 고찰하였다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1454**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

유기산 전해질을 사용한 양극산화법으로 제조된 산화 알루미늄 피막의 특성에 대한 연구The Study of Properties of Aluminium Oxide Film Fabricated by Anodization Method in Organic Acid Electrolyte

전병문 이병건

삼영전자공업(주) 박개발실

알루미늄 및 알루미늄 합금은 반응성이 매우 강한 금속이지만, 대기 중에서 표면에 보호성 자연산화막을 형성하는 밸브 금속의 일종으로, 뛰어난 내식성을 갖는다. 형성된 자연산화막의 두께는 매우 얇으므로 산업적으로 이용하기 위해 양극산화법을 사용하여, 두껍고 치밀한 산화막을 형성시킨다. 알루미늄의 양극산화에 있어서 중요한 요인 중 하나인 전해질에 대한 연구동향을 살펴보면, 피막 안정성이 좋은 붕산 전해질에서 높은 정전용량을 갖는 피막을 형성시킬 수 있는 구연산, 말론산, 타르타르산과 같은 유기산 전해질로 대체하는 연구가 활발하게 이뤄지고 있다. 본 연구에서는 기존의 붕산 전해질을 사용하여 형성된 양극산화피막과 유기산 전해질을 사용하여 형성된 양극산화피막의 전기적 특성을 비교하였다. 또한 피막의 형상과 결정성을 알아보기 위해 FE-SEM, TEM, FT-IR 분석을 실시하였다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1455**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Organic ion transport controled by electrochemical method with facial fabricated conducting polymer modified membrane

PIAOHUSHAN 손용근

성균관대 화학과

A lot of membrane separation methods were introduced in recent years. In this study, we went to perform a facile fabrication of conducting polymer modified membrane with immobile dopant ions. These modified membranes would be used for controling organic ion transport by adding constant and pulse potentials. First, gold was sputtered on the PC(polycarbonate) membrane and then a polypyrrole layer was electrochemically deposited on the Au surface in aqueous solution until the pores were covered perfectly. Then Methylene Blue(MB) permeation experiment progressed under various potential conditions. Since MB is a cationic dye, it's flux can be effected by the positive and negative potentials. In this study, we demonstrated that the organic ion permeate through the membrane can controled by adding constant and pulse potentials and proposed the ion transport mechanisms. 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)

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장소: 부산BEXCO

발표코드: **ELEC.P-1456**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, characterization and self-assembled monolayer of poly 8-(2,3-Dihydro-thieno[3,4-b][1,4]dioxin-2-ylmethoxy)-octane-1-thiol

Wang Wenxiu 손용근

성균관대 화학과

Due to the potential use of organic semiconducting materials as a low-cost alternative to silicon, so many groups exploring the field of organic electronics has exploded over the past decades. Ploythiophene is one of the most used conducting polymer in the fields of OFET, OLED etc. Polythiophene can be synthesized by either electrochemically or chemically methods using a simple oxidation process. Here we have synthesized the monomer EDTHM-8-SHA, and used electrochemical and chemical methods especially to obtain the polymer (PETHM-8-SHA). And the new monomer successfully forms a self-assembled monolayer on the gold electrode. The characterization of the monomer and polymer are used the CV and SEM test. 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)

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장소: 부산BEXCO

발표코드: **ELEC.P-1457**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High Surface Area of Nanoporous Platinum by alloying-dealloying method for Enzymatic Glucose Sensor

조혜진 손용근

성균관대 화학과

Nanoporous metals have recently attracted considerable interest in a wide variety of applications including catalysis, fuel cell, sensors etc. In this report, high surface area of nanoporous platinum electrode was fabricated by electrochemically alloying-dealloying method. Platinum is well known element that shows a significant electrocatalytic activity in many important applications. However, bare platinum has the shortcoming of low electrocatalytic activity towards the oxidation of glucose due to the poisoning effect of reaction intermediates, resulting in low sensibility, poor selectivity. So, we tried to use glucose oxidase to improve sensitivity.First of all, Zn nanoparticle was electrochemically deposited on Pt disc. Later then, Pt-Zn alloy was electrochemically dealloyed to obtain porous platinum surface. Glucose oxidase was immobilized on porous platinum. Then, to avoid leakage of glucose oxidase, Nafion was covered. We verify high surface area of the platinum electrode by showing response of H_2SO_4 and methanol. 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)

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장소: 부산BEXCO

발표코드: **ELEC.P-1458**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon supported cobalt oxide nanoparticles-iron phthalocyanine as alternative cathode catalyst for oxygen reduction in microbial fuel cells

Ahmed Jalal 김성현[1]

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The high cost and limited resources of precious metals as oxygen reduction catalysts (ORR) hindered the widespread use of microbial fuel cells (MFCs) in practice. Here, the feasibility of metal oxide assisted metal macrocyclic complex was investigated as a catalyst for ORR in an air-cathode MFC. Electrochemical results revealed that cobalt oxide (CoOx) incorporation increased the ORR activity of iron phthalocyanine (FePc). In MFCs, the maximum power density of 654±32 mW m^{-2} was achieved from the C-CoOx-FePc cathode, which was 37% higher than the power density of carbon supported FePc (C-FePc). The voltage output of the MFC only decreased to 85 % of its initial voltage after 50 cycles, suggesting that the synthesized catalyst showed acceptable long-term stability. The voltage drop partially resulted from the covering of biofilm on the catalyst layer. This work provided a potential alternative to Pt in MFCs for sustainable energy generation.

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장소: 부산BEXCO

발표코드: **ELEC.P-1459**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

구리 기판 위에 전착한 SnO2의 제조에 관한연구Tin oxide films directly deposited on copper substrate by electrodeposition

권병국

한국산업기술대 신소재공학과

SnO2 막을 전착법으로 구리 기판위에 직접 제조하였다. 20~30 mM 의 염화주석(SnCl2·H2O)과 100~150 mM 의 질산(HNO3)을 첨가한 수용액을 70~85℃로 가열하였으며 작업 전극으로 구리기판과 대전극으로 주석판을 사용하여 2 전극법으로 실험하였다. 전압이 0.4V 이상으로 하였을 때 비정질의 SnO2 막이 형성되었다. 전착 시간이 5 분이내로 짧을 경우 SnO2 막이 형성되었으나 이 보다 전착시간이 길어진 경우에는 금속 주석이 함께 형성되었다. 전압이 0.6V 이상에서는 금속 주석이 생성 되었다. 전착시간이 긴 경우 금속 주석이 형성되는 것은 전착이 진행되면서 전해액 내에 Sn4+의 농도가 낮아지고 Sn2+의 농도가 높아지기 때문으로 사료된다. SEM, EDS 분석 결과 생성물에는 다량의 염소가 검출되었으며 이로부터 전착 시 금속 주석과 뿐 아니라 염화물이 함께 생성된 것으로 생각된다. 전착이 진행됨에 따라 기판의 표면은 흰 색의 SnO2 막에서 노란 색의 생성물이 생기는 것을 관찰하였으며 400℃의 불활성 분위기에서 열처리 한 결과 검은 색의 상으로 변화하였다. 본 연구에서는 Scanning electron microscope (SEM)과 X-ray Diffraction (XRD) 분석을 통해 전착 조건에 따른 생성물의 상을 분석하고 이에 대한 기구에 대해 논의한다. 또한 구리 기판 위에 직접 제조한 SnO2 및 Sn 을 리튬-이온 전지의 음극재료로서 사용한 전지 특성에 대해 고찰한다.

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1460**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Laccase cathode with CNT incorporation for the electrocatalytic reduction of O2

김수정 신효설 강찬

전북대 화학과

An O2 reduction cathode on which laccase enzyme was wired by PAA-PVI-[Os(tpy)(dme-bpy)]2+/3+ (tpy = 2,2’;6,’2’’-terpyridine ; dme-bpy = 4,4'-dimethyl-2,2'-bipyridyl) redox polymer was constructed. The laccase enzyme electrode coated with a redox hydrogel film was prepared by dropping a mixture consisting of redox polymer, laccase and poly(ethylene glycol) diglycidyl ether (PEGDGE) over the carbon cloth-attached glassy carbon surface. In another way, a cathode, in which carbon nanotubes (CNTs) were incorporated, was also constructed. An optimal composition of redox polymer, CNTs, and laccase with the PEGDGE cross-linker content was determined. For the two prepared cathodes, electrocatalytic-reduction of O2 catalyzed by laccase was measured by rotating disk voltammetry under the condition of pH 5.0 0.2 M citrate buffer at 37℃. An enhancement of current density for O2 reduction on the laccase cathode with CNTs in comparison to that without CNTs was measured and the effect of CNT incorporation was characterized by controling conditions such as pH of the supporting electrolyte and the presence of halide ions.

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장소: 부산BEXCO

발표코드: **ELEC.P-1461**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Au Nanowire Electrodes: The Smallest Implant for Recording Neural Signal

강미정 강호석[1] 곽주현 김봉수

KAIST 화학과 [1]KAIST Chemistry

To improve the long-term functioning of neuroprosthetic devices and discrimination of different neural signals, reduction of the implant size is of great importance Here we report fabrication of nanoelectrodes made of single crystal gold (Au) nanowires (NWs) with a characteristic diameter of ~150 nm and demonstrate that it is possible to carry out measurements of neural signals from a brain of freely moving mouse using the Au NW electrodes. Since Au NW electrodes have high conductivity and small surface areas, we could observe the neural spikes with highly improved signal-to-noise (S/N) ratio compared to conventional W electrodes. Furthermore, the Au NW electrodes picked up distinctly different neural signals even when implanted as close as 1 mm apart inside a mouse brain, showing high space-selectivity. The perfect crystal Au NW electrodes could provide much improved information on the brain functions by sensitive neural recordings, and be employed in diverse biomedical fields including medical treatments by neural stimulation, brain machine interfaces, and in vivo monitoring of brain chemistry.

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장소: 부산BEXCO

발표코드: **ELEC.P-1462**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced electrogenerated chemiluminescence of phenylethynyl pyrenylethynylpyrene derivatives

주영원 유상욱 이연옥[1] 김종승[1] 김주훈

경희대 화학과 [1]고려대 화학과

우리는 phenylethynylpyrene 을 바탕으로 phenyl group 의 para-position 에 weak electron donating group 인 propyl group 을 도입한 화합물(1-5)들을 합성 하였습니다. 이 결과로 작용기가 많이 치환될수록 (1<4

THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ELEC.P-1463**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Study of TMA ad-structures depending on potential control with STM and theoretical calculation.

김잔디 신동완 이충균

충남대 화학과

Bottom-up architectures of 2D organic monolayers mainly rely on noncovalent bonds such as hydrogen bond, metal-ligand coordination and van der Waals interactions between the building-blocks.The information on the structures of organic monolayers, exculsively obtained using scanning tunneling microscopy (STM), would be a break-through to understand the interactions between the primary building-blocks and their useful properties such as nanopores in regular patterns, surface chiralities and reactivities. This work focus the adsorption of 1,3,5-Benzenetricarboxylic (Trimesic Acid, TMA) to a single crystal Au surface and interpretation with network structure of primary hexagonal TMAs at different potentials, using STM and theoretical calculation. The potential dependence of TMA structures was understood as a transition from molecular adsorption to anionic adsorption.

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장소: 부산BEXCO

발표코드: **ELEC.P-1464**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

셀레늄 전해석출 시 빛 조사의 영향

채원석 김승훈 정재구 한만소 박성호

대진대 화학과

수용액에서 FTO-glass 위에 셀레늄의 전해석출 시 빛의 영향을 제작된 전해용기로 확인하였다. 빛과 온도의 영향을 동시에 확인하기 위하여 용기의 아래 부분은 FTO-glass 를 장착 하였을 때 빛이 통과할 수 있는 구멍이 만들었고, 물자켓-비커를 이용하여 온도를 조절 하였다. 저온보다는 고온에서 셀레늄이 잘 석출되었으며, FTO-glass 의 뒷면에서 빛을 조사해 줄 경우 셀레늄의 전해석출 속도가 빨라지고 두께와 결정도가 향상되었다. 셀레늄 전해석출 시 순환전압전류법과 일정전압법을 사용하여 비교하였을 때 일정전압법에서 석출표면이 더 고르게 석출되는 것을 확인할 수 있었다. 셀레늄의 표면을 관찰하기 위하여 XRD, SEM, AFM 을 사용하였고, UV-Vis 분광기를 이용하여 밴드갭 에너지를 측정하였다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1465**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

STM의 tip 주사에 의한 POM-dodecane thiol 자기조립박막의 변형

신동완 김잔디 김종원[1] 이충균

충남대 화학과 [1]충북대 화학과

Au 표면에 형성된 thio 의 자기조립박막(SAM)에 대한 연구는, 나노 과학이나 나노 기술 분야에서 수 십년 동안 진행되어오고 있다. 주사탐침현미경(STM)을 이용한 자기조립박막의 연구는 분자 수준에서의 정보를 제공하며 특히, STM tip 을 사용해 tip-induced 탈착을 통한 lithography 에 응용할 수 있다. STM 의 tip bias 나 tunneling current 등의 파라미터들을 조작하여 자기조립박막의 부분적인 tip-induced 탈착을 제어할 수 있다.이 연구에서는 Au(111) 표면에 흡착시킨 SiMo- 타입의 polyoxometalate (POM)- dodecane thiolate 의 자기조립박막이 STM tip 에 의해 변형되는 것을 관찰하였고, POM 이 없이 dodecane thiol 만 자기조립된 Au 표면과 비교하여 POM 이 STM tip 으로 부터 주사되는 전자를 효과적으로 transfer 시키는 역할을 한다는 것을 알 수 있었다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1466**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Electrocatalytic Activity of Quantum-Sized Gold Nanoparticles Modified on ZnO nanorods/ITO Electrode for the Determination of p-Aminophenol.

백그린 고은솔 Prabhu 이동일

연세대 화학과

We here demonstrate the enhanced electrocatalytic activity of quantum-sized thiolate protected Au_{25} nanoparticles (Au_{25} NPs) modified on ZnO nanorods/ITO electrode. We recently revealed that Au_{25} NPs can be utilized for amperometric sensing because of the enhancement in electrocatalytic activity. To employ these special characteristics of Au_{25} NPs, initially well-aligned ZnO nanorod arrays are synthesized on indium-tin-oxide (ITO) surface through hydrothermal method followed by immobilization of Au_{25} NPs on ZnO nanorods/ITO electrode to achieve sensitive detection of p-aminophenol (AP). To clearly demonstrate the enhancement in signal associated with Au_{25} NPs, anodic current measurements of the alkaline phosphatase (ALP) enzyme catalyzed oxidation of 4-aminophenylphosphate (APP) to AP was investigated. The stable and reproducible modification of Au_{25} NPs on ZnO nanorods/ITO electrode resulted in a highly sensitive detection of AP which shows great potential for the ultrasensitive ALP biosensor applications.

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장소: 부산BEXCO

발표코드: **ELEC.P-1467**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Deposition and Photoluminescence of ZnS

채원석 정재구 김승훈 한만소 박성호

대진대 화학과

수용액에서 황화아연(ZnS)을 전도성 유리전극에 전기화학적으로 석출하였다. ZnS 의 전해석출은 순환전압전류법과 일정전압법으로 수행되었으며, 0.10 mol/L 의 $LiClO_4$ 가 지지전해질인 수용액의 온도는 70 도이고 $ZnSO_4$ 와 NaS_2O_3 을 사용하였다. 전해석출된 ZnS 는 짙은 회색을 나타내었고 5 분 정도의 짧은 시간에 매끄러운 박막을 얻을 수 있었으며, 전해석출 시간에 비례하여 XRD 세기가 증가하였다. 전자현미경의 관찰로 ZnS 의 표면은 구형 다발로 확인되었으며 광발광 측정에서 370 nm 의 들뜸광원에 대하여 최대발광 파장이 412 nm 인 발광스펙트럼을 확인하였다.

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장소: 부산BEXCO

발표코드: **ELEC.P-1468**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Highly Efficient Porphyrin Dyes for Dye-Sensitized Solar Cells

이시우

인천대 화학과

In view of the limited availability of fossil fuels and the disastrous environmental issues related with their combustion, it is imperative to develop renewable energy resources for the increasing global energy demand. The dye-sensitized solar cell (DSSCs) has attracted considerable attention as a promising technology for low-cost and high-efficiency photovoltaic cells. Significant efforts are now being made on the development of new sensitizer dyes to improve performance of DSSC for the purpose of possible commercialization. As such, it is necessary to elucidate the influence of dye structure on the device function. Porphyrins have been intensively investigated for use in DSSCs for over 12 years. The work was motivated in part by their central role in the photosynthetic reaction center as for light harvesting pigments. The achievement of an 11% solar-to-electric power conversion efficiency under standard condition (AM 1.5G, 100 mWcm-2) by using a judiciously tailored porphyrin dye is reported, which is comparable to that of other organic based dyes developed recently. Porphyrins are particularly appropriate for this application, because they show large absorption coefficients in the visible-near infrared (NIR) region, tunable redox and photophysical properties. In this presentation, we report the synthesis and characterization of a NIR porphyrin dye, focusing on one particular issue; the influence of dye structure upon tunable redox potential and photoinduced charge separation. We address this issue with employing a series of porphyrin dyes, which enable us to study the effect of dye structure on energy level and thus device performance.

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장소: 부산BEXCO

발표코드: **EDEC.P-1469**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

강산의 세기와 이온화 상수에 대한 교과서 내용 및 화학교사의 인식 분석Analysis of Textbook Content and Chemistry Teather's Cognition about Strength and Ionization constant of Strong Acid

전민철 백성혜

한국교원대 화학교육과

연구에서는 중등학교 화학 교사 50 명을 대상으로 강산의 평준화 효과, 이온화 상수에 대한 이해 정도를 알아보고, 개념 형성의 주된 근거가 무엇인지를 설문과 면담을 통하여 알아보았다. 그리고 교수요목기의 교과서부터 2009 개정 교육과정 화학Ⅱ 교과서의 서술 내용을 외국 교과서, 일반화학, 분석화학 및 유기화학 등 대학 교재, 화학 자료집 등의 서술 내용과 비교 분석하여 강산의 평준화 효과에 대한 교사의 인식의 차이를 찾고자 하였다. 연구 결과, 대부분의 화학 교사들은 강산의 평준화 효과와 이온화 상수에 대해 이해 정도가 매우 낮았고 이온화도와 이온화 상수 값이 호환되지 않는 현상에 대해 혼란스러워 하고 있었다. 교사들은 교과서에 제시된 강산의 이온화 상수 값을 별다른 비판적 사고을 거치지 않고 수용하고 있었다. 강산은 H_3O^+보다 산의 세기가 크므로 그 종류와 무관하게 물 속에서 평준화 효과에 의해 산의 세기가 같아진다. 그러나 화학 교과서에서는 별다른 부연 설명 없이 제시한 강산의 이온화 상수(HCl-10^7, H_2SO_4-10^2, HNO_3-20)를 그대로 믿는다면 강산의 평준화 효과와 모순되기에 과학적으로 신빙성 있는 자료로 보기 어렵다. 이러한 결과로부터 화학 교사들이 강산의 세기에 대해 올바른 인식을 가지기 위해서는 화학 교과서의 내용에 대해 비판적인 시각에서 사고하고 설명 상의 오류를 찾을 수 있는 능력을 길러 줄 수 있는 교사교육이 필요함을 알 수 있다.

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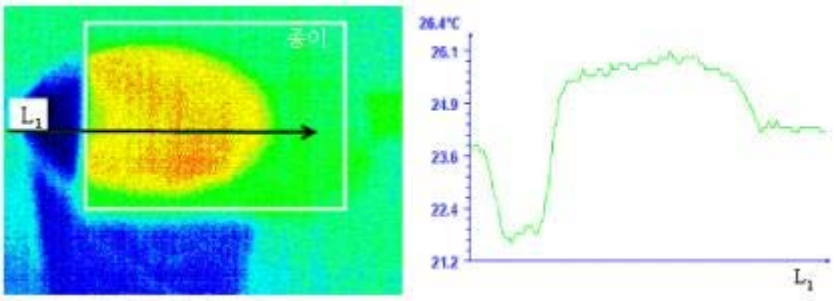
발표코드: **EDEC.P-1470**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

열화상 카메라를 이용한 화학 반응의 가시화Visualization of chemical reaction using thermal image camera

옥준석 강성주[1]

서울과학고 화학과 [1]한국교원대 화학과

본 연구에서는 과학 기술의 발달로 성능이 급속도로 향상되고 있으며, 그에 따라 장비의 활용 범위가 크게 확장되고 있는 적외선 열화상 카메라를 과학 교육 현장에 적용하는 방안을 마련하고자 하였다. 물질의 상태 변화와 화학 변화 과정에는 항상 열 출입이 수반되는데, 지금까지는 그 변화를 계가 평형에 도달한 후 측정되는 온도계의 눈금이나 수치로 읽을 수밖에 없었다. 본 연구에서 열화상 카메라를 이용한 결과 물질의 상태 변화 과정이나 화학 반응의 진행 과정을 실시간으로 시각적인 관찰을 할 수 있었다. 열화상 카메라의 중고등학교 교육 현장 활용은 학생들로 하여금 과학 실험의 정밀한 측정의 부담을 덜어줄 것이다. 또한 발생한 열에 의한 온도 변화가 색깔 변화로 나타나므로 학생들의 과학에 대한 흥미를 크게 제고할 것으로 기대한다.



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발표코드: **EDEC.P-1471**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

chemistry class using the sea water analysis

천만석 오진호[1]

한국과학영재학교 화학 [1]한국과학영재학교 화학생물학부

바닷물은 부산에서 쉽게 접할 수 있는 시료이다. 하지만 바닷물을 염의 농도가 너무 높아서 바로 측정하기 어렵고 또한 주성분의 분석을 위해서는 1000 배 이상을 희석해야 하기에 미량성분 분석이 안되는 문제점이 있다. 지구과학에서 해수에 대한 물리화학적인 실험이 있지만 바닷물의 화학 성분을 확인하는 실험에 관한 것은 잘 알려져 있지 않다. 화학의 증발, 저울 사용, 침전반응, 증류 작용, 적정, 희석과 오차 분석을 통하여 기본적인 화학 실험법을 익히고 적용하고자 한다. 특히 이러한 중학교 및 고등학교 교과과정 내용 및 도전적인 학생을 위한 정량 분석과 통계적인 접근법으로 실험 데이터의 처리에 대한 경험을 향상하고자 한다. 바닷물의 주성분은 물이며 1000 g 해수에 35 g 의 염분이 존재하며, Na^+, Cl^-, SO_4^{2-}, 가 주성분을 이루고 있다. 염분의 양을 증발을 이용하여 측정하여 참값 및 모둠별 값을 비교한다. 또한 용기의 변화에 따른 증발 시간의 변화 및 저울의 사용법을 익힌다. 또한 바닷물의 정성 분석으로 침전 반응을 이용하여 Ba^{2+} (SO_4^{2-}), Pb (CrO_4^{2-}), Ag (Cl^-, Br^-) 반응으로 확인을 한다. 간단한 증류 장치를 이용하여 증류한 후의 침전반응으로 증류 효과를 확인한다. 또한 증류 전 후의 염의 양을 정량하기 위하여 불꽃 흡광장치 (flame-AAS)를 이용한 Na 의 정량과, 이온크로마토그래피 (IC)를 이용한 Cl^-과 SO_4^{2-}의 양을 구한다. 또한 다량 성분인 염소량을 정량하기 위하여 질산은을 이용한 침전 적정을 실시하여 염소 및 할로겐화물의 양을 정한다. 알려진 바닷물의 농도와 비교하여 통계적인 방법을 통하여 차이를 토론한다.

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발표코드: **EDEC.P-1472**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

예비교사들의 변칙 사례 실험에서의 반응 유형과 과학과 실험의 본성에 대한 인식이 이에 미치는 영향

손수희 백성혜

한국교원대 화학교육과

이 연구의 목적은 예비 화학교사들이 변칙 사례 실험과 변칙 사례에 대한 원인을 밝히는 가설 검증 실험을 수행하는 과정에서 나타난 과학과 실험의 본성에 대한 인식을 알아보는 것이다. 이 실험은 예비화학교사의 예상에서 빗나가는 변칙사례 실험이다. 이를 위하여 화학교육과에 재학 중인 예비교사 9 인을 선정하여 중학교 1 학년 교과서의 실험을 수행하고, 이에 대한 보고서와 설문지, 반구조화된 면담 등의 질적 연구 방법을 통해 예비화학교사들의 실험 수행과 관련된 자료를 수집하였다. 수집된 자료는 전사 후 분석되었다. 연구 결과, 변칙사례 실험에서는 무시, 거부, 판단불가, 주변이론의 변화의 반응 유형이 발견되었다. 변칙사례에 대한 가설 검증 실험에서는 무시, 거부, 주변이론의 변화의 반응 유형이 발견되었다. 변칙사례에 대해 가설 검증 실험에서 실험에 대한 평가와 반성의 기회를 가짐으로써 일부 예비교사의 변칙사례에 대한 반응유형이 발전하였다. 하지만 3 명의 예비교사는 여전히 낮은 수준의 반응유형을 보였는데, 이들의 발전을 방해하는 요인으로는 과학 본성에 대한 인식, 실험측정의 본성에 대한 인식, 권위주의에의 의존, 낮은 수준의 추론 능력이 있다. 그리고 실험 후 면담과정에서 가설 검증 실험에서 발전하였던 예비교사들이 대부분 초기의 반응유형으로 회귀하였고, 그 이유로 대부분의 예비교사들은 대학 수준의 실험에 대한 불신을 들었다. 또한 법칙과 이론의 본성에 대해 도구주의적 관점과 상대주의적 관점을 가진 예비교사들은 변칙 사례 실험에서 높은 수준의 반응 유형을 나타나는 것이 관찰되었다. 이 연구를 통해 예비화학교사들이 예비교사 양성 교육기관에서 이루어지는 실험에 대해 불신하고 있으며, 예비교사 과학과 실험의 본성에 대한 인식이 실험실습에 대한 태도에 영향을 주었음이 나타났다.

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장소: 부산BEXCO

발표코드: **EDEC.P-1473**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

상태 변화와 용해에 대한 초등학생들의 개념 연구

강석진

전주교육대 과학교육과

이 연구에서는 초등학교 6 학년 학생 326 명을 대상으로 학생들이 상태 변화와 용해에 대해 어떤 선개념을 지니고 있는지 조사하였다. 학생들의 개념을 조사하기 위하여 선행 연구를 바탕으로 개념 검사지를 개발하여 사용하였다. 개념 검사지는 상태 변화와 관련된 3 문항(물의 끓음, 기화 시의 질량 변화, 수증기의 응결)과 용해에 관련된 2 문항(용해 시의 질량 변화, 용액의 균일성)으로 구성하였다. 연구 결과, 많은 학생들이 '물이 끓을 때 생기는 기포 속의 물질은 공기이다', '기체는 액체보다 가볍다', '컵 표면의 물방울은 얼음이 녹은 물이다', '설탕이 녹으면 가벼워진다', '소금은 무거우므로 소금물의 아랫쪽이 짜다' 등과 같은 다양한 선개념을 지니고 있는 것으로 나타났다.

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장소: 부산BEXCO

발표코드: **EDEC.P-1474**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

시각장애 초등학생의 용해 개념에 대한 사례 연구

김학범 차정호

대구대 과학교육학부

이 연구에서는 시각장애를 가진 초등학생의 용해 개념 특성을 조사하였다. 서울시 소재 시각장애 초등학교 5 학년 학생 4 명을 대상으로 용해의 정의, 균일 혼합물로서의 용액의 성질, 용해시 질량의 보존, 그리고 용해시 부피의 변화에 대하여 반구조화된 면담을 실시하였다. 모든 면담 상황은 녹화되었고 그 자료를 전사한 뒤 분석하였다. 면담을 분석한 결과, 시각장애학생들의 용해에 대한 이해는 대부분 현상에 의존하였고, 용해시 질량의 보존에 대해서는 알고 있었지만 그 이유를 설명하지는 못하였다. 포화 현상에 대해서는 이해하지 못하였으며, 과학적 용어의 사용이 미흡하였다. 모든 학생들이 부피 개념은 가지고 있었지만, 용해시 부피 변화에 대해서는 이해하지 못하였다. 전반적으로는 같은 학년의 정안 학생과 비슷한 양상을 보였으며, 시각장애가 있기 때문에 나타나는 특이한 개념 이해는 발견되지 않았다. 이러한 결과에 기초하여 시각장애 학생들의 개념 이해를 증진시키기 위한 방안을 논의할 것이다.

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발표코드: **EDEC.P-1475**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

대학생들의 창의적 사고력, 비판적 사고력, 학업적 자기조절 분석

방담이 박지은[1] 강순희[1]

가톨릭대 ELP학부대학 [1]이화여대 과학교육과

창의적 문제해결을 위해 필요한 사고력은 창의적 사고력과 비판적 사고력이다. 또한, 창의성과 내재적 동기의 관련성, 창의성과 외재적 동기의 관련성에 대해서는 저마다 다른 결과들이 제시되고 있다. 이 연구에서는 245 명의 대학생들(남 109, 여 136)의 창의적 사고력과 비판적 사고력, 그리고 학업적 자기 조절간의 관계를 분석하고 성별에 따른 차이를 알아보고자 하였다. 창의적 사고력 검사지로 Torrance 가 개발한 창의성 검사인 TTCT(Torrance Tests of Creative Thinking)를 사용하였으며, 비판적 사고력 검사지로 Watson-Glaser 의 Critical Thinking Appraisal 를 사용하였다. 학업적 자기조절에 대해서는 K-SRQ-A 검사지를 활용하였다. 창의적 사고, 비판적 사고, 학업적 자기조절(외적 조절, 부과된 조절, 확인된 조절, 통합된 조절, 내재적 조절)의 상관관계를 분석한 결과 창의적 사고는 확인된 조절, 내재적 조절과 상관이 유의미한 것으로 나타났으나 그 상관이 매우 낮았다. 비판적 사고는 확인된 조절, 통합된 조절과 상관이 유의미한 것으로 나타났으나 그 상관 또한 모두 낮게 나타났다. 마지막으로 창의적 사고와 비판적 사고 사이에는 유의미한 상관이 나타나지 않았다. 성별에 따른 창의적 사고력, 비판적 사고력, 학업적 자기조절의 차이를 분석하기 위하여 독립표본 t 검정을 실시한 결과 비판적 사고력은 남학생이 창의적 사고력은 여학생이 더 높은 것으로 나타났다($p<.05$). “이 논문은 2012 년도 정부(교육과학기술부)의 재원으로 한국연구재단의 지원을 받아 수행된 연구임(2012R1A1A2A10000454)"

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장소: 부산BEXCO

발표코드: **EDEC.P-1476**

발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

멘토링을 통한 멘티교사의 수업 실행 수준 변화 분석

남정희 이동원[1]

부산대 화학교육과 [1]부산대 대학원 과학교육과 화학교육전공

멘토링은 미국에서 1970 년 교육개혁의 문제점이 대두된 이후, 1980 년대 접어들어 미국과 유럽을 중심으로 초임교사 입문교육의 구체적 구현 전략으로 도입되어, 초임교사의 전문성 발달을 제도적으로 지원하고 개발하는 방법이 되고 있다. 멘토링 프로그램이 학교 현장에서 지속적으로 운영되었을 경우, 과학교사들이 실제 수업상황에서 보다 개선된 수업을 실천할 수 있는 실천적 지식을 새롭게 구성하는 과정을 통해 수업전문성 발달을 촉진하게 될 것으로 기대된다. 교사의 수업전문성 발달은 학교의 단위 수업 충실화를 실현하게 하여 결론적으로 학생들의 과학학습 향상에 긍정적인 영향을 주게 될 것으로 기대된다. 이 연구에서는 협력적 멘토링 프로그램을 개발하고 적용하여 그 효과를 검증하고 문제점을 분석하는 것을 목적으로 하였다. 이를 위해 7 개의 멘토와 멘티로 이루어진 멘토링 팀을 구성하여 4 회의 멘토링을 실시한 후 멘티 교사의 수업 실행 수준을 분석하였다. 멘티 교사의 수업 실행 수준 분석을 위해 수업 녹화 동영상 4 차시, 멘토, 멘티 협의회 전사본, 저널등을 분석하여 수업 실행 수준의 변화를 알아보았다.

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Teaching-Learning Effects on Scientific Inquiry, Scientific Attitude, and Scientific Achievement in Experimental Classes for Acid/Base Unit using Self-Regulated Larning Strategy

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The purpose of this study is to analyze the teaching-learning effects in experimental classes for the 'acid/base' unit of 11th grade chemistry-I textbook using self-regulated learning strategy. The experimental and the controlled groups were selected by the teaching-learning method established on self-regulated learning strategy and regular laboratory activity based on the teacher' instruction, respectively. After the laboratory activity for the unit using self-regulated learning strategy, the mean values of the scientific inquiry, scientific attitude, and performance assessment of the experimental group are larger than those of the control group. In the pre-test, there is not difference between the two groups. However, there is a little difference between the two groups in the post-test. By the results of the post-test for the experimental group, there has not been much relationship between the self-regulated learning strategy and the scientific inquiry, the scientific attitude, and the scientific achievement.

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사회적 구성주의 관점에서 전해질과 도체의 개념 형성에 대한 예비과학교사들의 인식변화 과정 분석

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구성주의는 과학지식이 자연 현상을 설명하는 과정에서 사회적 합의를 통해 구성된다고 본다(Bentley et al., 2000). 과학지식이 사회적 합의에 의해 형성되기 때문에, 학생들 역시 교실에서 과학지식을 토론하고 합의하여, 지식을 나름대로 생각하고 이해는 과정이 있어야만 한다. 교과서에 제시되었거나 교사가 전달하는 과학지식을 절대지식으로 받아들이고 사례를 암기 했을 뿐이라면, 그러한 과정으로 획득된 지식은 학생들에게 그 의미의 이해가 제대로 전달되지 못했을 것이다. 유사한 자연 현상을 설명하는 과학지식이라도 교과서 내에서 단원이 다르거나 설명하는 방식이 다른 경우, 이를 배우는 학생들은 과학지식들 간에 의미 있는 연결이 부족하고, 따라서 이들을 관련지을 때 사고의 혼란이 유발될 가능성이 높다. 전해질과 도체는 전통적으로 과학교과서에서 다른 단원으로 다루어지지만, 전기가 통하는 물질이라는 공통점을 가진다. 특히 2007 개정 과학교육과정 중학교 3 학년에서는 전해질과 이온단원이 도체를 다루는 전기단원 뒤에 제시된다. 따라서 이를 학습하는 학생들은 전기가 흐르는 물질이라는 공통점 때문에 도체와 전해질의 개념을 연결하여 이해 할 필요가 있다. 미래에 이를 가르치는 예비교사들 역시 도체와 전해질의 과학개념을 제대로 형성하고 있어야 한다. 이 연구에서는 예비교사들이 전해질과 도체의 개념을 어떻게 이해하고 있는지를 알아보고, 이를 통해 과학지식에 대한 인식을 알아보고자 한다. 예비교사들이 과학지식을 합의하는 과정을 경험함으로써, 예비교사 교육과정을 통해 과학지식의 본성에 대한 이해가 형성될 수 있는지 알아본다.

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대학교 분석화학 실험 수업에 적용해 본 문제중심학습 전략의 효과

윤회정 우애자

이화여대 과학교육과

문제중심학습(Problem-based learning, PBL)은 학생들이 능동적인 주체로서 실생활과 관련된 비구조화된 문제를 해결하면서 문제 해결 능력과 문제 해결에 관련된 지식을 습득할 수 있도록 하는 교수 전략이다. 본 연구는 PBL 전략을 대학교 실험 수업에 적용하여 기존 실험 수업에서 제기되는 여러 가지 문제점들을 극복함과 동시에 일반 수업 시간이 아닌 실험 수업에서도 PBL 의 긍정적인 학습 효과를 얻기 위하여 PBL 전략을 개발하고 그 효과를 검증하는 것을 목적으로 하였다. 기존의 분석화학 실험 수업 내용을 바탕으로 이를 포괄할 수 있는 세 개의 PBL 문제를 개발하였다. 실험집단의 학생들은 한 학기 동안 일련의 PBL 수업 단계에 따라 PBL 문제를 해결하였고, 비교집단의 학생들은 기존의 분석화학 실험 수업 방식에 따라 실험을 수행하였다. 연구 결과는 다음과 같다. 첫째, 실험집단 학생들의 창의적 사고력이 통계적으로 유의미하게 향상되었다(p

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The Preservice Teachers' Perceptions on Professional Development School (PDS) Course in Illinois State University

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It has been considered very important that in the pre-service teacher education program a practicum should provided pre-service teachers with supervised experiences such as applying the knowledge and the theory learned in a university/college to students and helped them to understand the full scope of teacher's role. However, pre-service teachers in Korea have not experienced the practicum meaningfully due to a short period of practicum, a lack of connectivity between university/college and elementary/secondary school, a teaching practice conducted without enough classroom observation and preparation, and a different regulation and culture between schools. Therefore it was required to prepare a plan for the effective operation of practicum; it was necessary to consider the Professional Development School (PDS).PDS, which has led educational reforms in the United States, was regarded as a ground of alternative pre-service teacher education that could enhance instruction professionalism through the collaborative relation between university/college and elementary/secondary school. In this study, we explored the perceptions of the pre-service teachers in the middle of a PDS course. We observed the pre-service teachers in the PDS course of Illinois State University in the United States and also conducted a survey and a semi-structured interview from September to December, 2011. The results revealed that the pre-service teachers as interns could develop the instruction professionalism by experiencing the intensive and extensive clinical experiences during one year. For example, mentors and interns cooperated for planning lessons, teaching, and reflecting. They were also able to increase the understanding about the students with a variety of characteristics and the culture of schools. Educational implications of PDS were discussed by considering the differences between United States and Korea's education system.

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단어 연상과 네트워크 분석을 이용한 중학생들의 화학 용어 인식 탐색 연구

김경진 김경은[1] 한재영[2]

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중학생들이 과학 시간에 배운 화학 용어를 어떠한 용어들과 연결해 기억하는지 알아보기 위하여, 단어 연상 검사와 네트워크 분석을 수행하였다. 중학교 1 학년과 2 학년 학생들에게 '화학'과 '확산'이란 용어를 접했을 때 떠오르는 단어를 5 개씩 적어보도록 하였다. 화학이란 단어를 가지고 연상하였을 때는 1 학년은 과학, 실험이 높은 순서로 나타났고, 2 학년 학생들은 물리, 실험이 높은 순으로 나타났다. 확산이란 단어를 가지고 연상하였을 때는 1 학년은 퍼진다, 냄새, 2 학년은 향수, 냄새가 높은 순으로 나타났다. 1, 2 학년 모두 많이 언급한 단어는 비슷하였으나 전체적으로 용어의 범주가 서로 달랐다. 보통 교과서에서 학습한 내용과 관련된 단어를 사용하는 경향이 보였다. 예를 들어 2 학년의 경우, 화학이란 단어를 가지고 연상하였을 때, 화학결합의 종류나 주기율표와 같은 단어의 빈도가 높음을 알 수 있었다. 1 학년의 경우는 아직 학습하지 않았기에 위와 같은 단어는 나타나지 않았다. 그리고 2 학년의 경우 과학적인 용어가 더 다양하게 쓰였음을 알 수 있었다. 확산이란 단어도 1 학년 과정에서 학습하게 되는데 1 학년은 대부분 확산과 관련되어 교과서에서 볼 수 있는 용어나 실험도구에 관한 단어가 많은 반면, 2 학년의 경우 과학적 용어 뿐 아니라 비과학적 용어의 사용이 많았고, 조금 더 넓은 범주의 확산에 관한 내용이 많다는 사실을 알 수 있었다. 그러나 응집도 부분에서는 1 학년보다 2 학년에서 높게 나타났다. 네트워크 분석을 통하여 보았을 때, 대부분의 학생의 용어가 연관을 가지고 주요 용어에 대하여 집중도가 높음을 알 수 있었다. 그러나 학급에서 1~2 명의 아이들의 용어는 다른 학생들과 연관성이 없음을 알 수 있었다. 1 개의 단어조차 친구들과 공통된 단어가 없는 학생들이 존재한다는 것이다. 그런 경우 이 학생이 과학 용어에 관해 정확하게 이해하고 있는 가에

대한 의문을 가질 수 있다. 네트워크 분석을 통해 교사는 학생들이 용어를 이해하는 방식을 알아볼 수 있고, 그로인해 수업을 계획함에 있어서 네트워크 분석결과를 활용하면 학생들의 이해도를 높일 수 있음을 기대할 수 있다.

대 한 화 학 회
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An effective explanation of the Tyndall effect using metal nanoparticle solutions

장낙한

공주대 화학교육과

It is very effective to explain the Tyndall effect for high school students using metal nanoparticle solutions because the size of particle can be diversely regulated in solution. I have prepared for gold and silver nanoparticle solutions to explain the Tyndall effect for high school students and have explained the dependence on the size of nanoparticles and the wavelength of an incident light. In a pure silver nanoparticle solution, the Tyndall effect was observed on both green(530nm) and red(670nm) light. But for a pure gold nanoparticle solution, the Tyndall effect was only observed on red light whereas it was almost not observed on green light. According to an increasing size of nanoparticles, the Tyndall effect was weakly observed on both green and red light. However, there was a little difference between gold and silver nanoparticle solution. The Tyndall effect was showed in gold solution much stronger than in silver solution for both green and red light. From an UV spectra of these nanoparticle solutions, this phenomenon should be attributed to the regularity of metal nanoparticles in solution. Namely, the regularity of gold nanoparticles was more constant than silver nanoparticles as a nanoparticle was aggregated by an adsorbate. The Tyndall effect was affected on the size of metal nanoparticles, the wavelength of an incident light and the regularity of metal nanoparticles in solution. Accordingly, this is educationally implicative because high school students can visually understand the relationship between the size of particle in solution and the wavelength of an incident light using metal nanoparticle solutions in the Tyndall effect.

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북한 교과서 물질 분야의 활동 분석

김은경 노석구[1] 박현주[2]

조선대 화학교육과 [1]경인교육대 과학교육과 [2]조선대 과학교육학부

이 연구는 북한 과학 교과서 내용 중 물질 분야에서 제시된 활동을 클로퍼(Klofer) 탐구활동의 분석틀에 따라 조사하고 분석하여, 통일 후 또는 탈북 학생들의 과학교육을 위한 기초자료로 제공하기 위함이다. 2002 년에 발행된 북한의 인문학교 3 학년, 4 학년, 제 1 중학교 3 학년, 제 1 중학교 4 학년, 제 1 중학교 5 학년, 제 1 중학교 6 학년을 분석 대상으로 교과서에 제시된 활동을 개수와 내용 분석 등을 포함한 양적 및 질적으로 분석하였다. 연구결과에 따르면, 북한 교과서에는 탐구 활동과 관련된 영역이 별도로 제시되어 있지 않고, 본문과 더불어 간단한 해보기 수준으로 제시되었다, 활동 또한 간단한 실험만을 주로 제시하고 있고, 실험기구나 시약의 수, 종류 등이 제한적으로 이용되고 있었다. 클로퍼의 다양한 탐구 영역에서 교육의 기회를 제공하기 보다는, 관찰이나 간단한 수행 등과 같은 극히 제한적 탐구 영역의 활동이 제공되고 있었다.

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Exploring the optimum conditions of experiment measuring size of a molecule with oleic acid in scientifically gifted education program

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The size of molecules is too small to measure directly. According to 5th national science curriculum, the experiment measuring molecule size with the oleic acid was included in science textbook. These days, the experiment can't be found in science textbook, but it is found in scientifically gifted education programs. The purpose of this study was to find optimal experimental conditions in the experiment measuring the size of molecules with oleic acid to perform successful experiments in the laboratory. The first research question is to find the best concentration of oleic acid diluted with ethanol. The second research question is to determine which amount of lycopodium powder affect the shape of oleic acid spreaded on the water. The results of the study was as follows. First, varying concentrations of oleic acid, 1 / 500 dilution of the concentration of oleic acid revealed to be the most accurate results. Second, the quantity of lycopodium powder in the water affects the appearance of the spread of oleic acid. If there was too much lycopodium powder on the water, oleic acid does not spread into a circular but irregular shape. These results provide some implications on experiments measuring the size of oleic acid molecules that can be performed more successfully.

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예비화학교사들의 개인차 요소, 성격, 학습양식 및 과학학습전략 분석과 교과 선호도와 학업성취도의 상관성

곽옥금 김봉곤

경상대 화학교육과

인지심리학에 바탕을 둔 개인차 요소는 학생들의 학습활동뿐만 아니라 교사들의 교수활동에도 매우 큰 영향을 미친다. 따라서 본 연구에서는 사범대학 화학교육과에 재학중인 예비화학교사들의 개인차 요소인 사고양식, 성격, 학습양식 및 과학 문제해결 능력을 분석하였다. 아울러 이들 예비교사들이 선호하는 교수양식을 조사 분석하였다. 학생들의 사고양식과 성격유형은 집단 별 유의한 차이를 보였으며, 정보처리학습이론에 근거한 학생들의 학습유형은 학생들의 전공과목에 따른 성취도와도 높은 상관성을 보였다. 아울러 이들의 개인차 요인은 자신의 선호 교수방법에 매우 밀접한 상관성을 보였다.

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예비교사의 교재연구과정에서 나타난 2009 개정 과학과 교육과정 화학1 과목 내용요소에 대한 인식

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전북대 화학교육과 [1]호남제일고

교사 전문성에 대한 중요성이 부각되고 그에 대한 연구도 활발히 진행되고 있다. 여러 연구들에서도 알 수 있듯이 교사 전문성은 교사의 수업에서 발현되며, 예비교사교육과정에서 경험한 교육의 내용은 교사의 수업 전문성 제고를 위한 기본적인 토대가 된다. 수업의 질은 수업 전 선행되는 교재연구의 질에 영향을 받는다고 할 수 있는데, 현재 교사나 예비교사의 교재연구 방법에 대한 연구는 드물다. 따라서 이 연구에서는 교원자격이수를 위한 필수과목인 강의에서 교재연구와 수업실제를 경험하는 중에 나타나는 교육과정 내용요소에 대한 인식을 예비교사의 교재연구 전후로 나누어 알아보고, 예비교사들이 경험한 여러 가지 교재연구방법에 대한 인식을 예비교사의 관점에서 분석해보고자 한다. 교재연구가 완료되었음에도 불구하고 예비교사들이 여전히 어려워하는 내용요소가 무엇인지 나타나면 이를 예비교사 교육과정에서의 교재연구수업에서 활용할 수 있을 것이고, 교재연구 방법에 대한 인식을 토대로 효과적인 예비교사 교육방법에 대한 토대를 마련할 수 있을 것이라고 기대한다.

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기체의 밀도와 관련된 고등학생과 예비과학교사의 개념 분석

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전북대 화학교육과 [1]호남제일고

이 연구는 고등학교 수준에서 요구되는 기체의 성질 중에서 온도, 압력, 부피 변화를 포함하여 확산과 관련된 기체의 밀도에 관한 고등학생과 예비과학 교사의 개념 이해 수준을 분석하였다. 대학수학능력시험에서 요구되는 수준의 개념 이해 정도를 분석하기 위하여 기출문제와 모의고사 및 EBS 교재에 포함된 기체 관련 평가 문항에서 문제부 의 진술문을 완성형으로 변형한 뒤, 응답에 대한 이유를 진술하는 10 개의 문항을 사용하여 학생들의 개념을 조사하였다. 연구 결과, 고체와 액체의 밀도를 측정하고 상대적인 크기를 비교하는 문항에서는 높은 이해 수준을 보였으며 밀도를 정의하고 밀도식과 단위 큰 어려움을 보이지 않는 고등학생과 예비교사들도 기체의 밀도와 관련된 문항에서는 이해 수준이 낮게 나타났다. 대표적인 오개념으로는 기체의 압력과 밀도를 동일시 하거나, 기체의 종류와 상관없이 상대적으로 분자수가 많으면 질량이 크기 때문에 밀도가 크다는 것 등이 나타났다. 또한 밀도와 관련된 부피와 질량의 변화에 대한 물리적 검토 없이 여러 가지 기체 관련 법칙을 진술하거나 수식에 대입하려는 경향이 매우 높게 나타났으며, 확산과 관련된 3 개의 유사한 문항에 대해서도 다른 성취수준을 보였다. 이는 실제 고등학교 화학 수업시간에 진행되는 문제풀이 과정은 대학수학능력시험에서 요구되는 개념의 적용과 자료 해석 능력 향상을 목적으로 이루어지고 있지만 기본 개념에 대한 이해와 적용보다는 수식에 의한 알고리즘식 문제풀이 과정에 집중함에 따라 학생들은 실제 여러 가지 기체의 물리적 성질이나 변화 과정에 대한 이해 수준이 낮은 것으로 나타났다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

남한과 북한 과학 중 물질 교육 내용의 분석

박현주 김은경[1] 노석구[2]

조선대 과학교육학부 [1]조선대 화학교육과 [2]경인교육대 과학교육과

이 연구는 남한과 북한 과학 중 물질 교육 내용을 학습내용, 탐구활동, 용어 등을 분석하고 남한과 북한의 학년별, 수준별 차이를 조사하하여, 통일 후 또는 탈북 학생들의 과학교육을 위한 기초자료로 제공하기 위함이다. 남한의 2007 개정 과학과 교육과정, 교육과정 해설서, 교과서, 그리고 북한의 2002 년에 발행된 인문학교 3 학년, 4 학년, 제 1 중학교 3 학년, 제 1 중학교 4 학년, 제 1 중학교 5 학년, 제 1 중학교 6 학년을 분석 대상으로 내용을 분석하였다. 연구결과에 따르면, 북한의 물질 교육 내용은 초등학교는 남한보다 북한이 간단하고 쉬운 지식과 용어를 교육하지만, 중학교와 고등학교는 초등학교의 수준에서 비약적으로 발달된 심도 있는 지식과 용어를 제공하고 있는 것으로 조사되었다.

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발표분야: 초중등교사・화학교육

발표종류: 포스터, 발표일시: 수 16:00~19:00

The Analysis of 9th grade Science's Gender Difference Representative Items of NAEA

김현경

한국교육과정평가원 교육평가본부

The purpose of this study is to examine characteristics of National Assessment of Educational Achievement of Science according to gender. This study is investigated the gender achievement difference, 2010 the National Assessment of Educational Achievement(NAEA) of science, a ratio of correct answers within each contents domain and behavioral domain, and the items which show high difference between male and female. As a results, first, for academic achievement of science females outperformed males. Second, for the ratio of correct answers within all area of science females outperformed males, especially in constructed-response items. Third, the highest ratio of correct answer among each area of science was chemistry. For interpreting date, males outperformed females. For classification property of materials, a similar items with daily life, items related to memorize rules, females outperformed males. This information of properties according to gender will be able to complement the weak point of students when they study science, and support instructional methods on science.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Mechanistic study on oxidation of diclofenac by iron sulfide mineral catalyzed Fenton reaction

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Iron sulfide mineral (FeS2) catalyzed Fenton-like reaction was investigated to rapidly and completely degrade diclofenac, one of the most frequently detected pharmaceutical in sewage treatment plant, without formation of toxic products. The FeS2 provided proper pH condition (pH 3?4) and appropriate amount of aqueous Fe(II) which led to the complete oxidation of diclofenac in 120 sec. The continuous dissolution of aqueous Fe(II) from FeS2 surface seems to be a key factor to complete the oxidation of diclofenac by continuously producing the OH? and inhibiting quenching reactions. The major aromatic intermediates such as 2,6-dichlorophenol and 2-chloroaniline were also rapidly degraded by the OH? attack and successfully mineralized to HCl and CO2 during the degradation reaction.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Peacock-Shaped TiO2 Light Scattering Layer with TiO2 Nanorods Film for Dye-Sensitized Solar Cells

강순형

전남대 화학교육과

Nowadays, the exploration of new photoelectrode 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 one-pot synthesis of peacock-shaped TiO2 light scattering layer with TiO2 nanorods film for dye-sensitized solar cells by hydrothermal method controlling the acid ratio of HCl and CH3COOH. In the case of 1:2 ratio of HCl:CH3COOH, the one-dimensional (1-D) TiO2 nanorods (NRs) film was synthesized with a length of 2 μm, whereas 1-D TiO2 NRs film with peakcock shaped TiO2 nanobundles as a light scattering layer (LSL) was acquired in the 2:1 ratio of HCl:CH3COOH. This LSL showed the remarkably dual functions in an aspect of high light harvesting attributable to the large surface area due to micrometer-sized TiO2 nanobundles consisting of small-sized TiO2 NRs with approximately 30~40 nm sized diameter and light scattering effect in the long wavelength of 550-700 nm. Accordingly, this dual functions of LSL result in the sharp increased conversion efficiency (3.93 %) about above two times compared to that (1.49 %) of TiO2 NRs film synthesized in 1:2 rato of HCl:CH3COOH.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Organic Dyes containing Bridge(π) for Dye-sensitized Solar Cells.

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화석연료의 사용으로 환경오염 및 지구온난화에 따른 기후변화 문제가 부각되고 있다. 에너지 관련 환경 문제에 대응하기 위해 대체 에너지원 개발이 시급한 상황 속에서 신재생 에너지인 태양에너지의 개발이 기대되고 있으며 염료감응태양전지(Dye-sensitized solar cells; DSSCs)는 차세대 대체에너지로서 친환경적, 고효율의 장점을 가지고 있어 많은 각광을 받고 있다. DSSCs 의 핵심재료 중 하나인 염료에는 유기염료와 유기금속염료가 있으며 유기염료는 유기금속염료에 비해 자원적인 제약이 없고, 저가합성 가능, 다양한 구조의 염료로 디자인이 용이, 가시광선 영역에서 높은 흡광효율을 가진다는 장점이 있어 유기염료의 연구가 많이 진행되고 있다. 본 연구의 유기염료는 donor(D)로 9-ethyl cabazole 을 사용하여 D-D 구조를 가지는 bis 형태로 합성하였고 bridge(π)는 thiophene, acceptor(A)로는 -COOH 그룹을 도입하여 acceptor 를 하나만 가지는 형태인 유기염료(BECZ3)와 두 개를 가지는 유기염료(BECZ4)로 합성하였으며, NMR 과 Mass 를 통해 구조를 확인하였고 유기염료의 광전변환효율을 측정하였다.

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Life cycle assessment on Pyroprocess, a reprocessing technology of nuclear spent fuels

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In this work, we use the Life Cycle Assessment (LCA) to simulate a potential comprehensive environmental impact of the reprocessing. Although many studies have analyzed the environmental impacts of nuclear power plants, their analyses have been missing the nuclear waste treatment and the reprocessing phases. This is mainly due to the fact that reprocessing is actually being conducted only in a few countries, and most spent fuels are stored in the water pool of the reactor facility. In order to fill the gap, it is necessary to include the reprocessing phase as a part of the complete life cycle of the nuclear power technology. The target technology is Pyroprocess which is highly advantageous because of its proliferation resistance. However, Pyroprocess is still under development, and there is no commercial facility yet so that it is unavailable to use a general way of collecting life cycle inventory (LCI). We set a framework for LCA of Pyroprocess based on a demonstration facility and experimental results. System model is composed of seven processes including Decladding, Voloxidation, Electro-reduction, Electro-refining, Salt treatment, Off gas treatment, and Electro-winning. These engineering processes compose the life cycle of the complete Pyroprocess. In addition, a utility system such as illumination, a cooling system, an HVAC system, etc. is allocated for the seven processes equally because all processes are installed at the same utility system and share it. We used EcoInvent V2 data for the analysis. A functional unit is 1 MT-U reprocessed, and 98wt% of Uranium is recycled into nuclear fuels. The result will help policy decision makers when they consider adapting reprocessing technologies for the 4th generation of nuclear power plants.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon source effect on the methylmercury bioaccumulation in the Mekong River food web

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The objective of this study was: 1) to examine the trophic transfer of mercury (Hg) and methylmercury (MeHg) for benthic and pelagic organisms collected from the Mekong River, and 2) to determine the linkage between carbon source characteristics and the bioaccumulation factors (BAFs) of MeHg. For these purposes, concentrations of Hg and MeHg in river water, sediment, and organisms, and δ15N and δ13C in organisms were determined in the dry and wet seasons of 2011 in the Mekong River. Hg and MeHg distribution in sediment ranged from 18 to 48 ng/g, and from 0.090 to 1.5 ng/g, respectively. For benthic organisms, Hg and MeHg levels ranged from 20 to 700 ng/g, and from 7.3 to 400 ng/g, respectively. Hg and MeHg levels in organisms showed positive correlations with δ15N (6.2 ? 13‰), suggesting trophic transfer of Hg and MeHg along the river food chain. The MeHg log BAFs ranged from 2.3 to 3.4 for pelagic biota, and from 0.60 to 3.4 for benthic biota. There was a negative correlation between sediment organic carbon and the MeHg BAFs of benthic organisms, indicating that organic carbon reduces MeHg mobility from sediment to biota. Regarding carbon source effects, the biota with more benthic carbon sources (heavier δ13C) accumulated less MeHg than those with more pelagic carbon sources (lighter δ13C). A pelagic-based diet appears to result in more efficient MeHg trophic transfer than a sediment-based diet.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Divalent mercury reduction by reduced quinone in anoxic environments

이세용 Hieu Van Duong[1] 한승희

광주과학기술원 환경공학과 [1]Hue University

It was reported that Hg(II) can be reduced to Hg(0) by humic substances in the natural anoxic environment; however, the role of reduced quinone moieties in Hg(II) reduction has not yet been studied. In this study, aqueous Hg(II) reduction experiments were carried out under anoxic conditions using chemically and microbially reduced anthrahydroquinone-2,6-disulfonate (AH2QDS) to understand the importance of reduced quinone compound in the reduction of Hg(II). Approximately 93% and 49% of the total Hg(II) were reduced by chemically and microbially reduced AH2QDS, respectively, within 2 hours. In contrast, only

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Fabrication of reduced graphene oxide based carbonaceous materials with high porosity for energy storage

문건희

포항공과대 화학공학과

Carbon-based materials possessing unique properties involving high surface area, high conductivity, high porosity, and omnipresence have been actively investigated for developing new types of materials for energy and environmental applications. Among a variety of carbonaceous materials, graphene as having been rightly considered as a rising star since it had been observed is a monolayer carbon sheet consisting of sp2-hybridized carbon atoms in a two-dimensional honeycomb lattice, which exhibits distinct properties such as high mobility of charge carriers, high mechanical strength, high thermal conductivity, and high specific surface areas. Therefore, various kinds of composites based on 2D graphene sheets have been developed and tested for various purposes. Herein, new carbon-carbon assembly, hollow carbon spheres embedded in reduced graphene oxide (r-GO) sheets, is accomplished by removal of inorganic templates and tested to check its capacitive behavior. As a result, the composite shows the enhancement for electron storage due to high surface area and high porosity during charge and discharge cycling compared with bare hollow carbon spheres or r-GO sheets.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Photoactivity and Changed Band-gap by N, Nb-TiO2: Experimental and Theoretical Understanding

임종훈

포항공과대 환경공학부

Bare, N-doped, Nb-doped and N,Nb-codoped TiO2 was synthesized by conventional sol-gel method and characterized by using XRD (X-ray diffraction), DRUVS (Diffuse reflectance UV/Visible absorption spectroscopy), XPS (X-ray photoelectron spectroscopy). The changed electronic structure of all samples was confirmed by experimental Mott-Schottky plot and theoretical Density of State calculation (DOS). The photocatalytic activity under visible light was tested using the photocatalytic oxidation of iodide, 4-chlorophenol and reduction of chromate (VI) in aqueous phase. The changed electronic structure and enhanced visible light absorption of N,Nb-TiO2 can be caused by modification of CB and VB. Nb doping can induce the red-shift of CB, slightly and N doping can increase the visible light absorption by inducing the NOx species. Furthermore, when N and Nb are simultaneously doped on TiO2, impurity level is less formed because of charge neutrality. This result can reduce the formation of recombination center. Ti4+ + O2- = Nb5+ + N3-And also, as we confirmed in DOS data, the width of VB is broaden reveling that the mobility of photogenerated hole is increased. Consequently, the photocatalytic activity of N,Nb-TiO2 is higher than that of bare TiO2 and mono doped TiO2 under visible light irradiation ($\lambda > 420$nm).

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

The Arsenite(III) oxidation by UV Photolysis of NO_2^- and NO_3^-

김동효 최원용

포항공과대 환경공학부

Concerns about Arsenic contamination have been increased due to the need for safe drinking water in developing countries. Prior to removal process of arsenic compounds from wastewater, oxidation process should be firstly done since oxidized species (arsenate) has so higher affinity for adsorbents that it can be easily removed by coagulation or precipitation. In this work, the photooxidation of As(III) under UV ($\lambda >$ 295 nm) irradiation was investigated in the presence of NO_2^- and NO_3^- (typically 200 μM or about 9.2 ppm). The As(III) oxidation was highly enhanced in the presence of NO_2^- as compared with that in the presence of NO_3^-, whereas the direct photooxidation in water was negligible. Since the As(III) oxidation induced by NO_2^- photolysis is mainly driven by the in situ generated oxidants from dissociation of NO_2^-, the removal of NO_2^- and concurrent production of NO_3^- were monitored by ion chromatography. The As(III) oxidation by NO_2^- photolysis has an advantage to be applied to the solution with wide pH conditions. The HNO_2 with higher quantum yield for ?OH can be involved in the As(III) oxidation under acidic condition. On the other hand, it was reported and observed that the photo-conversion of NO_3^- to NO_2^- is faster under alkaline condition so that NO_2^- can be reused. The excitation of NO_2^- under UV irradiation led to the generation of ?OH and e_{aq}^-, which seem to be involved in the oxidation reaction of As(III). It was observed that the photo-oxidation of As(III) was efficient in an air-or N_2O-saturated solution as compared with that in the N_2-saturated solution. It means that O_2 or N_2O reacted with aqueous electron to make $O_2?^-$ or ?OH, respectively since the reaction by aqueous electrons is highly dependent on electron acceptors (O_2, N_2O). In addition, the addition of excess tert-butanol (?OH radical scavenger) decreased the photooxidation rate, which implies that ?OH was also involved in the As(III) oxidation.

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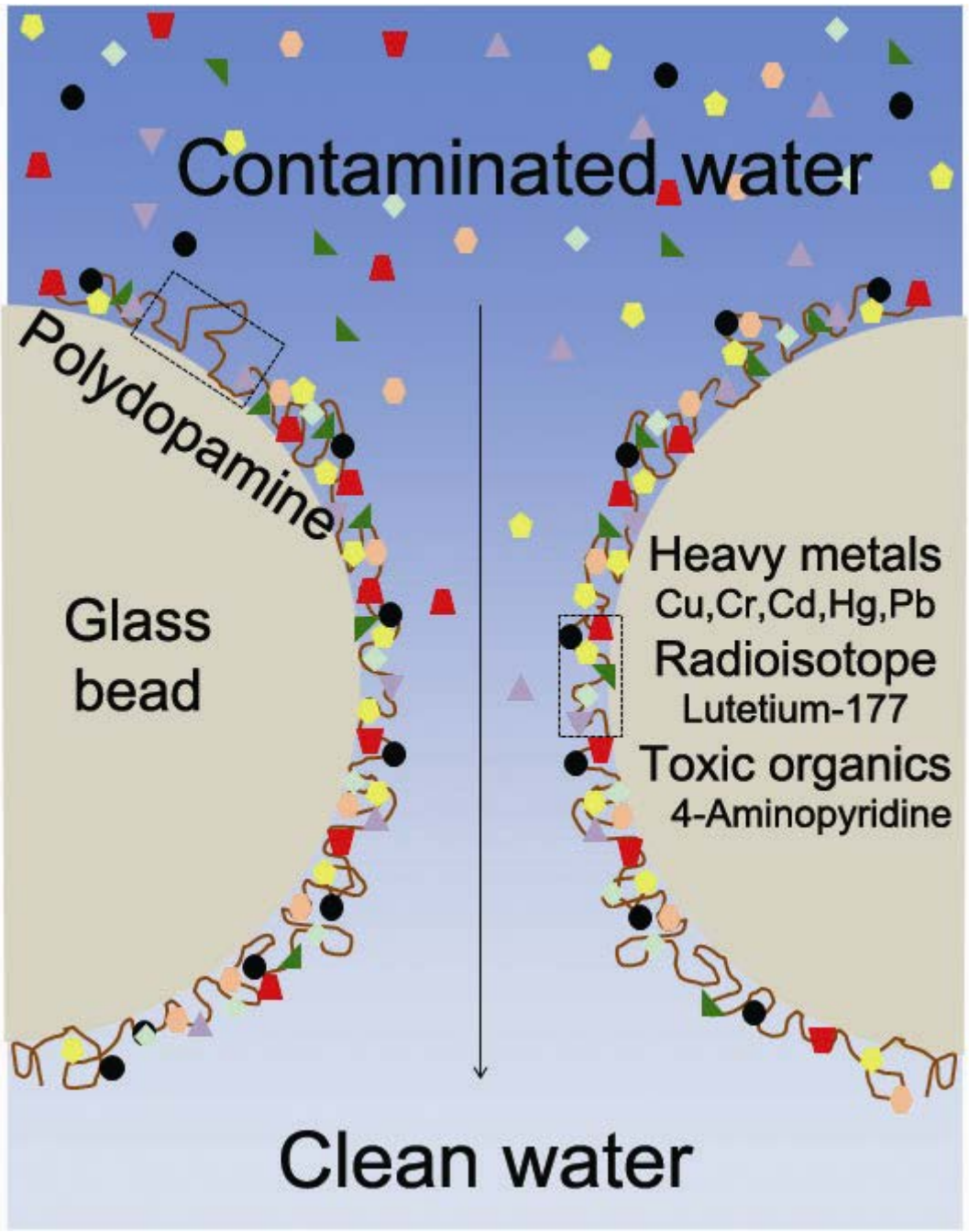
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 수 16:00~19:00

Water Detoxification by a Substrate-Bound Catecholamine Adsorbent

이미현 홍선기 이해신

KAIST 화학과

As technology develops, a demand for clean water has been continuously increased. The water utilized by industry is irreversibly contaminated by a wide variety of toxic chemicals such as heavy transition metals, radioisotopes and synthetic organics. Thus, there has been a large effort to remove such toxic chemicals. Examples include alginate, in which the abundant carboxyl group chelates metals, and activated carbon which is highly porous and therefore a good absorbent. We previously reported that polydopamine has the versatile coating ability on a wide range of substrate materials, which makes it an attractive candidate for various applications. Here, we demonstrate a simple and effective method of removing toxic chemicals from contaminated water. The polydopamine coated micro-size beads exhibit high absorbing capacities for various types of toxic chemicals: heavy metals(Cu, Cr, Hg and Pb), synthetic organics(4-aminopyridine) and radioisotope (177-Lutetium). In addition, this polydopamine filter was easily regenerated by treatment of acid or hydrogen peroxide.


Contaminated water
Polydopamine
Glass bead
Heavy metals
Cu,Cr,Cd,Hg,Pb
Radioisotope
Lutetium-177
Toxic organics
4-Aminopyridine
Clean water

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Algal oil extraction from Chlorella and biodiesel preparation

김소은 김종득[1]

KAIST(KAIST) 생명화학공학과 [1]KAIST 생명화학공학과

Fatty acid methyl esters and methanol are mixed up with diverse composition as a new type of extractant. A novel extraction method which extracts lipid from dried Chlorella by mixing it with biodiesel/methanol is developed. Th new extraction method exhibited high extraction efficiency against dried Chlorella. A study is conducted to find the optimized composition between biodiesel and methanol in extraction solvent. The extraction efficiency with biodiesel/methanol is 1.06 times higher than that of chloroform/methanol and yield is higher than 95 percent.

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발표코드: **ENVR.P-1501**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photo-chargeeable and dischargeable TiO_2 and WO_3 heterojunction electrodes

김성훈 박현웅[1]

경북대 물리학과 [1]경북대 에너지공학부

TiO_2 and WO_3 heterojunction electrodes are studied for their bi-functionality on harvesting light and storing energy. Both semiconductors are fabricated either mixed electrodes or two different electrodes galvanically coupled in a mixed electrolyte of 0.1M Sodium formate and 0.1M Sodium chloride. Irradiation of AM 1.5-light shifrs the open circuit potentials(OCPs) of the mixed and coupled electrodes from around -0.1V_{SCE} (dark OCPs) to a potential range between -0.8 and -0.5V_{SCE} , which slowly return to their respective dark OCPs over a period of around 14h. Such discharging periods are significantly influenced by the irradiation time and weight or area ratios of TiO_2 and ht or area ratios of TiO_2 and WO_3. When the TiO_2 and WO_3 mixed electrodes are galvanically coupled to stainless steel electrodes for application to anticorrosion, the mixed potentials of the couple are maintained at ca. -0.4V_{SCE} over 10h even after light off. The measure galvanic currents verify that the photogeverated electrons of TiO_2 flow to WO_3 and even overflow to the steel during the irradiation, while the stored electrons at WO_3 flow to the galvanically coupled steel electrodes directly or through the TiO_2 upon light off.

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장소: 부산BEXCO

발표코드: **ENVR.P-1502**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

DRIVING FACTORS OF ENERGY CONSUMPTION IN KOREAN CITIES

이민진 안태규

성균관대 에너지과학과

Energy efficiency improvement is paid great attention as the most powerful and essential solution to deal with climate change mitigation and energy security issues. Although many researches covered energy efficiency in national level and end-use device level, only few investigated sub-national level. However within a nation, there exists heterogeneity of energy use patterns between rural and urban areas. Thus a better understanding of energy use in each rural and urban area is necessary for appropriate energy efficiency policy. In particular, globally rapid urbanization is forecasted to significantly contribute to increase of energy consumption in many scenario analysis. Therefore, this research addresses three key questions with focusing on urban area energy use : What factors contribute to change of urban energy use? Why energy use patterns differ between cities? And How did the driving forces change its impact to energy use by urbanization phases. Six Korean major cities is used as a empirical analysis.

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발표코드: **ENVR.P-1503**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Reduction of chromate in the presence of zero-valent magnesium under neutral pH conditions

박재선 이기현

연세대 지구시스템과학과

Zero-valent magnesium (ZVMg) is a powerful reductant, which provides several advantages for remediation of environmental contaminants compared to zero-valent iron (ZVI). This study examined the reduction of 5 - 100 uM $[Cr(VI)]_0$ in the presence of 50 mg/L ($[Mg^0]_0$ = 2.06 mM) ZVMg particles at pH 7 buffered with 50 mM Na-MOPS. The reduction of Cr(VI) was completed within 60 min with $[Cr(VI)]_0$ = 4.9 or 9.6 uM but substantially retarded at > 120 min with higher $[Cr(VI)]_0$ (49.9 or 96.9 uM) likely due to the rapid dissolution and the surface passivation of ZVMg in water. The effect of dissolved oxygen was negligible on the rate and extent of Cr(VI) reduction. Experimental results indicated that Cr(VI) was reduced not directly by ZVMg but by reactive intermediates produced from water reduction by ZVMg. The extent of Cr(VI) reduction observed in this study suggests that ZVMg can reduce Cr(VI) more effectively than iron-based reductants under the experimental conditions employed in this study.

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발표코드: **ENVR.P-1504**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly conductive current collector for Li-battery applications.

정성훈 정범균[1] 박동원[2] 이재영[3]

광주과학기술원(GIST) 솔라에너지 연구소(RISE) [1]광주과학기술원(GIST) 환경공학부 [2]광주과학기술원 솔라에너지연구소 [3]광주과학기술원 환경공학과

Current collector is a primary component in electrochemical energy storage device such as capacitors, batteries, and fuel cells. Aluminum (Al) metals are commonly employed as current collectors of positive electrodes, regard to its excellent electrical conductivity and chemical stability by forming a passive oxide film. However, Al has a high interfacial contact resistance (ICR) with the carbon-based active materials, due to the low wettability between Al and carbon, which gradually fades its capacity. Thus, the formation of intermediate layer between Al and carbon is highly important to ensure battery performance and safety. In this work, we introduced a highly conductive pyrolytic carbon layer that penetrates into nanoporous alumina channels and strongly adheres to an Al current collector via the following process: Al anodization, alumina etching, catalyst deposition, and pyrolytic carbon chemical vapor deposition (CVD). To further explore the stability of these current collectors in electrolyte, preliminary results on the battery application based on the transverse resistance and electrochemical tests are discussed.

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장소: 부산BEXCO

발표코드: **ENVR.P-1505**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Co, Cu, Ni-doped ceria catalysts; CO Oxidation Reaction Performance vs. M-doped and MM'-codoped Effects

박요한 손영구

영남대 화학과

최근 급격한 산업화로 인해 NOx, CO 같은 산화물 형태의 여러 환경오염 물질이 부산물로 많이 생성된다. 특히 이들 산화물은 불완전한 산화 상태로 환경뿐 만 아니라 인간의 생활에도 영향을 주는 경우가 많다. 이 때문에 이들 산화물을 인체에 무해한 상태로 만드는 촉매에 대한 연구가 활발하게 이루어지고 있다. 본 실험에서는 단일 산화물로도 좋은 성능을 가진 CeO2(Ceria)를 지지체로 사용하여 다양한 금속들(Co, Cu, Ni)을 도핑시킨 물질을 가지고 CO 의 산화반응에 대한 효율을 알아 보고자 한다. 이를 위해 다음과 같은 내용을 바탕으로 효율이 좋은 촉매를 찾아 볼 것이다. 1) 하이브리드, 2) 하이브리드 금속의 상대적 양, 3) MM' 혼합 하이브리드. 이 세 가지 항목에 대한 논의를 위해 XRD(X-ray diffraction), SEM(scanning electron microscopy), UV-visible absorption, BET 를 이용하여 합성한 물질의 기본물성을 알아보고, CO TPR 과 GC-MS 분석을 통하여 실질적인 효율을 알아볼 것이다.

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장소: 부산BEXCO

발표코드: **ENVR.P-1506**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

The removal method of aromatic compounds in naphtha using mixtures of ionic liquid and organic solvent.

김진형

호남석유화학(주) 연구4팀

The separation of aromatic compounds from C_4 to C_{10} aliphatic compound mixtures is challenging since these compounds have boiling points in a close range and several combinations from azeotropes. In this work, we investigated the separation of aromatic hydrocarbons (benzene, toluene, ethylbenzene and xylenes) from naphtha by liquid-liquid extraction with mixtures of ionic liquid and organic solvent. Several extractants are suitable for extraction. The results, extraction degree of aromatic compounds from aliphatic compounds are higher compared to those obtained with sulfolane and glycols which are the most industrially used solvents for the extraction of aromatic hydrocarbons from a mixed aromatic/aliphatic hydrocarbon stream.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Generation of toxic Cr(VI) from sparingly soluble $Cr(OH)_3(s)$ mediated by surface catalyzed Mn(II) oxidation

남궁선이 이기현

연세대 지구시스템과학과

This study examined $Cr(OH)_3(s)$ oxidation coupled with surface catalyzed Mn(II) oxidation as a potential pathway of soil and groundwater contamination by Cr(VI) without any anthropogenic activity. The suspensions of 1.0 g/L $Cr(OH)_3(s)$ and/or 50 ?M Mn(II) were prepared in 50 mM $NaNO_3$ at pH 7 - 9 in the presence or absence of dissolved oxygen. No Cr(VI) was produced from $Cr(OH)_3(s)$ under anaerobic conditions at all pHs both in the presence and absence of dissolved Mn(II). In the presence of oxygen, by contrast, $Cr(OH)_3(s)$ was oxidized and produced Cr(VI) at pH $\geq$ 8. The oxidation of $Cr(OH)_3(s)$ was substantially accelerated in the presence of dissolved Mn(II) and increased with increasing pH. Our results show that the oxidation of Mn(II) by dissolved oxygen is catalyzed on the surface of $Cr(OH)_3(s)$ and that sparingly soluble $Cr(OH)_3(s)$ can be oxidized by the products of Mn(II) oxidation. In addition, the rate and extent of $Cr(OH)_3(s)$ oxidation would likely be controlled by those of surface catalyzed Mn(II) oxidation.

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장소: 부산BEXCO

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발표분야: 환경에너지

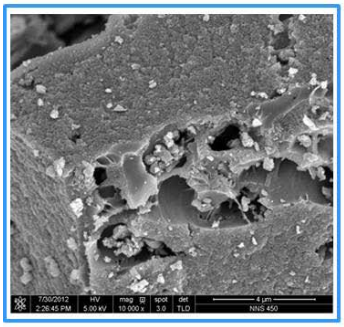
발표종류: 포스터, 발표일시: 수 16:00~19:00

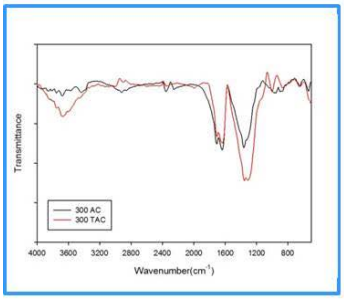
Activated carbon/self-decomposition material as a biological substrate for adsorption and dechlorination of trichloroethylene

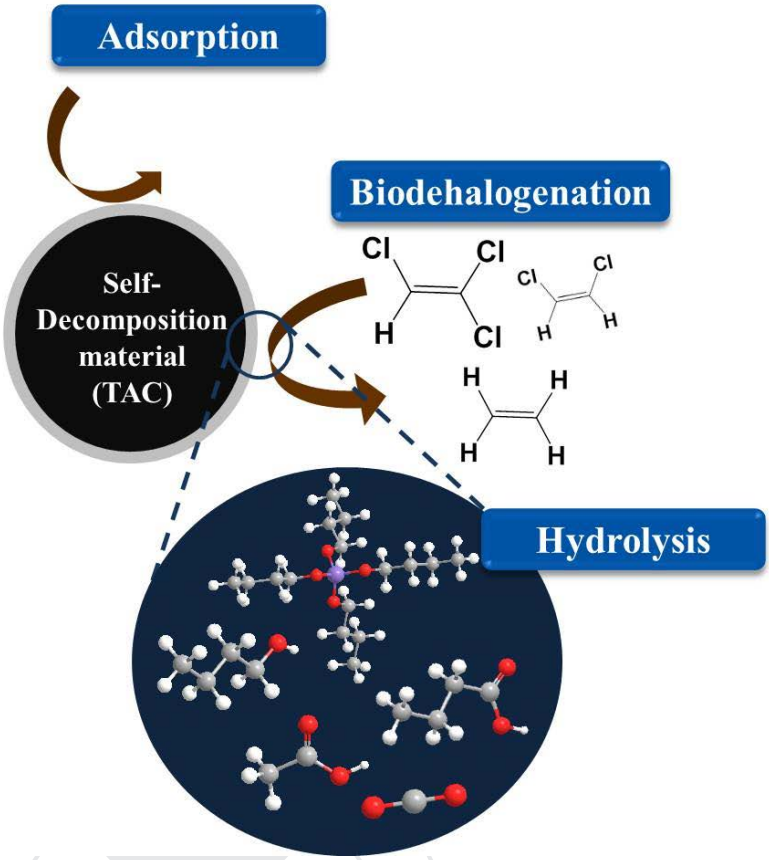
조은경 박재우[1]

한양대 건설환경공학과 [1]한양대 토목공학과

Activated carbon (AC) adsorption technology is often used for the urgent removal of persistent organic pollutants (e.g. PCE, TCE). Various organic compounds, such as organic acids, alcohols have been studied as potential electron donors to enhance biological dechlorination. Tetraalkoxysilanes are a group of silicon-based compounds as a self-decomposition material, which can be utilized as a biological substrate that contain four oxygen bridges from the central silicon atom to the corresponding organic (alkoxy) group. They can be transformed to bioavailable substrate as alcohol by hydrolysis. These by-products can promote biological dechlorination. This study was designed: i) to synthesize the self-decomposition material surface modification activated carbon (TAC), ii) to investigate the abiotic transformation of tetrabutoxy silane (TBOS) and the TCE adsorption capacity at TAC. Maximum adsorption capacity (qMax) was calculated as 278.34 mg/g from the Langmuir isotherm model. The hydrolysis rate was to observed to be 0.0117 day-1. This result showed that TBOS could be used a self-decomposition material in the natural sites.







THE KOREAN CHEMICAL SOCIETY

일시: 2012년 10월 17~19일(수~금) 3일간

장소: 부산BEXCO

발표코드: **ENVR.P-1509**

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PEMFC용 고분산/고효율 전극촉매 합성기술 개발

박병일 김해리[1] 김세훈[1] 차문순[1]

오덱(주) 기술연구소 [1]오-덱(주) 기술연구소

전극촉매기술은 연료전지 부품 소재 개발의 핵심 기술 중 하나로서, 상업화에 가까워짐에 따라 성능은 동일하며 가격을 낮출 수 있는 전극촉매 기술에 대한 연구가 다양하게 이루어지고 있다.본 연구에서는 백금의 분산도를 향상시키기 위하여 백금전구체와 카본과의 흡착방법 및 전구체 환원조건을 조절하여 효과적인 합성방법을 개발하였을 뿐 아니라 저렴한 단가의 팔라듐을 사용한 백금-팔라듐 촉매의 합성방법을 개발하여 촉매성능과 가격경쟁력 확보를 위한 연구를 진행하였다.백금분산도 향상을 위해 백금전구체와 카본과의 흡착방법 및 전구체 환원조건을 조절하여 효과적인 합성방법을 개발하였다. 개발된 전극촉매 합성방법은 자체개발된 백금전구체를 이용해 카본표면에 1 차적으로 물리적 고착을 진행하고 2 차적으로 화학적인 고착기술을 적용하여 원하는 백금 함량을 담지시키는 기술로 어떤 카본 담지체를 사용하더라도 고분산된 전극촉매를 얻을 수 있었으며, 합성공정도 간단해져 대량생산에도 유리한 장점을 가진다.또한 원가절감을 위한 저백금 촉매 기술로 Pt-Pd alloy 합성 기술을 개발하였으며, 특히 개발된 촉매기술은 일반적으로 두 번이상의 공정을 거치는 합금촉매 합성과는 달리 1 회의 합성공정으로 공정부분에서도 유리한 장점을 가진다. 본 연구에서는 1 회의 공정으로 촉매합성이 가능한 두 가지 Type 의 Pt-Pd alloy 전구체를 개발하여 전극촉매에 도입하였다.합성된 전극촉매들은 XRD, TEM, TGA 를 이용하여 물성평가를 진행하였으며 전기화학적 평가가 가능한 Unitcell Test 를 이용하여 활성평가를 진행하였으며 그 결과, 상용촉매와 동등수준의 성능을 보임을 확인하였다.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 16:00~19:00

Photocatalytic reduction of Carbon Dioxide to methane by synthesized Titanium Dioxide photocatalyst

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Titanium dioxide (TiO) is an efficient photocatalyst and can reduce carbon dioxide(CO) to produce hydrocarbon compounds such as methane, methanol, and so on. We synthesized modified TiO and irradiated ultra violet (UV) to reduce CO to methane. Photoreduction of CO was carried out in an aqueous solution under UV light irradiation. Synthesized TiO was prepared in a 30 cm height and 7cm diameter quartz vessel reactor. UV light irradiation was with a Xe lamp placed above the reactor. The products were analyzed with gas chromatography. Reduction of CO experiments were carried out using a TOGA 6500 series (Younglin Co.) equipped with a methanizer and a flame ionization detector (FID).

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Study on the effects of UV light on Crude oil's chemical compositions by high resolution mass spectrometry and comprehensive 2D GC MS

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Every year significant amount of petroleum enters into the environment as a result different incidents. Once the oil is spilled, it goes through various physical and chemical changes such as bio degradation, photo degradation, and emulsification etc. So, It is very important to analyze the changes in order to have an idea of the effect of the spilled oil on environment. Crude oil (Iranian heavy oil) was used for our experiment. As photo oxidation plays a vital role in the changes of crude oil, we decided to investigate the effect by irradiating the oil using UV spectrometer. This oil was kept to the exposure of UV light for 35 hours and the oil was fractionated into four fractions; saturate, aromatic, resin and asphaltene. The fractions were characterized by use of 15 T FTICR MS. APPI Positive and ESI negative modes were used for ionization. The results show that nitrogen and sulfur species decreased. 2D GC Mass spectrometer was also used to analyze saturate fraction and the results shows that aromatic compounds were vastly decreased after photo degradation.

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Photocatalytic Degradation of Organic Dyes by Tin Porphyrins Immobilized on Mesoporous Materials

박범혁 김희준

금오공과대 응용화학과

A photocatalyst that is active under visible light is of paramount importance as an essential element of solar photoenergy utilization. Diverse approaches are being made in search of visible light active photocatalysts. In this study, tin porphyrin was explored as an efficient visible light photocatalyst for an environmental remediation. Visible light photocatalysis using water-insoluble tin porphyrins immobilized on mesoporous material MCM-41 was investigated for the degradation of several organic compounds in water. The photocatalytic activities of tin porphyrins on MCM-41 will be presented in detail.

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Recovery of platinum from wastewater coupled with power generation using a microbial fuel cell

최찬수

대전대 응용화학과

To verify the feasibility of cost-effective recovery of platinum metal from wastewater a dual chambered microbial fuel cell (MFC) was studied. The anode chamber contained anolyte with 12.2 mM acetate and phosphate buffer media, and the cathode chamber contained catholyte with different concentrations of Pt(IV) and 0.2 M NaCl. The anode was carbon brush electrode bio-catalyzed with anerobic microorganisms and the cathode was carbon cloth. The onset shift in potential is highly dependent on the $[PtCl_6]^{2-}$ concentration, which is dissimilar from other kinds of reactions, such as that involving Ag(I) and $[PdCl_4]^{2-}$, previously studied in this lab. The current densities of Pt(IV) as $[PtCl_6]^{2-}$ concentration indicated by the kinetic- and diffusion-controlling regions of voltage vs. current density (V-J) curves greatly increased from 200 ppm to 1000 ppm. Hence, all electrochemical parameters improved, resulting in high power generation with the increase of the initial concentration. The maximum power of 5.04 W/m^2 with a fill factor of 0.64 was achieved with 500 ppm initial concentration. A maximum voltage of 0.333 V, a maximum current density of 15.2 A/m^2 at the maximum power point, and an internal resistance of 138 Ω were achieved at 500 ppm Pt(IV) concentration. After 6 hours reaction, the recovery rates of 98.69% and 99.59% were achieved for initial concentrations of 50 ppm and 200 ppm, respectively. With the fed-batch system having an initial concentration of 500 ppm, discharge curves indicated electric energy greater than about 17.2 Wh/Kg as a byproduct.

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

Preparation of ITO powder from waste ITO target

최동철 손용근

성균관대 화학과

LCD, a flat panel display, is used widely in most of modern instruments such as TV, cell phone, camera, car navigation system, and etc. ITO glass is one of the most important parts of the LCD. The ITO glass is a transparent electrode can apply voltage between both end of liquid crystal. In and Sn are most important elements used in ITO glass fabrication. As the production grows in LCD industry, the price of those elements are raised rapidly. Especially these days several counties in the world monopolize the In and Sn market. So It is very important to secure the supply of these resources. One way to avoid the supply difficulty is the recycling methode of the materials for the discarded IT instruments or waste or sludge of the sputtering target. We have tried to prepare ITO powder from the waste of ITO target for resource recycling purpose. ITO powder was successfully prepared by using In/Sn hydroxide coprecipitation and heat treatment up to 300℃ for 24hr. XPS, EDX, XRD, TGA and ICP were done for this sample.

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발표분야: 환경에너지

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Photoelectrochemical water oxidation using metal doped BiVO4 electrodes

정혜원 박현웅[1]

경북대 물리및에너지학부 [1]경북대 에너지공학부

Photoelectrochemical (PEC) water oxidation has received growing attention as a mean to produce solar fuel via water splitting, which has been considered one of the grandest challenges in contemporary science. PEC water oxidation, however, suffers from low efficiency due to kinetically hindered four-electron transfer for oxygen evolution at a low power density of solar spectrum in nature. With this in mind, this study focuses on the preparation of metal-doped BiVO4 photoanodes and comparison of the dopant effects on the PEC efficiency in 0.1 M phosphate at pH 7 under a simulated solar irradiation (1 Sun, AM 1.5). Cr, Mo, and W were selected as primary dopants and their doping levels varied. To further improve the efficiency, naturally abundant water-oxidizing electrocatlaysts were coupled the optimized BiVO4 electrodes.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of bilayered structure composed of TiO2 nanotubes and nanoparticles for dye-sensitized solar cells

안보은

전남대 화학교육과

Bo Eun Ahn and Soon Hyung Kang*Department of Chemistry Education, Chonnam National University, Gwangju 500-757, KoreaE-mail address: skang@jnu.ac.krIn Dye-sensitizied solar cells(DSSCs) comprising TiO2 nanoparticles, the considerably large surface area of NPs ensures a high dye loading for light harvesting, but the injected photoelectrons in TiO2 perform a random walk over the disordered framework of NPs, leading to increased scattering and recombination with a reduction of electron collection efficiency. Because of these drawbacks of the NPs, the TiO2 nanotubes-based DSSCs have been studied more often. One of the significant advantages of NT-based DSSCs is the higher charge collection efficiencies owing to less scattering and recombination probability, due to electrons direct pathways to be transported through the ordered tubes. However, these ordered NTs usually have a relatively small surface area in comparison with NPs, therefore leading to lower dye loading and diminished light harvesting. So we would like to improve the shortcomings of nanotubes.Dye-sensitized solar cells (DSSCs) invented by Michael Gr?tzel have been widely examined 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. This point can be overcome exploring one-dimensional TiO2 nanotube (TONT) by electrochemical two-step anodization in 0.25 wt% NH4F of ethylene glycol. Furthermore, to complement low surface area of TONT, the overcoating of TiO2 nanoparticle were introduced. This bilayered TiO2 nanotube/nanoparticle film was characterized by XRD, FE-SEM, and J-V analysis.

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Colloid formation monitoring during interaction between U(VI) and nZVI

신영호 이우진

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Radioactive contamination of soils, sediments, and groundwater is a arising global issue as a results of a number of activities including U mining, the production and use of depleted U for military purposes. Uranium is the one of the major radioactive elements related environment contamination and the chemical reduction of uranium from soluble U(VI) to insoluble U(IV) has been widely studied as a potential mechanism for its immobilization/stabilization in situ. Recently, many research groups have reported that nZVI can successfully remove soluble U species from aqueous phase and it was attributed to reductive precipitation of U(VI) and adsorption of U(VI) to iron corrosion products. However, relatively few studies have examined on the adverse effect of nZVI usage for U(VI) immobilization/stabilization. The formation of pseudo-colloids can stabilize U ion, therefore, colloid-facilitated transport in which actinides' long-distance transport in groundwater could lead hundreds times of higher mobility compared to U ion transport. In this study, the reaction mechanism between U(VI) and nZVI was elucidated and the colloid formation during the reaction was monitored by laser induced breakdown detection (LIBD). As a results of monitoring, mostly smaller than 20nm Fe(II) colloids were generated from nZVI surface by cation exchange between U(VI) and Fe(II).

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Nitrate reduction by bimetallic Pd-Cu catalyst supported on iron soil mineral

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KAIST(KAIST) 건설 및 환경공학과 [1]KAIST 건설환경공학과 [2]KAIST 건설 및 환경공학과

The contamination of surface water and groundwater by nitrate has gradually increased due to excessive consumption of fertilizer in the world. Nitrate should be removed from our natural and engineered water system because it can be converted into nitrite which may cause serious diseases to human being such as blue baby, cancer, and hypertension. Nitrite can be generated as an intermediate product in the nitrate reduction processes and then it can be converted to both ideal product (nitrogen gas) and to undesirable product (ammonia). Even though many studies have shown the successful catalytic removal of nitrate, more efforts are needed to improve the selectivity of nitrogen gas. In this study, the nitrate reduction and its selectivity to degradation products was investigated by bimetallic Pd-Cu catalyst supported on iron soil mineral. The effect of environmental factors such as hydrogen flow rate, metal ratio and the amount of catalyst was evaluated using 30 different experimental conditions. Different removal efficiency (46 to 100%) was obtained during the catalytic degradation of nitrate with the various nitrogen selectivity (0 to 72%) at 1.5 h. 31.34cc/min of hydrogen flow rate, 0.5/2.05 wt.% of Pd/Cu ratio, and 0.26 g of the amount of catalyst were selected as a optimal condition for nitrogen gas selectivity (72%) in this study.

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Oxidative degradation of gas-phase toluene in pyrite Fenton system

최경훈 이우진

KAIST 건설 및 환경공학과

Oxidative degradation of gas-phase toluene was investigated to model a treatability of gaseous contaminants emitted from the soil and groundwater remediation sites in Fenton-like reaction using pyrite as an iron source. Gas-phase toluene was continuously flowed into pyrite Fenton system at a concentration of 30 ppm and it was removed by minimum 83% during 4 hr. Toluene volatilized from pre-contaminated sand at a concentration of 300 mg/kg was completely removed by the pyrite Fenton system in 4 hr. During the oxidative degradation of toluene, there were no specific gas-phase products, while benzyl alcohol and benzoic acid were found in liquid-phase as intermediates. OH radical was identified as an effective radical species on degradation of gas-phase toluene in pyrite Fenton system. The longevity of pyrite as a catalyst in Fenton-like system monitored to estimate the replacement time for the catalyst was 1 day, revealed through the analysis of the concentrations of gas-phase toluene (gas chromatograph), surface analysis of pyrite (x-ray diffraction), and sulfide dissolution rate in pyrite (ion chromatograph). The results can be used to provide basic knowledge to understand heterogeneous Fenton reaction to treat volatile organic compounds produced from soil and groundwater treatment processes.

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