

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PLEN-1**

발표분야: 기초강연

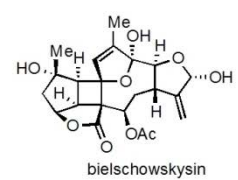
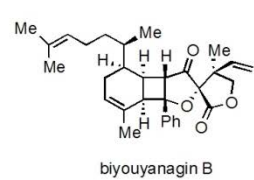
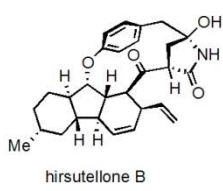
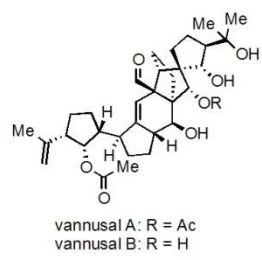
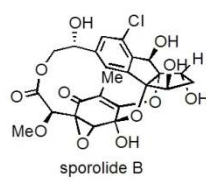
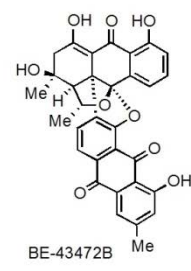
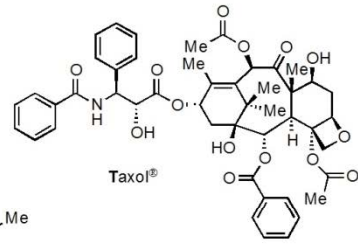
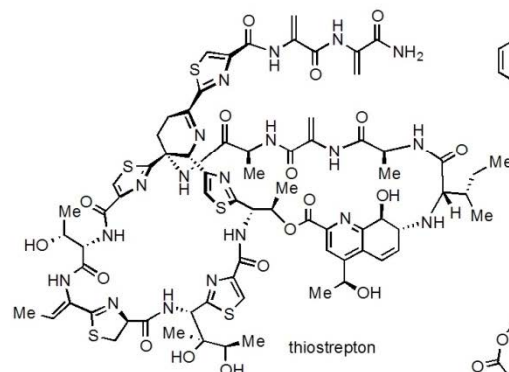
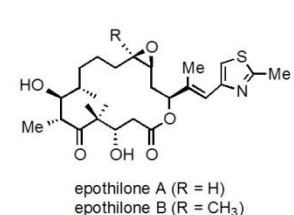
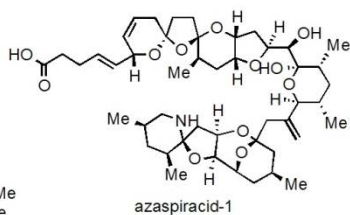
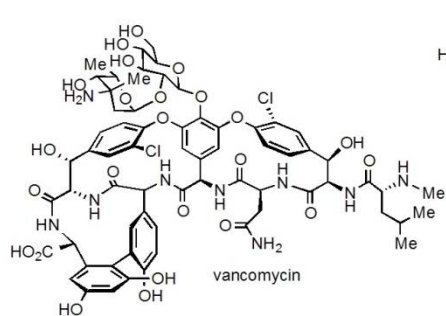
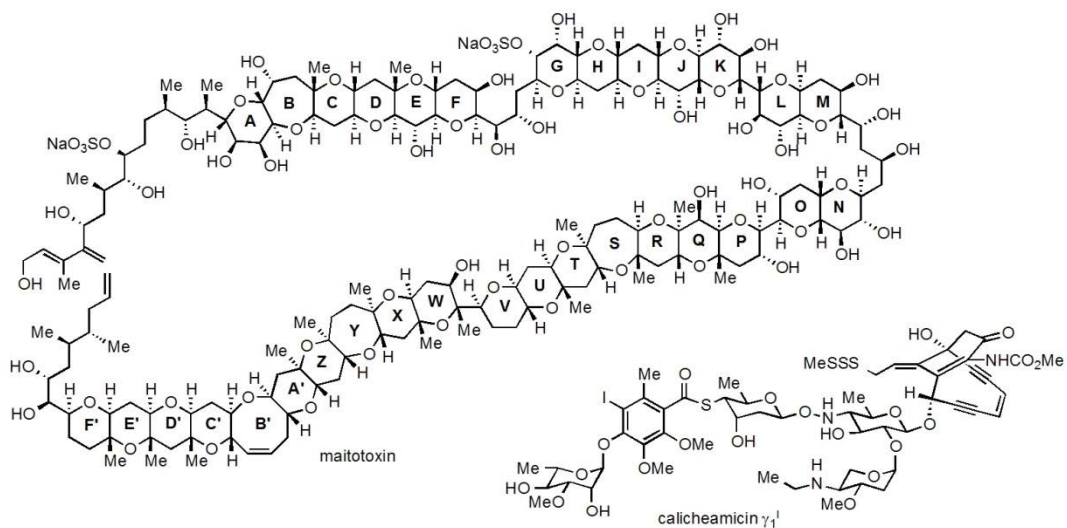
발표종류: 특별강연, 발표일시: 목 13:30, 좌장: David Yu-Kai Chen

## Total Synthesis of Biologically Active Molecules

**K. C. Nicolaou**

*Department of Chemistry, The Scripps Research Institute & Department of Chemistry and Biochemistry,  
University of California, USA*

Intelligent drug discovery from nature has been in practice for millennia and has a glorious history in terms of medical breakthroughs.<sup>1-4</sup> Such natural products provide fertile ground for discovery and development in the area of chemical synthesis, chemical biology and medicine. These opportunities continue to fascinate and inspire new science as new structures come under scrutiny by synthetic organic chemists. In this lecture, a number of total synthesis endeavors will be highlighted with emphasis on mechanistically-based design of new cascade reactions and synthetic strategies. Examples may include calicheamicin, Taxol<sup>®</sup>, vancomycin, epothilones A and B, azaspiracid-1, thiostrepton, BE-43472B, sporolide B, vannusals A and B, hirsutellone B, biyouyanagin B, bielschowskysin, and maitotoxin.



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발표코드: AWARD-1

발표분야: 학술상 기념강연

발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 주태하

## Recent Developments in the Theory of Diffusion-Influenced Reaction Kinetics

이상엽

서울대 화학부

Many reaction processes occurring in viscous media and solids are influenced by the diffusive transport rates of reactant molecules. Over the years from early 80's to present we have developed new and refined theories on the various aspects of the diffusion-influenced reaction kinetics. We laid down the rigorous theoretical framework for the reversible diffusion-influenced reactions and constructed many-particle kernel theory which gave almost exact results for several types of reactions. We derived the most successful theories for the excluded volume effects on the intrapolymer reactions, and for the subdiffusion-assisted reactions occurring in disordered media with energetically disordered trapping sites and spatial constraints. We also reformulated the theory of the diffusion-influenced bimolecular reactions completely by starting with the classical Liouville equation for the reactants and explicit solvent molecules. The structures of reactant and solvent molecules may be arbitrarily complicated with full atomistic details retained, and the sink function describing the reaction event may also be arbitrarily

complicated. Nevertheless, we were able to obtain a formally exact expression for the bimolecular reaction rate coefficient, and analyzed general properties of the rate coefficient, such as the long-time behavior and the upper and the lower bounds. The theory thus provided a rigorous and efficient molecular dynamics simulation method for calculating the rates of complex reactions involving proteins and polymers. More recently, we have devised a new method of solution for the Fredholm integral equations of the second kind. The method would be useful when the direct iterative approach leads to a divergent perturbation series solution. By using the method, we obtained an accurate expression of the propagator for diffusive dynamics of a pair of particles interacting via an arbitrary central potential and hydrodynamic interaction. The method has been found to give most accurate rate expressions for the bulk and geminate recombination reactions as well as for the reactions with long-rang reactivity like electron and energy transfer reactions.





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발표코드: POLY1-1

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 강영종

## Low band gap conjugated polymers and poly-electrolytes for polymer solar cells

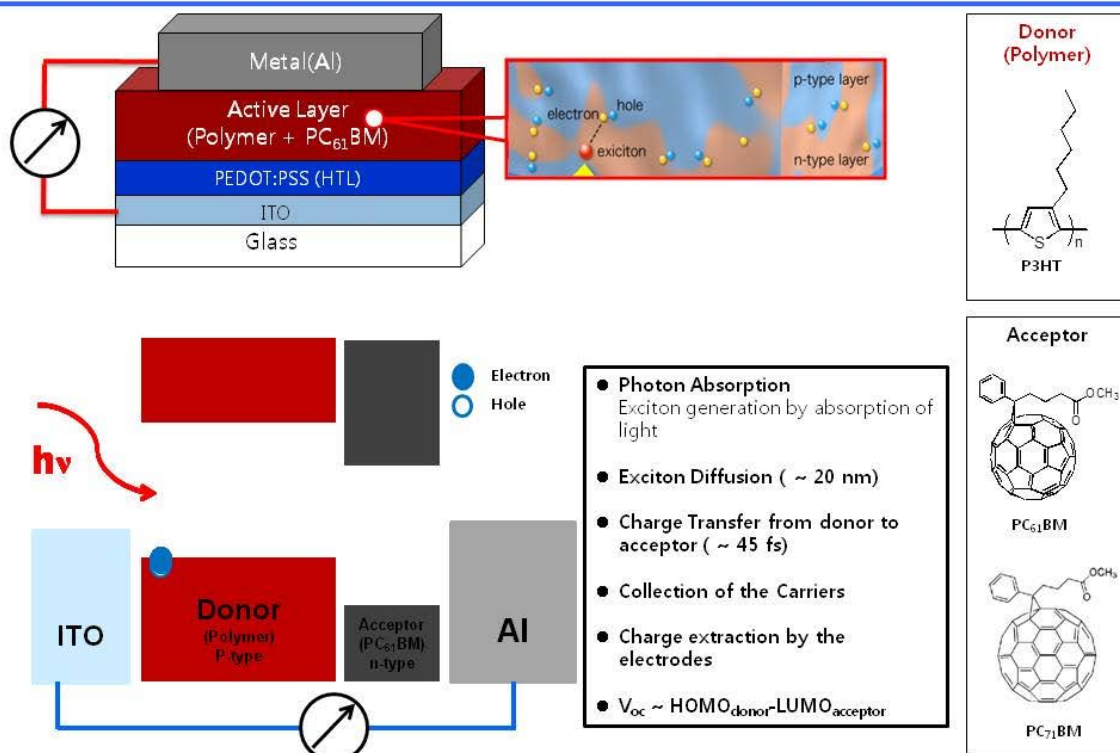
김주현

부경대 응용화학공학부/고분자공학과

지난 몇 십 년간 공액 시스템을 기반으로 하는 고분자 소재는 LEDs, solar cells, thin film transistors 와 같은 분야에 널리 응용되어 왔다. 최근 공액 시스템을 기반으로 하는 고분자 소재를 이용한 태양전지의 연구가 활발히 진행되고 있으며 눈에 보이는 발전을 거듭하고 있으며, 상용화의 가능성까지 보이고 있다. 수 많은 합성연구자들은 태양광을 효과적으로 흡수하여 고효율의 태양전지를 구현 할 수 있는 작은 밴드 갭(low band gap)을 갖는 신규 공액고분자에 대한 연구와 태양광에 위해 형성된 여기자로부터 효과적으로 전자를 이동시킬 수 있는 C60 을 기반으로 하는 신규 전자 받게 소재에 관한 연구가 활발히 진행되고 있다. 또한 디바이스 연구자들은 활성층(공액고분자와 C60 블렌드 층)의 morphology 거동의 연구 및 활성층과 각 전극의 계면 조절을 통한 효율 향상에 집중하고 있다. 지난 몇 년간 본 연구실에서는 활성층의 주요 요소인 작은 밴드 갭(low band gap)을 갖는 고분자와 활성층(active layer)과 전극과의 계면 특성의 향상을 위한 수용성 고분자의 합성에 대한 연구를

수행하였다. 본 연구발표에서는 지난 몇 년간 수행한 가은 밴드 갭을 갖는 고분자와 수용성 고분자 소재의 합성 및 합성한 소재들을 이용한 태양전지의 특성에 대하여 논의 하려 한다.

## Polymer Solar Cells (Bulk hetero-junction type)



OOM Lab. (Organic Optoelectronic Materials Laboratory)



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발표코드: POLY1-2

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 강영종

## Self-assembled Hybrids Comprising Ge Nanoparticles and Polymer Composites for Anode Materials of Advanced Lithium-Polymer Batteries

박문정

포항공과대 화학과

A facile synthetic route toward binder-free anode materials comprising Ge nanoparticles (GeNPs) and amorphous carbons is developed for high capacity lithium batteries. Confinement of butyl-capped GeNPs (ca. 10 nm) within poly(styrene-*b*-isoprene) (PS-PI) block copolymer particles is successfully achieved with aid of thermoset polymers. Each PS-PI particle with characteristic size of 120 nm contains 5~8 GeNPs. The internal structure of the composites was locked up by simple thermal curing process and all polymeric materials were turned into carbons by subsequent pyrolysis. The resulting anode contains well-dispersed GeNPs, embedded in carbon matrix and exhibits smooth surface in the absence of binders. It has been revealed that the GeNPs/carbon hybrid 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 hybrid anode also shows rate capability during repeated cycles at 1C, 2C, 5C,

and 10C rates. The elimination of polymeric binders in the fabricated anode would greatly rule out the issues arising from non-conducting nature of the binders and inhomogeneous distribution of active materials in the anode.



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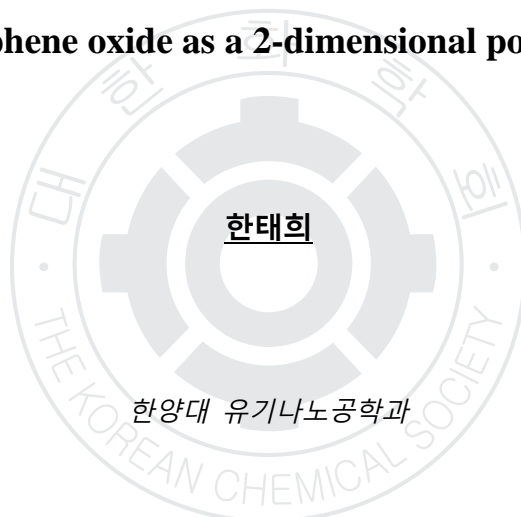
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발표코드: POLY1-3

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 강영종

## Graphene oxide as a 2-dimensional polymer



Oxidative etching of graphene flakes was observed to initiate from edges and the occasional defect sites in the basal plane, leading to reduced lateral size and a small number of etch pits. In contrast, etching of highly defective graphene oxide and its reduced form resulted in rapid homogenous fracturing of the sheets into smaller pieces. Based on these observations, a slow and more controllable etching route was designed to produce nanoporous reduced graphene oxide sheets by hydrothermal steaming. The degree of etching and the concomitant porosity can be conveniently tuned by etching time. Etched graphene oxide patterns strongly support that graphene oxide sheets can be regarded as a 2-dimensional random block copolymer. In contrast to nonporous reduced graphene oxide annealed at the same temperature, the steamed nanoporous graphene oxide exhibited nearly two orders of magnitude increase in the sensitivity and improved recovery time when used as chemiresistor sensor platform for NO<sub>2</sub> detection. The results underscore the efficacy of the highly distributed nanoporous network in the low temperature steam etched graphene oxide.

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발표코드: POLY1-4

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 10:15, 좌장: 강영종

## Materials development for energy Storage: Cathode materials in lithium ion batteries



강병우

포항공과대 신소재 공학과

Energy is essential entity for human being like food, air, and water. However, today energy has been challenged by the lack of supply and the growing demand. Further serious problem of energy is the strong dependence of supply on non-renewable sources that generate tons of CO<sub>2</sub> causing unexpected climate change. Energy storage can help us to address these challenges because it can store energy for a later use and convert energy to be a better quality. By utilizing these functions, energy storage can make renewable sources more reliable and easier to use leading to the increase of supply. Furthermore, energy storage enables vehicles to utilize the electricity instead of oil through the burgeoning electric vehicles' technology. Among other energy storage technologies, lithium ion batteries are very attractive because they cover a wide range of energy spectra and have high energy density. The development of lithium ion batteries is crucial task for addressing energy challenges. In this talk, I will focus on the development of cathode material, which is a key component for the performance of lithium ion batteries. In the advent of

new applications such as plug-in electric vehicles (PHEV) or electric vehicles (EV), a lot of attention has gone to  $\text{LiFePO}_4$  because of its excellent safety and its inexpensive cost. However,  $\text{LiFePO}_4$  suffers from poor power capability which is essential requirement in vehicles. I will discuss what factors affect power density and how to improve it in  $\text{LiFePO}_4$ . Through these understandings simple approach had been developed. With this approach  $\text{LiFePO}_4$  shows very high power capability. Developing materials brings up new possibilities such as the electrification of vehicles in lithium ion batteries which really help to address energy challenges.



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발표코드: POLY1-5

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 김동하

## Well-dispersed Anatase TiO<sub>2</sub> Nanoparticles for Photovoltaic Applications

이원목

세종대 화학과

Zero-dimensional TiO<sub>2</sub> nanoparticle possesses significant importances in many industrial fields due to its photophysical and photochemical properties. Typical properties of nanocrystalline TiO<sub>2</sub> nanoparticles are 1) photocatalytic activity, 2) high refractive index, 3) electron transporting property, 4) UV absorbance, etc. Despite its importance, preparation of well dispersed TiO<sub>2</sub> nanoparticles in liquid matrix is not straightforward due to its hardly controllable kinetics during synthesis. In this presentation, two synthetic approaches for TiO<sub>2</sub> nanoparticles will be introduced, and some of successful applications will be discussed. Aim of this study was the preparation of transparent TiO<sub>2</sub> nanoparticles dispersions in aqueous or organic media toward practical applications such as photoelectrodes for dye sensitized solar cell, hole blocking layer for organic solar cell, and reflectors for micro-lasers.



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발표코드: POLY1-6

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 김동하

## Hole Extraction Layers to Improve the Device Lifetime of Organic Photovoltaic Cells



이태우

포항공과대 신소재공학과

In organic bulk heterojunction solar cells, hole extraction and device lifetime are critically related with the hole extraction layer which is inserted between a photoactive layer and a positive electrode. In this study, conducting polymer-based hole extraction layers (HELs) with high work function were employed for organic solar cells based on poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole): [6,6]-phenyl C61-butyric acid methyl ester (PCDTBT:PCBM). With our HELs, the Open circuit voltage ( $V_{oc}$ ) was significantly increased. We also demonstrate that our HEL greatly improve the device lifetime under continuous irradiation of AM 1.5-100 mW/cm<sup>2</sup> simulated sunlight.

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발표코드: POLY1-7

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 김동하

## New Photocatalyst for Artificial Photosynthesis



Nature utilizes solar energy for the synthesis of various compounds, which remains as a target model for the development of artificial photosynthetic system. In biocatalysis systems, enzymes catalyze and build intricate products with high specificity in environmentally benign conditions. Many enzymes, particularly, the oxidoreductases depend on nicotinamide co-factors such as NAD (nicotinamide adenine dinucleotide) and NADP (nicotinamide adenine dinucleotide phosphate) for their biological/industrial functions. The high cost of these co-factors, however, remains as one of the major hurdles in industrialization of many promising enzymatic processes. Therefore, an efficient method of their in situ regeneration has long been expected to provide a means of making the process economically and industrially feasible. In the regeneration of co-factors, so far, a number of strategies such as enzymatic, electrochemical methods etc., had been devised and investigated, but these strategies are still associated with their own drawbacks. The use of light energy for the regeneration of co-factors is envisioned to provide the opportunity of harnessing the clean and abundant solar energy. Therefore, we developed the photocatalyst-redox enzyme

coupled bioreactor system that exemplified solar synthesis in a simple heterogeneous system. Generating NADH in non-enzymatic light-driven process and coupling it to the enzymatic dark reaction catalysis for chemical synthesis via photobiocatalysis, the present work remains conceptually a novel model. Also it demonstrates successfully a new and potentially promising visible-light driven artificial photosynthesis system for the ultimate goal of utilization of solar energy in chemical synthesis.



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발표코드: POLY1-8

발표분야: Current issues in environment/energy fusion technologies

발표종류: 심포지엄, 발표일시: 목 12:05, 좌장: 김동하

## **Titanium-embedded layered double hydroxides as highly efficient water oxidation photocatalysts under visible light**

강정구

KAIST 신소재공학과

Here, we have synthesized the new titanium-embedded layered double hydroxides (LDHs), such as (Ni/Ti)LDH and (Cu/Ti)LDH. First of all, the formation of LDH structures and the bonding nature for a mixed oxide structure of LDHs are explored in this work. Also, it is determined that our LDHs show two absorption bands in the red and blue regions under visible light, thus different from those of a pure titanium oxide with absorption bands in only the UV region. We found that the (Ni/Ti)LDH with the high surface area showed a higher reaction rate, producing 49 mmol O<sub>2</sub> in water oxidation by using 200mg of the photocatalyst and 1 mmol of AgNO<sub>3</sub> as a sacrificial agent. Also, the (Cu/Ti)LDH showed a good reaction rate and produced 31 mmol of O<sub>2</sub> under the same condition. On the other hand, conventional TiO<sub>2</sub> nanoparticles generated a very small amount of oxygen within the error range under this visible light irradiation. Consequently, these results imply that absorption bands in the visible

range and the large surface area of an LDH could result in the high water oxidation photocatalytic activity under visible light.



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장소: 일산KINTEX

발표코드: POLY2-1

발표분야: International symposium on supramolecules and self-assembly

발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 박태호

## Fluorescent Conjugated Polymers as Chemical and Biological Sensing Platforms



이택승

충남대 유기소재섬유시스템공학과

Fluorescent conjugated polymers are being extensively investigated for their potential applications in the fields of optoelectronics, microelectronics, and chemical and biological sensors. Especially, water-soluble conjugated polymers have been attracted a great deal of attention because of their unique optoelectronic properties, which may serve as a basis for a new generation of optoelectronic devices and biochemical detection such as DNA, proteins, and biological agents. Their peculiar properties stem from the combination of optoelectronic properties of conventional conjugated polymers and water solubility induced by ionic nature of polyelectrolytes. Their optoelectronic properties can be easily tuned through the structural alteration of the conjugated structure of the polymer backbones, and the ionic functionality endows them with exceptional features such as electrostatic interaction with oppositely charged species, a high sensitivity toward fluorescence quenchers and fluorescence change with aggregation.

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발표코드: POLY2-2

발표분야: International symposium on supramolecules and self-assembly

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 박태호

## Covalent self-assembly of nanostructures materials



김기문

포항공과대 지능초분자연구단, 화학과, WCU 첨단재료과학부

We have developed a novel method to synthesize nanostructured polymer materials including polymer nanocapsules, free-standing two-dimensional polymers, and polymer nanorings using covalent self-assembly. Without relying on any pre-organized structures or templates, polymerization of monomers with a flat core and multiple polymerizable groups at the periphery directly produces polymer nanocapsules, two-dimensional polymers, or polymer nanorings depending on reaction medium, bending rigidity of monomers and/or intermediates produced, and degree of in-plane symmetry of monomers. The details of the work will be presented.

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발표코드: POLY2-3

발표분야: International symposium on supramolecules and self-assembly

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 박태호

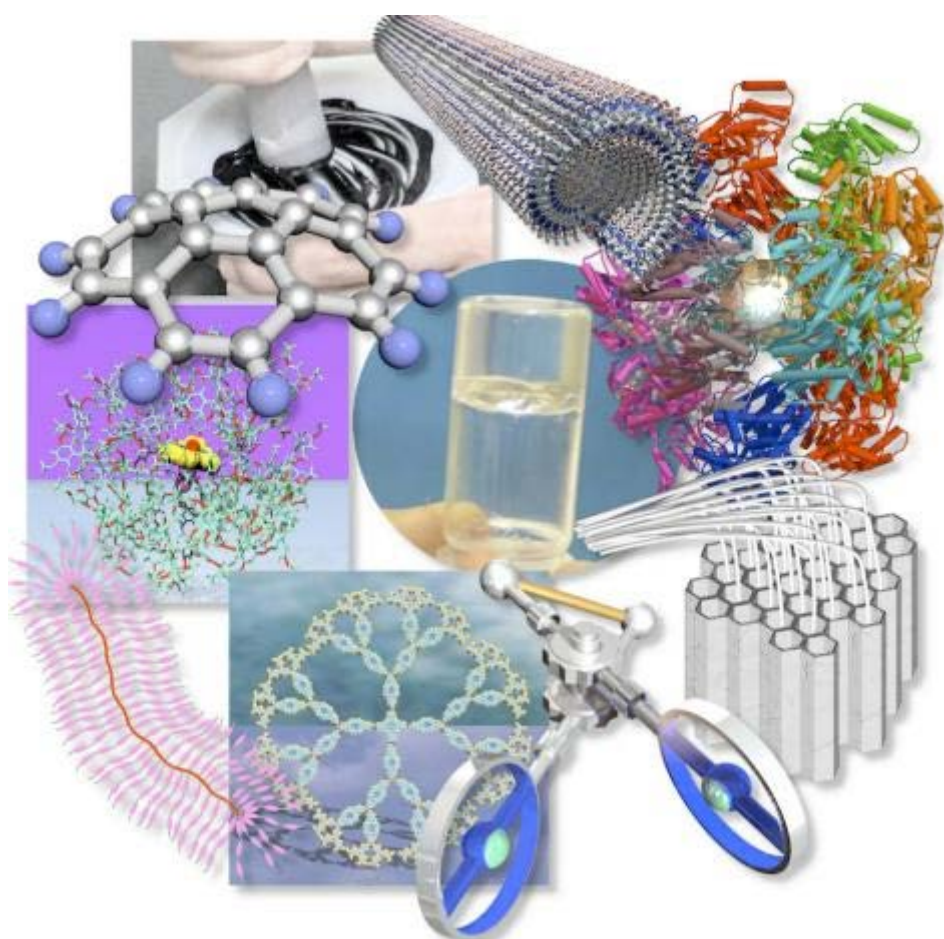
## Advanced Molecular Assembly for Functional Materials

**Takuzo Aida**

*The University of Tokyo and Riken Advanced Research Institute*

Owing to a tremendous progress in supramolecular chemistry, one may now construct and tailor a variety of desired nanostructures, where assembling events mostly operate thermodynamically. However, if one may consider developing materials for practical applications, we certainly need to design kinetically preferred hierarchical structures in a macroscopic scale. Here we report some of related achievements in our recent study. [1] Nature 2010, 463, 339. [2] Science 2010, 330, 808. [3] Science 2011, 334, 340. [4] Science 2012, in press.





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발표코드: POLY2-4

발표분야: International symposium on supramolecules and self-assembly

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 박태호

## Switchable Supramolecular Systems from Self-Assembly of Dendritic Oligomers

이명수

서울대 화학과

Supramolecular events take place through molecular assembly process in which molecular modules spontaneously form ordered aggregates through various types of intermolecular interactions. Among many self-assembling systems, aromatic rigid building blocks have proven to be particularly interesting due to their great potentials to construct smart nanostructures. Because the self-assembly of the rod blocks arises mostly from subtle anisometric interactions, the small variations in local environments trigger rapid transformation of the equilibrium features. Along this line, we have made an effort to construct dynamic supramolecular systems by introducing oligoether dendrons into aromatic rod building blocks. We have shown that rod amphiphiles with oligoether dendrons self-assemble into various well-defined nanostructures that are able to respond to environmental changes by changing their shapes and macroscopic properties. We have also shown that bent-shaped rigid segments can adopt hexameric macrocycles with a dynamic mechanical motion triggered by temperature. In this symposium, our

progress to exploit switchable nanostructures in aqueous solution will be presented together with their practical implications. References [1] H.-J. Kim, E. Lee, H.-s. Park, M. Lee, *J. Am. Chem. Soc.* 2007, 129, 10994 [2] E. Lee, J.-K. Kim, M. Lee, *Angew. Chem. Int. Ed.* 2008, 47, 6375. [3] E. Lee, J.-K. Kim, M. Lee, *Angew. Chem. Int. Ed.* 2009, 48, 3657. [4] J.-K. Kim, E. Lee, M.-C. Kim, E. Sim, M. Lee, *J. Am. Chem. Soc.* 2009, 131, 17768. [5] E. Lee, J.-K. Kim, M. Lee, *J. Am. Chem. Soc.* 2009, 131, 18242. [6] H.-J. Kim, S.-K. Kang, C. Seok, M. Lee, *Angew. Chem. Int. Ed.* 2010, 139, 8471. [7] H.-J. Kim, T. Kim, M. Lee, *Acc. Chem. Res.* 2011, 44, 72.



일시: 2012년 4월 25~27일(수~금) 3일간

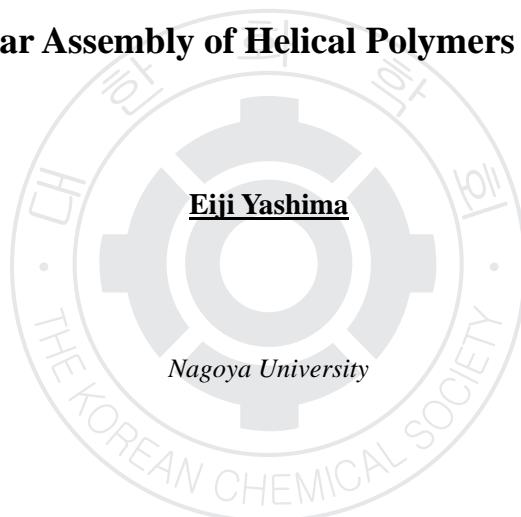
장소: 일산KINTEX

발표코드: **POLY2-5**

발표분야: International symposium on supramolecules and self-assembly

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 박태호

## Supramolecular Assembly of Helical Polymers and Oligomers



Unique macromolecules and oligomers that fold into a preferred-handed single- and double-stranded helical conformation induced by chiral substituents covalently bonded to the main-chains or external chiral stimuli followed by memory of the helical chirality are presented. The direct observations of helical structures of artificial helical polymers by atomic force microscopy (AFM) will be also presented. A series of double helices composed of different components and sequences that exhibit specific functions, such as chirality sensing, chiral recognition, enantioselective asymmetric catalysis, anisotropic spring-like motion, and remote-stereocontrol are also described.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND1-1

발표분야: Carbon Materials Chemistry

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박수진

## In Situ Synthesis of Thermochemically Reduced Graphene Oxide Polyimide Composites

구본철

KIST 복합소재기술연구소

Highly conductive reduced graphene oxide (GO) polyimide nanocomposites are synthesized by a well-organized in situ thermochemical synthesis technique. The surface functionalization of GO was carried out with aryl diazonium salt including 4-iodoaniline to form phenyl functionalized GO (I-Ph-GO). The thermochemically developed reduced GO (R-I-Ph-GO) has five times higher electrical conductivity (42,000 S/m) than typical reduced GO (R-GO). We also demonstrate a R-I-Ph-GO/polyimide (PI) composites having more than  $10^4$  times higher conductivity ( $\sim 1$  S/m) compared to a R-GO/PI composites. Finally, our on-going researches with functionalized GO (I-Ph-GO) and applications will be introduced and discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

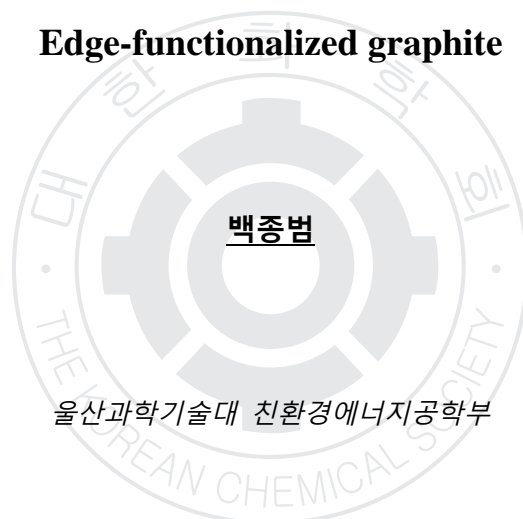
장소: 일산KINTEX

발표코드: IND1-2

발표분야: Carbon Materials Chemistry

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 박수진

## Edge-functionalized graphite



울산과학기술대 친환경에너지공학부

High-yield “direct” exfoliation of graphite has so far remained a challenge to graphene research community. Here, we demonstrate a “direct” covalent attachment of organic molecular wedges to the edges of pristine graphite instead of graphite oxide (GO). The approach is the first case of “direct” functionalization of pristine graphite and a step toward high-yield exfoliation of three-dimensional graphite into two-dimensional graphene sheets. The resultant edge-selectively functionalized graphite is readily dispersible in common organic solvents with a concentration in the range of 0.27-0.80 mg/mL. The improved dispersibility is driven by a strong interaction between the polar functional groups on graphite and the polar solvent. The resistance of resultant graphene films upon solution cast and subsequent heat-treatments is 0.5-3 k $\Omega$ /sq with 65-95 % of optical transmittance, whose value is several orders of magnitude better than reduced GO (rGO). Our findings suggest that the edge-selectively functionalized graphite can be prepared and conveniently used as base materials for a wide range of applications from wet chemistry to device applications.

일시: 2012년 4월 25~27일(수~금) 3일간

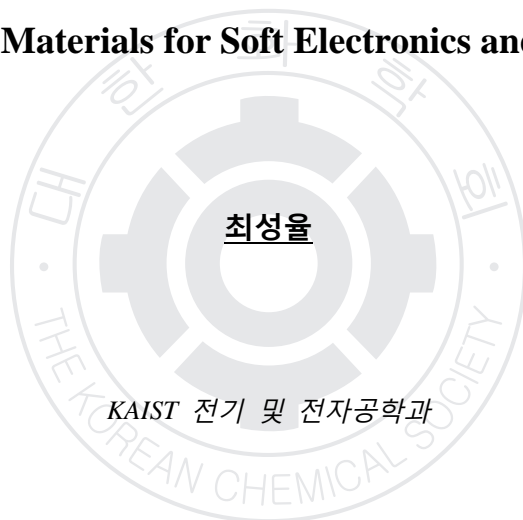
장소: 일산KINTEX

발표코드: IND1-3

발표분야: Carbon Materials Chemistry

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 박수진

## Graphene Materials for Soft Electronics and Photonics



Graphene, two-dimensional one-atom-thick planar sheet of carbon atoms densely packed in a honeycomb crystal lattice, has attracted attention due to its extraordinary electrical, optical, and thermal properties. In addition graphene's outstanding tensile strength allows graphene-based electronic and photonic devices to be flexible, stretchable, and foldable. In this talk, we discuss a novel platform and architecture for the development of high-performance graphene-based flexible devices and components. We have reported flexible electronic devices based on graphene materials, i.e. field-effect transistors, gas sensors, and nonvolatile memory devices, in which versatile properties of graphene materials have been incorporated into a flexible electronic platform. Recently, we also have demonstrated the graphene-based plasmonic waveguide for high-performance optical interconnection in flexible optoelectronic devices. We conclude that graphene-based electronic and photonic devices have huge potential to be exploited further for development of next-generation human-friendly soft optoelectronic systems.

일시: 2012년 4월 25~27일(수~금) 3일간

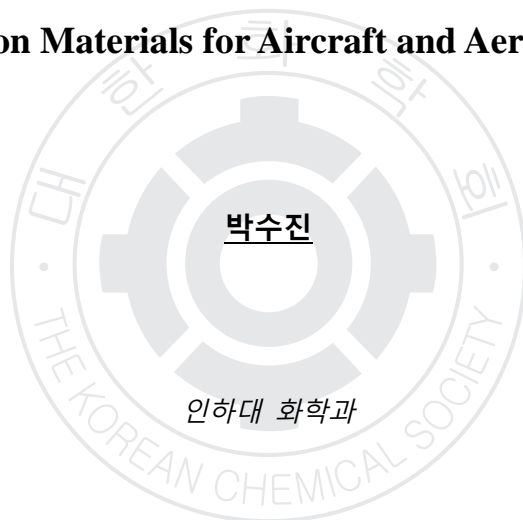
장소: 일산KINTEX

발표코드: IND1-4

발표분야: Carbon Materials Chemistry

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 최성율

## Carbon Materials for Aircraft and Aerospace



Aerospace engineering is changing. Traditionally, aeroplanes have been made out of metal-alloys of aluminum; now however, carbon fibers-reinforced plastic composites (CFRP) have been increasingly substituted for the take-up of them and expected to make the next generation across the aerospace industry. These materials can provide a much better strength-to-weight ratio than metals by as much as 20% better. The prodigious strength of the individual strands of carbon would be five times in comparison with the aluminum alloys (the ultimate strength of aerospace grade: 450 MPa). Additionally, the CFRP are only 60% of the density of aluminum. Thus, the CFRP have the best combination of strength and cost. In this presentation will cover the widespread introduction of CRFP for aircraft and aerospace and their development status.



일시: 2012년 4월 25~27일(수~금) 3일간

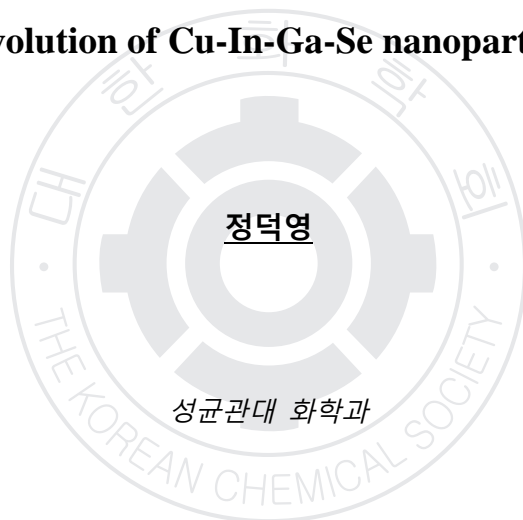
장소: 일산KINTEX

발표코드: IND2-1

발표분야: Non-Vacuum-Processed Inorganic Thin Film Solar Cells

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김진영

## Structural evolution of Cu-In-Ga-Se nanoparticle syntheses



Nanoparticles of the  $\text{Cu(In,Ga)Se}_2$  (CIGS) were synthesized by ultrasound irradiation under ambient pressure and characterized by powder X-ray diffraction, scanning electron microscopy, Raman spectroscopy and X-ray fluorescence analyses. The samples have chalcopyrite and/or zinc blende crystal structures. Synthetic conditions were determined for the crystallized CIGS nanoparticles formation to prevent from  $\text{Cu}_2\text{Se}$ ,  $\text{Cu}_{2-x}\text{Se}$ , and  $\text{CuSe}$  etc. In solution syntheses, the different crystalline phases were obtained, depending on pH, concentration of starting materials.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND2-2

발표분야: Non-Vacuum-Processed Inorganic Thin Film Solar Cells

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 김진영

## CIGS 박막 태양전지의 개발 동향 및 이슈

윤재호

한국에너지기술연구원 태양에너지연구단

CIGS 박막 태양전지는 결정질 실리콘 태양전지 보다 제조단가가 낮으면서도 저가형 태양전지중에서 가장 효율이 높다. 따라서 가격 경쟁력과 응용가능성 측면에서 여타 태양전지에 비해 발전 가능성이 매우 높은 태양전지로 인식되고 있다. 실험실 수준에서 20% 이상의 효율이 보고됨으로써 고효율 태양전지로서의 가능성이 입증되고 있으며 비진공 프린팅 공정의 적용으로 인하여 저가 태양전지로서의 가능성 또한 증명되고 있다. 따라서 전세계적으로 'cost-effective'한 CIGS 박막 태양전지를 제조하기 위한 경쟁이 매우 치열하다. 특히 비진공 프린팅을 이용한 CIGS 박막 태양전지는 기존의 진공 공정을 이용한 CIGS 박막 태양전지에 비해 초기 투자비용이 적을 뿐만 아니라, 공정중에 사용되는 소재의 이용율이 높기 때문에 태양전지의 제조단가를 크게 낮출 수 있다. 하지만 진공 공정 대비 효율이 낮기 때문에 고효율화를 위한 기술 개발이 필요하며 이와 함께 roll-to-roll 공정을 구현할 수 있는 기반기술의 개발도 필요하다. 본 발표에서는 CIGS 박막 태양전지의

연구동향과 및 최근의 이슈들을 살펴보고고 이를 통하여 CIGS 박막 태양전지의 발전 방향을 모색하고자 한다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND2-3

발표분야: Non-Vacuum-Processed Inorganic Thin Film Solar Cells

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김진영

## 스프레이 기반 CIGS 태양전지 제조

김준호

인천대 물리학과

CIGS 태양전지는 박막형 태양전지 중에서 최고효율을(~20%) 보이고있다. 현재, 저가 고효율 제조 방법에 대한 연구가 활발하다. 우리는 스프레이 열분해법을 이용하여 CIGS 태양전지 제조연구를 해오고 있는데, 우리의 태양전지는 ITO/ZnO/In<sub>2</sub>S<sub>3</sub>/CIGS/Mo/glass 구조를 가진다. 여기서,CIGS 와 In<sub>2</sub>S<sub>3</sub> 는 스프레이 열분해법을 통해서 제조된다. 우리는 CIGS 와 In<sub>2</sub>S<sub>3</sub> 의 제조온도에 따른 태양전지 변환효율에 대해서 발표하고자 한다. 특히, In<sub>2</sub>S<sub>3</sub> 의 경우 증착온도가 높을 수록 제조된 태양전지의 효율이 높게 나타난다. 또한 제조된 태양전지의 I-V,C-f 특성 측정을 통해 제조된 태양전지의 defect 특성을 논의하고자 한다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND2-4

발표분야: Non-Vacuum-Processed Inorganic Thin Film Solar Cells

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 김준호

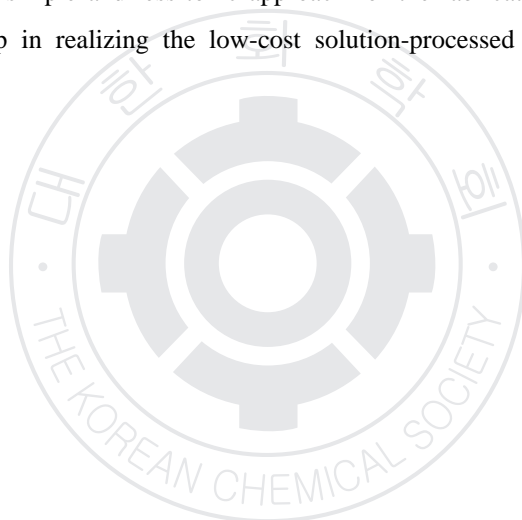
## Non-Vacuum Deposition of Nontoxic and Abundant $\text{Cu}_2\text{ZnSnS}_4$ for Thin-Film Solar Cells

문주호

연세대 신소재공학과

Copper zinc tin sulfide ( $\text{Cu}_2\text{ZnSnS}_4$ , CZTS) is a very promising material as a low cost absorber alternative to other chalcopyrite-type semiconductors based on Ga or In because of the abundant and economical elements. In addition, CZTS has a band-gap energy of 1.4~1.5eV and large absorption coefficient over  $\sim 10^4 \text{cm}^{-1}$ , which is similar to those of  $\text{Cu(In,Ga)Se}_2$  (CIGS) regarded as one of the most successful absorber materials for high efficient solar cell. Most previous works on the fabrication of CZTS thin films were based on the vacuum deposition such as thermal evaporation and RF magnetron sputtering. Although the vacuum deposition has been widely adopted, it is quite expensive and complicated. In this regard, the solution processes such as sol-gel method, nanocrystal dispersion and hybrid slurry method have been developed for easy and cost-effective fabrication of CZTS film. Among these methods, the hybrid slurry method is favorable to make high crystalline and dense absorber layer. However, this method has the demerit using the toxic and explosive hydrazine solvent, which has severe

limitation for common use. With these considerations, it is highly desirable to develop a robust, easily scalable and relatively safe solution-based process for the fabrication of a high quality CZTS absorber layer. Here, we demonstrate the fabrication of a high quality CZTS absorber layer with a thickness of 1.5~2.0  $\mu\text{m}$  and micrometer-scaled grains using two different non-vacuum approaches. The first solution-processing approach includes air-stable non-toxic solvent-based inks in which the commercially available precursor nanoparticles are dispersed in ethanol. Our readily achievable air-stable precursor ink, without the involvement of complex particle synthesis, high toxic solvents, or organic additives, facilitates a convenient method to fabricate a high quality CZTS absorber layer with uniform surface composition and across the film depth when annealed at 530  $^{\circ}\text{C}$ . The conversion efficiency and fill factor for the non-toxic ink based solar cells are 5.14 % and 52.8 %, respectively. The other method is based on the nanocrystal dispersions that are a key ingredient in the deposition of thermally annealed absorber layers. We report a facile synthetic method to produce phase-pure CZTS nanocrystals capped with less toxic and more easily removable ligands. The resulting CZTS nanoparticle dispersion enables us to fabricate uniform, crack-free absorber layer onto Mo-coated soda-lime glass at 500  $^{\circ}\text{C}$ , which exhibits a robust and reproducible photovoltaic response. Our simple and less-toxic approach for the fabrication of CZTS layer, reported here, will be the first step in realizing the low-cost solution-processed CZTS solar cell with high efficiency.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND2-5

발표분야: Non-Vacuum-Processed Inorganic Thin Film Solar Cells

발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 김준호

## Electrochemical Deposition of Semiconductor Thin Films for Solar Cell Applications

김진영

KIST 광전하이브리드센터

The electrochemical deposition is one of the popular synthetic approaches for preparing semiconductor thin films. However, depositing semiconductor films on the conducting nanostructured electrodes is challenging owing to the preferential deposition on the outer surface of the electrode and the subsequent pore clogging. In this presentation, a mechanistic study on the factors governing the deposition morphology during the electrochemical deposition of semiconductor films on the electrically conducting nanostructured electrodes will be introduced in terms of the in-situ electronic properties of semiconductors and electrodes. Some of our recent efforts on the electrochemical deposition of chalcogenide thin films for the application to thin film solar cells will also be introduced.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR1-1

발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이진석

## Quantum-Sized Gold Nanoparticles



Metal nanoparticles containing a few to a few hundreds of atoms have been the focus of recent investigations because of their novel electronic, optical, and catalytic properties. They appear to represent the bulk-to-molecule transition region where electronic band energetics yield to quantum confinement effects and discrete electronic states emerge. In the first part of this talk, I will present recent advances in the synthesis of quantum-sized gold nanoparticles and their size-dependent electrochemical and optical properties. In the second part, I will present their use in photocatalysis and electrochemical sensing. A new class of metal-semiconductor composites was prepared by anchoring uniform gold nanoparticles on ZnO or TiO<sub>2</sub> nanoparticles. These composites exhibited significantly enhanced photocatalytic activity in degrading organic substrates in both oxidative and reductive pathways. The photocatalytic activity was found to be controlled by the size of gold nanoparticles. For electrochemical sensing applications, well-defined modified electrodes were prepared using quantum-sized gold nanoparticles that act as a redox



mediator as well as an electronic conductor. The gold nanoparticles exhibited excellent mediated electrocatalytic activity that was utilized for amperometric sensing of biologically relevant analytes.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR1-2**

발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 이진석

## Synthetic Strategy and Optical Property Characterization of Complex Nanorods

박성호

성균관대 화학과

In this talk, we represent a novel approach to investigating intra-nanorod surface plasmon coupling with control over block compositions. The multi-component rod-like nanostructures, which consist of optically active components (Au and Ag) and optically less active component (for example, Ni) in UV-vis-NIR spectral window, showed interesting optical response depending on each block length and the total length of the structure. By controlling the composition and relative lengths of the blocks that comprise these structures, we can tailor the overall optical properties. Depending on the relative fraction of Au and Ag blocks, the intensity of the transverse modes varied without noticeable peak shifts. However, the strong intraparticle surface plasmon coupling resulted in the collective appearance of longitudinal LSP modes, including higher-order modes. The experimental observations were confirmed by theoretical calculation, using a discrete dipole approximation method. In addition, we will briefly discuss how the complex

psuedo-1-dimensional nanostructures can be synthesized by using electrochemical deposition and hard templates.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR1-3

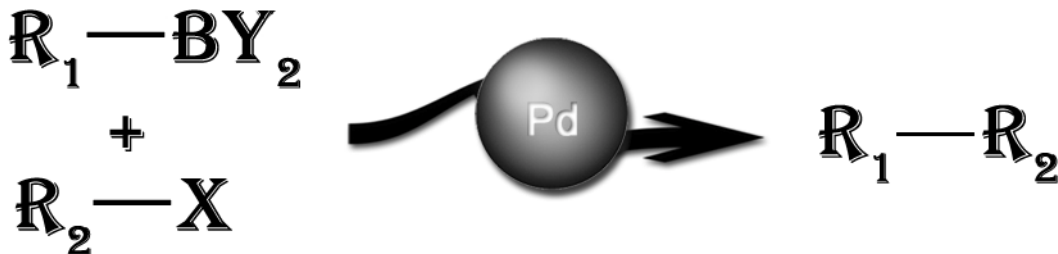
발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 이진석

## Nanocatalyst for Suzuki Coupling Reactions



The Pd nanostructures were employed in Suzuki coupling reactions with various substrates, and they served as good catalysts in these reactions.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR1-4

발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 박강현

## 2D Nanosheets of Inorganic Solids and Graphene: Emerging Building Blocks for Efficient Visible Light Active Photocatalysts

황성주

이화여대 화학·나노과학과

A variety of hybrid-type visible light active photocatalysts are synthesized by self-assembly between two oppositely charged low-dimensional nanostructured semiconductors including 2D nanosheets and 0D nanoclusters. As building blocks, the 2D nanosheets of layered metal oxide, layered double hydroxide (LDH), and reduced graphene oxide (RGO) are synthesized by the exfoliation process of the pristine layered inorganic solids and graphite. The obtained 2D inorganic/RGO nanosheets are reassembled with each other or hybridized with other 0D nanoparticles like transition metal hydroxide nanoclusters or CdS quantum dots. The band structure and surface area of wide bandgap layered titanate can be effectively tailored through the hybridization with LDH 2D nanosheets or transition metal oxide/metal chalcogenide 0D nanoparticles. The obtained nanohybrids show promising photocatalytic activity to effectively decompose organic compounds or to produce H<sub>2</sub> and O<sub>2</sub> gases under the irradiation of visible light.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR1-5

발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 박강현

## **p-InP Nanopillar Photocathodes for Highly Efficient Water Splitting**



The production of hydrogen from the photoelectrochemical (PEC) water splitting can provide abundant, renewable, clean source of energy for the future. Here, the photoelectrochemical evolution of hydrogen using p-InP nanopillar arrays decorated with metallic co-catalyst is explored. The nanopillar devices exhibit an great enhancement in the conversion efficiency, as compared to planar substrates. This behavior is mainly attributed to 1) the high current density by low surface reflectivity of nanopillar arrays along with the enhanced surface area for catalytic reaction and 2) the favorable positive shift in the onset potential by newly exposed orientation and surface modification during the reactive ion etching (RIE) process. Of particular importance to this architecture is the use of InP as the absorber layer, which is known to have a low carrier surface recombination velocity, thereby minimizing the loss of photogenerated carriers at the surfaces. Furthermore, TiO<sub>2</sub> protection layers are applied by atomic layer deposition to suppress the photocorrosion.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR1-6

발표분야: Recent Advances in Inorganic/Material Science

발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 박강현

## Research on the Adhesion, Development and Outgrowth of Hippocampal Neurons on Nanostructured Surface

이진석

숙명여대 화학과

Nervous systems are composed of microstructured scaffolds with three-dimensional nanofeatured textures. These textures enable the systems to give nanometer-scaled physical cues to the overlying cells, along with biochemical cues. However, it is practically very difficult to investigate the topographical environments in vivo in the biological systems and/or to mimic them precisely in vitro. Recently, the acceleration of neuronal development and neurite outgrowth was revealed by recent works from us on various types of nanotopographies. Concrete understanding of the topographical effects on neuronal development and neurite outgrowth would be intensively beneficial for the biomedical applications. However, there were few systematic studies about these nanotopographical effects on neuronal developments in a feature size-dependent manner. Herein, we report a nanoscale-resolved study of nanotopographical effects on development of hippocampal neurons. In this study, we use substrates with packed glass beads by rubbing method for generating highly periodic nanotopographies with various sizes.

We found that acceleration of neuritogenesis appeared only on the beads larger than 200 nm in diameter, and observed that filopodial thickness was comparable with this scale. This study is expected to be essential to elucidate the nanotopographical effect on neuronal development.





일시: 2012년 4월 25~27일(수~금) 3일간

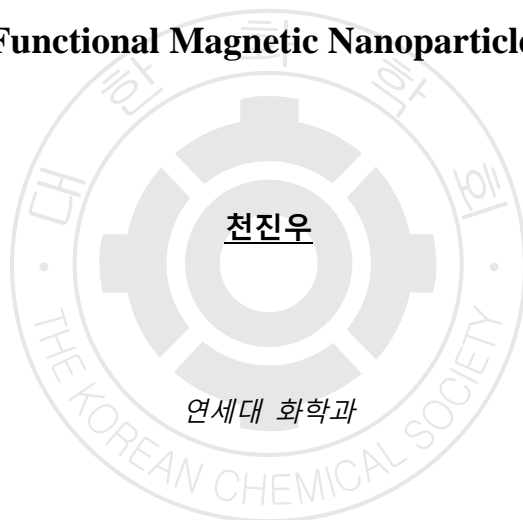
장소: 일산KINTEX

발표코드: INOR2-1

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 최희철

## Functional Magnetic Nanoparticles



One of the important trends of next-generation nanomedicine is theranostics that is defined by the combination of therapeutics and diagnostics on a single platform. Magnetic nanoparticles are among one of the most essential platforms for targeted imaging, therapy, and simultaneous monitoring of therapeutic efficacy. In this talk, I will discuss magnetic nanoparticles as a core platform material for theranostics and add a variety of functionalities such as drug, targeting moiety, and gene to enhance their performance. Their unique utilization in highly accurate dual-modal MR imaging, therapeutic hyperthermia of cancer cells, controlled drug release, gene delivery, and molecular level cell signaling and cell fate control will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

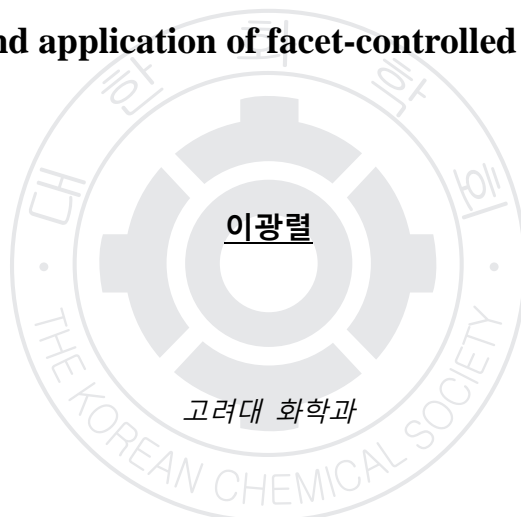
장소: 일산KINTEX

발표코드: INOR2-2

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 최희철

## Synthesis and application of facet-controlled nanocrystals



The formation process of nanoparticle is affected by various kinetic and thermodynamic parameters, which are determined by the intricate interplay of precursors, surfactants, and reaction temperature. Whilst the variation of surfactant and reaction temperature has been a preferred approach for synthesis of new nanoparticles, more exotic methods, namely, elemental exchange, doping-assisted kinetic control, surface-stabilization by non-surfactants, epitaxial growth, and etching, are being developed to fine-control nanocrystal growth and to overcome the dearth of precursors. In this seminar, I will describe non-conventional synthetic strategies for crystallographically well-defined noble metal nanocrystals as well as nanocrystal application in catalysis.

일시: 2012년 4월 25~27일(수~금) 3일간

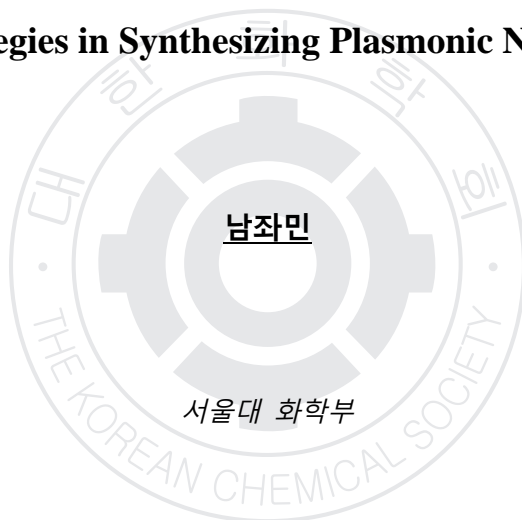
장소: 일산KINTEX

발표코드: INOR2-3

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 최희철

## DNA-Based Strategies in Synthesizing Plasmonic Nanogap Structures



Here, I will describe DNA-based synthetic strategies to build up new types of plasmonic nanogap Au/Ag structures. I will also show and discuss the use of these plasmonic nanostructures as excellent optical signal enhancement platforms for surface-enhanced Raman scattering and metal-enhanced fluorescence.

일시: 2012년 4월 25~27일(수~금) 3일간

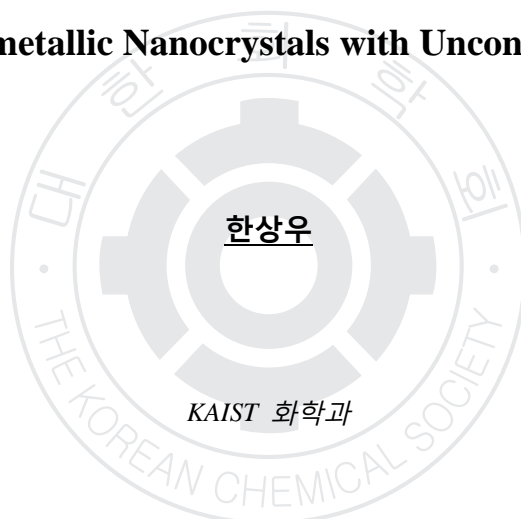
장소: 일산KINTEX

발표코드: INOR2-4

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 최희철

## Two in One: Bimetallic Nanocrystals with Unconventional Shapes



During the past decade, bimetallic nanocrystals (NCs) with a core-shell and alloy structures have received a great deal of attention owing to their remarkable optical and catalytic properties, which are superior to those of monometallic NCs. In particular, the catalytic activity and selectivity of NCs can be tuned by controlling their morphology, because the exposed surfaces of the NCs have distinct crystallographic planes (facets) that can determine their overall catalytic properties. Accordingly, shape-controlled synthesis of bimetallic NCs has been extensively studied in efforts to optimize their properties. However, the control of the size, shape, and composition of NCs has been limited due to the complex kinetics in the reduction of cationic metal precursors and to the difficulty in finding suitable stabilizing agents. Therefore, development of an efficient synthesis route for the preparation of monodisperse bimetallic NCs is still a radical issue to study their properties and applications. Here we report several facile wet-chemical synthesis strategies to prepare bimetallic NCs with well-defined morphologies and their inherent structural, optical, and catalytic characteristics.

일시: 2012년 4월 25~27일(수~금) 3일간

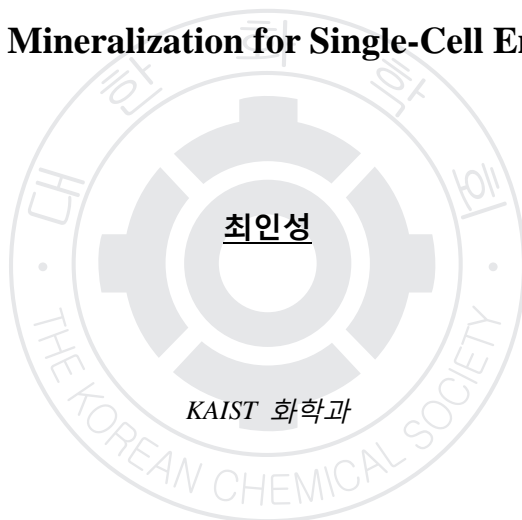
장소: 일산KINTEX

발표코드: INOR2-5

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 남좌민

## Bioinspired Mineralization for Single-Cell Encapsulation



It is bioinspired mineralization that makes it possible to interface living cells with inorganic materials at the single-cell level, maintaining the cell viability. The hybrid structures, with inorganic materials as a shell and cells as a core, show emerging properties compared with native, bare cells, such as enhanced viability and protection against external stresses. This approach suggests an approach to the formation of a new class of hybrid structures, mimicking the natural endospores, called “artificial spores”.

일시: 2012년 4월 25~27일(수~금) 3일간

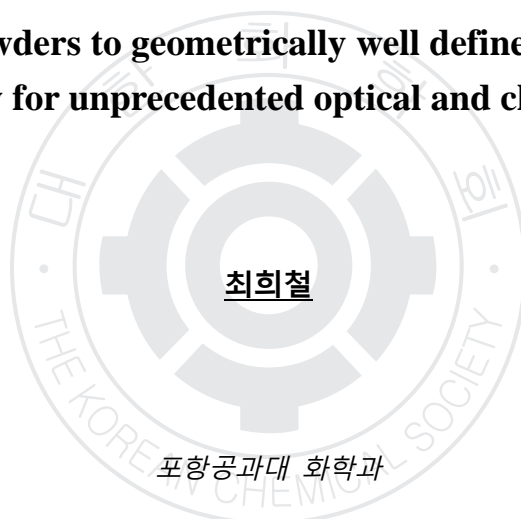
장소: 일산KINTEX

발표코드: INOR2-6

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 남좌민

## From organic powders to geometrically well defined low-dimensional structures: A way for unprecedented optical and chemical properties



Scaling-down the size of a bulk material into a quantum size regime grants new optical and electrical properties due to the emergence of discrete electronic energy states according to the quantum size effect. Another way to secure new optical and electrical properties that has been recently proposed is to design and grow crystalline low dimensional structures from individual ensemble molecules, which is known as meso size effect. The meso size effect is especially of great interest for highly conjugated molecules. For example, we have recently demonstrated that C70 cubes are directly crystallized from individual C70 molecules in solution phase, and the C70 cubes emit strong photoluminescence (PL) due to the reduced exciton scattering sites by the crystallization. In this presentation, I will introduce new examples that exhibit unprecedented optical and chemical properties upon the crystallization of individual multi-phenyl ring molecules and macrocyclic molecules into 1D wires. The synthetic method, crystal plane-dependent

PL activity and crystal structure-dependent intermolecular interaction change that are primarily induced by the crystallization will be discussed in detail.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR2-7

발표분야: New Synthetic Strategies of Functional Inorganic Nanostructures

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 남좌민

## Flexible and Stretchable Electronics and Applications for Biomedical Devices

김대형

서울대 화학생명공학부

High quality single crystal inorganic materials for high performance electronics and optoelectronics are intrinsically stiff and brittle, while biological systems are soft and curvilinear. This abstract describes methods of deterministic assembly of inorganic nanomaterials onto flexible and stretchable substrates to solve this fundamental mechanical mismatch between electronic devices and bio-system. To achieve flexible and stretchable bio-integrated electronic systems with comparable performance to state-of-the-art, wafer-based devices, ultrathin shape single crystal nanomaterials are transferred on flexible and stretchable substrates using dedicated dry transfer-printing technology. This system minimizes the induced strain in active area while successfully isolates strain to highly stretchable interconnection regions. In addition to unconventional device designs, various materials and substrates, including bio-resorbable silk film, minimally invasive silicone balloon catheter and ultrathin elastomeric materials whose modulus is similar with epidermis, are utilized to deduce the successful integration with bio-



system. The concepts of flexible and stretchable bio-integrated devices are illustrated through application examples including soft and conformable electrophysiological monitors integrated with hearts and brains, and tattoo-like epidermal electronics with mechanical properties matched to the epidermis.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS1-1**

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 분과기조강연, 발표일시: 목 09:30, 좌장: 강상욱

**[발표취소] Designing Organic Materials for Photovoltaic Devices  
Based on Electronic Energy Transfer**

**Anthony Harriman**

*Newcastle University, School of Chemistry*

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS1-2**

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 심포지엄, 발표일시: 목 10:05, 좌장: 심상덕

## **Comparative Study of Charge Recombination Dynamics in DSSCs Prepared with Various TiO<sub>2</sub> Electrodes**



조대원

건국대 건국대-프라운호퍼 태양전지 연구소

We have prepared the dye-sensitized solar cells (DSSC) consist of N719 on modified TiO<sub>2</sub> electrodes. The electron transfer dynamics showed strong correlation with device photovoltaic performance, which is studied by transient absorption spectroscopic methods. We find the charge recombination dynamics are dependent upon the modification of TiO<sub>2</sub> electrodes employed in the device. So we investigated the effects of thickness, size, and introducing of nanostructure TiO<sub>2</sub> for charge recombination process. From photodynamic point of view, the higher DSSC device performance is obtained when the dye-regeneration and electron diffusion are fast enough to reduce charge recombination losses, thereby optimizing the conditions of electrode in the device.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: PHYS1-3

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 심상덕

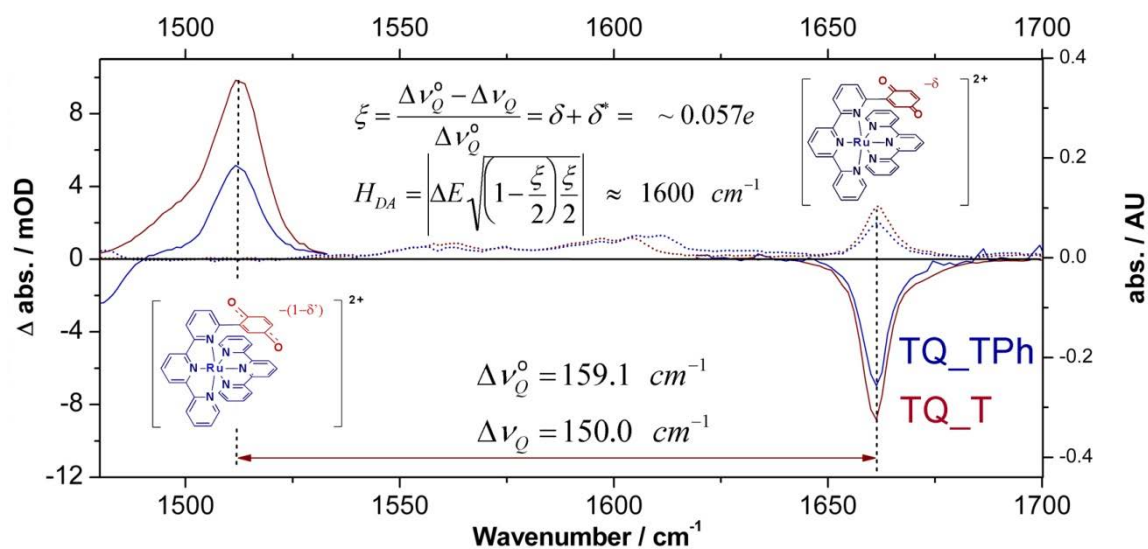
## Probing Ground-to-CT State Electronic Coupling by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy; Application to Sensitizer-Semiconductor Interfacial Electronic Coupling

강윤경

상명대 화학과

New pi-stacked  $[\text{Ru}(\text{tpy})_2]^{2+}$  (T\_T)-benzoquinone (Q) donor-acceptor (D-A) systems,  $[\text{Ru}(6-(2\text{-cyclohexa-2',5'-diene-1,4-dione)-2,2':6',2''\text{-terpyridine})(2,2':6',2''\text{-terpyridine})][\text{PF}_6]_2$  (TQ\_T), have been synthesized and characterized. Orthogonal alignment of Q to the tpy ligand imposes this unit juxtaposed cofacially on the central pyridyl ring in another tpy with a typical van der Waals distance. The low energy electronic absorptions of these complexes are mainly metal-to-ligand charge transfer (MLCT) in nature, similar to that observed in T\_T benchmark system, and do not exhibit distinguishable metal-to-Q charge transfer (MQCT) absorption in spite of the proximal location of the electron acceptor unit (Q) to the electron donor unit (T\_T). Due to the negligible intensity of MQCT bands, evaluation of  $H_{\text{DA}}$  between ground and lowest energy MQCT states are not available through conventional Mulliken-Hush analysis. For such systems,  $H_{\text{DA}}$  values were successfully evaluated from the relative difference ( $\xi$ ) of the carbonyl

stretching frequency between the neutral Q and its one electron radical anion, which was determined by an ultrafast visible-pump/mid-IR-probe (TrIR) spectroscopic method. TrIR results showed that the partial charge localized on Q moiety in the MQCT state was  $\sim -0.97e$  and the corresponding  $H_{DA}$  was  $\sim 1600\text{ cm}^{-1}$ <sup>1</sup>. Extending this methodology provides useful information regarding sensitizer-semiconductor interfacial electronic coupling in dye-sensitized solar cell, which cannot be precisely evaluated by conventional electron transfer rate measurement.



일시: 2012년 4월 25~27일(수~금) 3일간

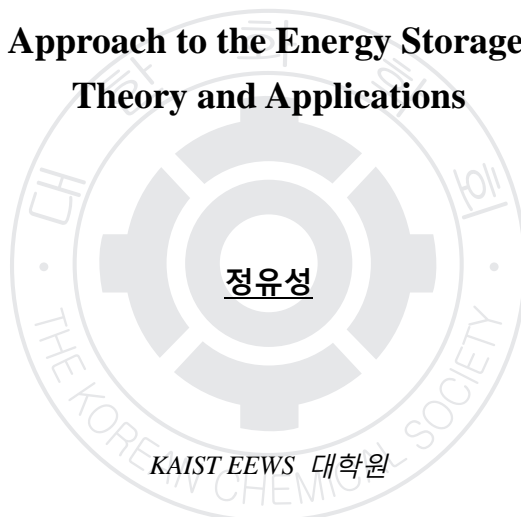
장소: 일산KINTEX

발표코드: **PHYS1-4**

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 조대원

## **First Principles Approach to the Energy Storage and Utilization: Theory and Applications**



Obtaining chemical accuracy (0.04 eV) to quantify key chemical quantities (e.g. heats of formation, bond dissociation energies, and reaction barrier heights) using quantum mechanics has been a major focus in the development of the theory. This has led to, for example, the Gn method that approaches to this accuracy. Because G3 is a coupled cluster based method, it scales on the order of  $N^7$ , where N measures the system size, limiting to fairly small molecules for routine use. Present-day density functional methods are generally believed to provide a sweet spot between feasibility and accuracy, yet still lead to significant errors for some systems. For example, current density functionals give a poor description of London dispersion, which is essential to predict the packing of molecules into solids, and the binding of drug molecules to proteins. They are also poor in predicting the magnitude of reaction barriers often cases. In this talk, I will present a new doubly hybrid density functional we developed which includes the perturbative correlation treatment of opposite-spin electrons only and therefore provides a unique

combination of high accuracy and speed. As applications of new electronic structure methods, I will discuss issues related to designing high capacity energy storage materials.



일시: 2012년 4월 25~27일(수~금) 3일간

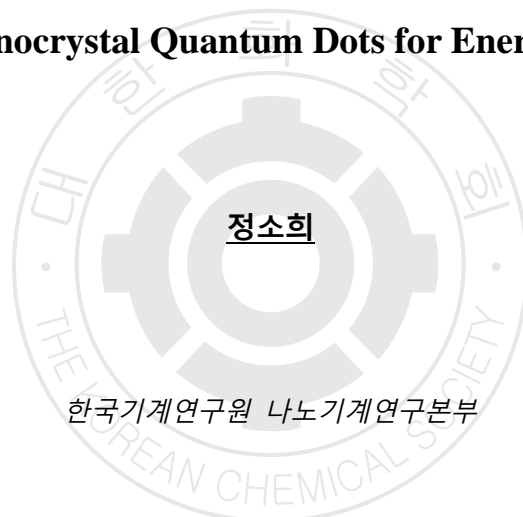
장소: 일산KINTEX

발표코드: **PHYS1-5**

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 조대원

## Assembled Nanocrystal Quantum Dots for Energy Applications



Colloidal Nanocrystal Quantum Dots (NQDs) have been considered ideal building blocks for functional materials because of their physical properties based on quantum confinement effect. Recent advances in the use of hot carriers and multiple-exciton from the high energy photon in NQDs have demonstrated potential efficiency improvements when used in photovoltaics. Here, strategies to facilitate carrier transfer/transport while preserving optical characteristics of isolated NQDs will be discussed. Specifically, synthesis and characterizations of 1) the fabrication of neat NQD solids (assembled NQD films) with modified surfaces by attaching ligands or by applying physical processes such as heat annealing [J. Phys. Chem. C (2011), 115(3), 607] and 2) coupling NQDs to one-dimensional nanostructures such as single-walled carbon nanotubes (SWNTs) [ACS Nano, (2010) 4(1), 324] will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS1-6**

발표분야: Energy conversion and solar cell: physical chemist's view

발표종류: 심포지엄, 발표일시: 목 11:45, 좌장: 조대원

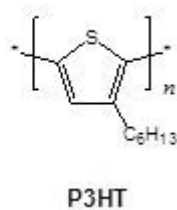
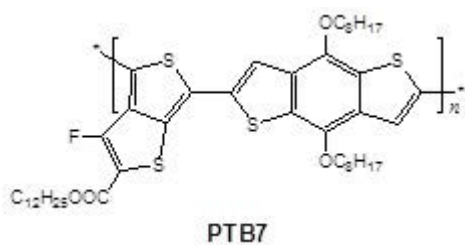
## Ultrafast Exciton Dynamics in PTB7 and P3HT; Effect of Excess Energy on Exciton Diffusion in OPV polymers

조성 Lin X. Chen<sup>1</sup>

전남대 화학과 <sup>1</sup>Northwestern University, USA

Over the past few decades, semiconducting polymers have been investigated to materialize efficient molecular photonic and electric devices such as organic solar cells, printing electric circuit, organic light-emitting diodes, and so on. Among those, considerable efforts have been devoted to organic solar cells as a substitute energy source to overcome an energy crisis. Bulk heterojunction (BHJ) organic photovoltaic (OPV) cells have various advantages, low cost, ease fabrication, and small environmental impact relative to silicon or heavy metal based solar cells. The solar energy conversion efficiency of OPV cells is improving and especially polymer-based OPV cells are promising for commercialization. We have investigated two representative OPV polymers, poly(thienothiophenebenzodithiophene) (PTB7) and poly-3-hexylthiophene (P3HT), which are alternating copolymer and homopolymer, respectively (Scheme 1). This work revealed that the initial excited states of PTB7 and P3HT after photoexcitation are emissive and that their origins can be assigned as optically allowed exciton states. Interestingly, the initial excitons

with excess energy in PTB7 coherently diffuse before vibrational relaxation and then the cold excitons sequentially show incoherent exciton diffusion processes to neighboring local state. On the other hand, although P3HT show efficient deactivation processes, these processes are not involved in exciton diffusion. This contrary feature results from that the initial excitons are experimentally generated on long conjugated local sites with low electronic energies and thus they are energetically isolated by neighboring short local sites and that there is no conformational motions within a few picoseconds.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS2-1**

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

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 최명룡

## Ultraviolet-Ultraviolet Hole Burning Spectroscopy for Ions Stored in a Quadrupole Ion Trap

김남준

충북대 화학과

We have developed a new technique of ultraviolet-ultraviolet (UV-UV) hole burning (HB) spectroscopy applicable for ions stored in a quadrupole ion-trap (QIT). The UV-UV HB spectroscopy has been extensively employed for neutral molecules produced in a supersonic jet to obtain the conformational specific electronic spectra. However, the HB spectroscopy has never been applied for ions in an ion trap because of the difficulty in distinguishing the fragment ions produced by the pump laser from those by the probe. Because all of the fragment ions produced by both of the pump and probe lasers are trapped again in the ion trap, the fragment ion signal by the pump converges into the fragment ion signal by the probe, which is irradiated with a certain time delay from the pump. However, we found that some fragment ions are not trapped but escape from the ion trap with the kinetic energy deposited from the photodissociation right after irradiation of the pump pulse and can be detected separately from those by the probe using a reflectron time-of-flight mass spectrometer next to the ion trap. Using this technique we successfully

obtained the UV-UV HB spectrum of dibenzo-18-crown-6-ether complexes with alkali metal cations and confirmed the presence of only a single conformational isomer for each of those complex ions in the gas phase.



일시: 2012년 4월 25~27일(수~금) 3일간

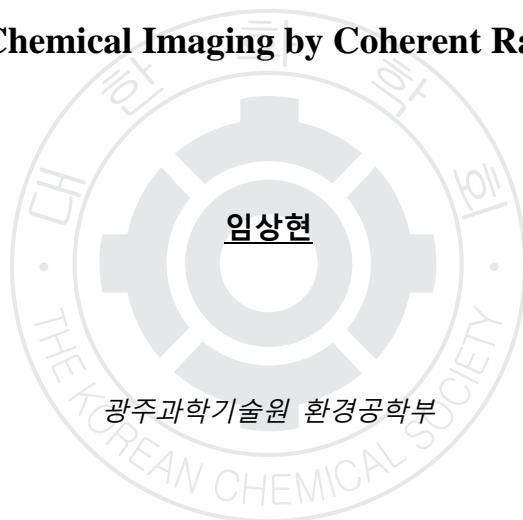
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발표코드: **PHYS2-2**

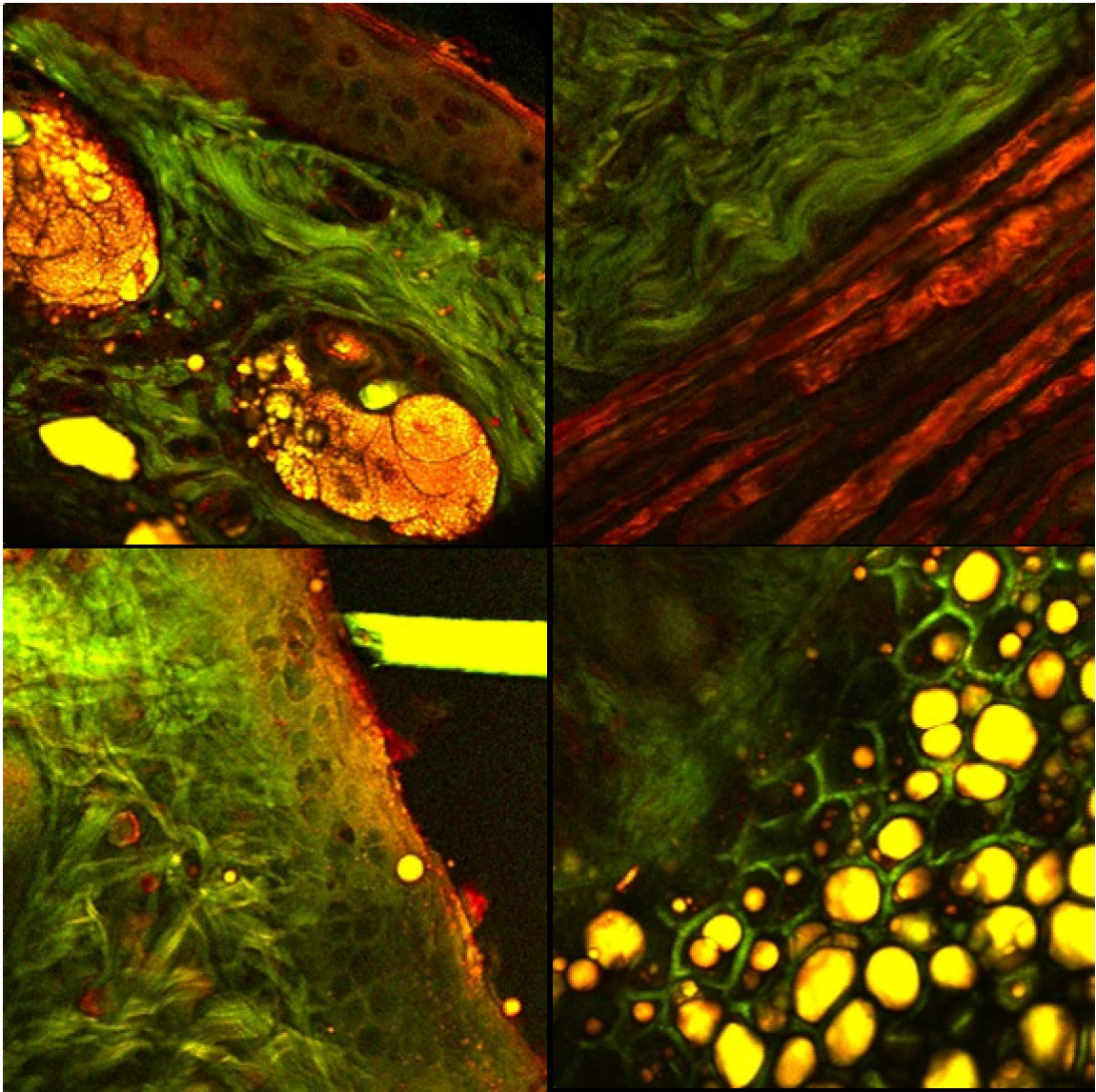
발표분야: New Trends in Physical Chemistry: Young Physical Chemist Symposium

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 최명룡

## Bond-Selective Chemical Imaging by Coherent Raman Microscopy



Coherent Raman Microscopy (CRM) can map out distributions of multiple chemical components via characteristic vibrational responses of each species. We acquire such chemical maps from unstained cells and tissues by analyzing CRM images obtained at a few vibrational frequencies. The spectral focusing method is utilized to achieve both high spectral resolution and fast vibrational frequency scanning. We have developed a novel image processing protocol to generate background-free color images, where the color code represents the relative distributions of protein and lipid and the brightness corresponds to sample concentrations. Preliminary CRM images from various animal tissues show great promises for its label-free histology applications. I will also discuss remaining technical issues and future development directions.



TEAN CHEMICAL

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS2-3**

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

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 최명룡

## 이차원 적외선 분광학을 이용한 단백질의 구조 동역학연구



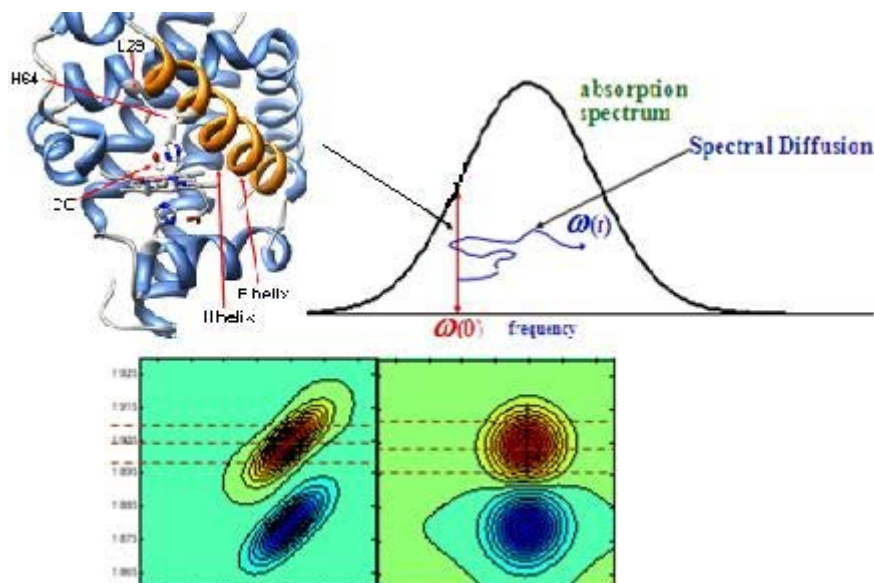
곽경원

중앙대 화학과

3 차 비선형 분광학의 한 방법인 초고속 적외선 이차원 분광법은 열적 평형상태에서 일어나는 단백질과 같은 생체분자의 빠른 구조 동역학을 연구할 수 있는 가장 좋은 분광법이다. 용액 상에서의 구조 동역학에 대한 연구는 이차원 분광 스펙트럼의 시간에 따른 변화를 관측함으로써 이루어진다. 이러한 스펙트럼의 변화는 실험에서 관측되는 분자 진동수의 변화에 의해서 유발된다. 하지만 다양한 종류의 스펙트럼의 모양을 변화시키는 요인들이 스펙트럼 모양의 분석을 통하여 진동수 변화와 동역학의 분자수준의 기술을 연결하는 진동수-진동수 상관함수(Frequency-frequency correlation function)의 정확한 결정을 어렵게 만든다. 또한 넓은 선폼을 가지는 적외선 스펙트럼에서 각기 다른 진동수 영역에 따라 달라지는 동역학을 개별적으로 관측하는 것도 스펙트럼의 모양을 관측해서는 불가능하다. 이러한 약점들을 극복하고자 이차원 분광스펙트럼으로부터 진동수-진동수 상관함수를 직접적으로 얻어내는 이론적 방법이 개발되었다. 이 새로운 방법의



실험으로부터의 관측대상은 스펙트럼 모양의 변화가 아니라 이차원 분광 스펙트럼의 중심부를 통과하는 중심선의 기울기이다. 이러한 기울기의 변화가 진동수-진동수 상관함수와 직접적으로 비례한다는 것이 이론적으로 보여지고 있다. 또한 이러한 새로운 중심선 기울기의 측정은 실험적 제한으로부터 유발되는 여러 가지 오차요인들에 무관함이 입증되어졌다. 이러한 진동수 기울기의 측정은 근본적으로 스펙트럼의 모양변화에서 동역학을 연구하던 것과는 다르게 이차원 스펙트럼의 각 슬라이스 스펙트럼의 봉우리 위치에서 실험적 정보를 얻기 때문에 여러 가지 스펙트럼의 모양변화를 유발하는 오차원인으로부터 자유롭고 정확한 진동수-진동수 상관함수의 측정을 도와줌으로써 이차원 분광법을 이용한 동역학 연구에 가장 좋은 분석방법을 제공하고 있다. 본 발표에서는 새롭게 개발된 구조 동역학을 분석하는 방법의 장점을 소개하고 단백질의 구조 동역학 분석에 응용된 결과들을 소개한다.



AN CHEMICAL



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS2-4**

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

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 권찬호

## Unimolecular Dissociation of Peptide Ions Facilitated by Laser-induced Surface Heating

한상윤

한국표준과학연구원 나노바이오통합연구단

We investigated the mechanical aspects involved in laser-induced thermal desorption of peptides from flat surfaces, in pursuit of new ionization that may offer an alternative to the conventional MALDI method. A comparative study on laser desorption/ionization (LDI) from surfaces with different thermal properties was carried out. In addition, the internal energies of resulting LDI ions were determined using a series of thermometry preformed ions, which was also compared with the MALDI method. The study revealed that thermal desorption promoted by laser-induced surface heating is the main driving force for the observed LDI processes of thermally labile molecules with large molecular masses. The results also indicated that laser-induced thermal desorption can further provide a means to increase the internal energies of generated peptide ions, giving rise to unimolecular decomposition of peptide ions. This work demonstrates that the thermal mechanism is indeed important for LDI of thermally labile molecules, and can also offer

a way to cause a post-source decay, which is suitable for peptide sequencing using TOF/TOF mass spectrometry.



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장소: 일산KINTEX

발표코드: PHYS2-5

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

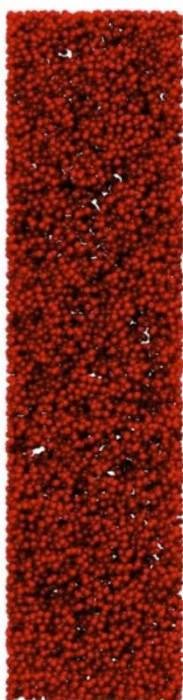
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 권찬호

## **CROWDING-INDUCED PHASE SEPARATION OF SELF-ASSOCIATING PARTICLES: IMPLICATIONS TO NUCLEAR COMPARTMENTALIZATION**

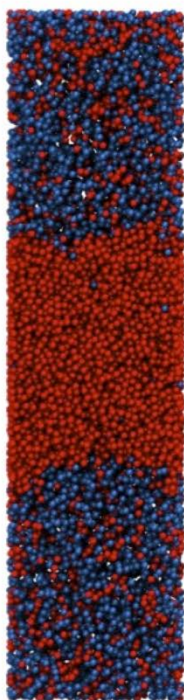
김준수

이화여대 화학나노과학과

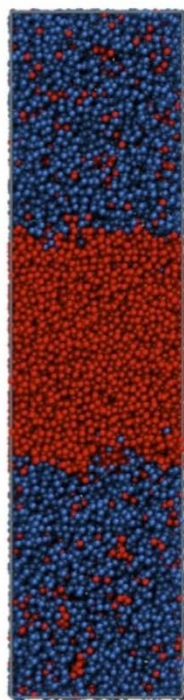
세포내의 혼잡한 환경은 세포내의 구조체 형성과 그 기능에 큰 영향을 미친다. 본 연구에서는 컴퓨터 시뮬레이션을 통해서 Lennard-Jones (LJ) 입자들의 상분리가 혼잡한 환경에 의해 어떤 영향을 받는지 연구하였다. 세포내의 혼잡한 환경을 묘사하기 위해서, 상분리하는 LJ 입자들 외에 추가적으로 여러가지 상호작용력을 가지는 입자들을 더해주면서 LJ 입자들의 상분리 변화를 연구하였는데, 이러한 혼잡 물질들의 존재로 인하여 LJ 입자들의 상분리가 촉진되는 것을 관찰할 수 있었다. LJ 입자의 상분리 현상과 세포핵 내의 구조체 형성의 유사성을 바탕으로, 혼잡한 세포내의 환경이 세포핵 내의 구조체 형성에 중요한 영향을 미친다는 것을 결론지을 수 있었다.



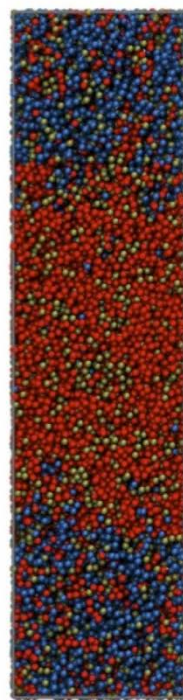
(a) No  
Crowding



(b) Repulsive  
 $\phi_B = 0.05$



(c) Repulsive  
 $\phi_B = 0.10$



(d) Mixed  
 $\phi_B = 0.05$   
 $\phi_C = 0.05$



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장소: 일산KINTEX

발표코드: ANAL1-8

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 분과기념강연, 발표일시: 목 17:00, 좌장: 이광필

## Studying Structures and Conformation Dynamics of Proteins Using Spectrometric Analysis



김준곤

포항공과대 화학과

In this presentation, we provide our on-going studies of structural dynamics of proteins using supramolecular chemistry and spectrometric techniques. Cucurbit[6]uril (CB[6]) and 18-crown-6 (18C6) are neutral cyclic molecules, which are efficient host molecules in molecular recognition and have high affinity for positively charged or cationic compounds. We have investigated the host-guest chemistry of CB[6] and 18C6 to lysine residues of proteins and its applications to study protein structure dynamics using various spectrometric techniques including mass spectrometry, ion mobility mass spectrometry, circular dichroism spectrometry, and fluorescence spectrometry. For example, the propensity of a series of isobaric poly-alanine based peptides with a Lys to form a helix in the gas phase is improved via host-guest chemistry with 18C6. Low energy collision induced dissociation of a CB[6]-protein complex yields highly selective fragments and additional MS<sub>n</sub> spectra reveal details of the CB[6] binding sites, which

allow us to deduce the protein structures and their population in the solution phase. Further applications of supramolecular chemistry related to controlling protein structure dynamics will be discussed.



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장소: 일산KINTEX

발표코드: ANAL1-1

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김성환

## **Nanomaterial-Assisted Electrochemiluminescence and Surface-Enhanced Raman Scattering toward Ultrasensitive Biosensor**

오정욱 김하석<sup>1</sup> 남좌민

서울대 화학부 <sup>1</sup>대구경북과학기술원 에너지시스템학과

Nanomaterial offers tremendous potential for the development of the optical signal enhancement due to its characteristic property. Electrogenenerated chemiluminescence (ECL) and surface-enhanced Raman scattering (SERS) are very promising tools for ultrasensitive biosensors. The ECL signal was significantly enhanced by the dendritically conjugated dye-doped silica nanoparticles and nanoglass patterned electrode. Nanogap-imbedded metal core-shell structure generated reproducible and highly enhancing SERS signal, which can be applicable to the ultrasensitive biosensor.

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발표코드: ANAL1-2

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김성환

## Supramolecular Electrochemistry for the Design of a Highly-Sensitive Biosensor

신익수 홍종인

서울대 화학부

Though significant advances have been made in supramolecular recognition, most of researches are focused on their photochemical changes upon target recognition. If the chemical probe is manipulated via electronic operation so that the binding event for a specific target is programmed or read out via electronic signal, one can develop molecular-level electronic sensors. Electrochemistry can provide the answer to this requirement, since electrons/holes, besides supplying the energy needed to make a device work, can also be useful to “read” the state of the system and thus to control and monitor the operation of the device. In the talk, electrochemically sensing approach using supramolecular probes will be discussed. Some results of supramolecular electrochemical sensing investigated in our laboratory will be reviewed.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ANAL1-3

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 김성환

## **An ultrathin platinum film as a novel chemodosimetric platform**

**김양래 정택동**

서울대 화학부

Chemodosimeters on an ultrathin platinum film have been successfully used as molecular switches for the fluorescent sensing of target ions. In addition, the colorimetric response of chemodosimeters-immobilized platinum film can be detected by the naked eye because platinum film displays optical transparency in the visible spectral region. Electrochemically controlled release of chemodosimeters attached to patterned platinum film is also confirmed using fluorescence and impedance methods.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ANAL1-4

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김성환

## Enzymatic Digestion of Single-DNA Molecules in Nanopores

이승아 강성호

경희대 응용화학과

Enzyme digestion of single DNA molecules in nanopores was directly observed in real time at the single-molecule level. The platform within solid-state nanoporous membrane was used to trap or entrap the individual lambda-DNA molecules labeled with the fluorescent dye, YOYO-1, and enzyme molecules. The digestion rates calculated from the decrease in fluorescence intensity showed different values according to the environment of nanopores. For example, when one end of the DNA molecule was inserted into a nanopore, it was possible to monitor the digestion process outside, near and inside the pore, where the individual DNA molecules showed different characteristic digestion rates. Enzymatic digestion at the chemisorbed nanopores such as L-cysteine or mercaptoethanol also exhibited different rates. These results provide that enzymatic digestion depend on environment as chemical property of the surface or steric restrictions.

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장소: 일산KINTEX

발표코드: ANAL1-5

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 이광필

**[발표취소] Recent advances in oil spill environmental forensics**



임운혁

한국해양연구원 남해특성연구부

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ANAL1-6

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 이광필

## 일회용 전기삼투펌프의 활용

신운섭

서강대 화학과/바이오융합협동과정/ 이오프로우㈜

Ag/Ag<sub>2</sub>O 전극의 도입으로 가스발생 없이 낮은 전압에서 안정되게 작동되는 전기삼투펌프(electroosmotic pump)의 구현이 가능했다. 예를 들어 두께 2 mm, 지름 8 mm의 펌프는 1 전자당 14,000 개의 물분자의 이동을 가능케 하였고, 0.3~2.0 V를 걸었을 때 5~40  $\mu$ L min<sup>-1</sup>의 유속을 가능케 하였다. 이 펌프는 Ag/Ag<sub>2</sub>O가 입혀진 다공성탄소전극과 실리카 멤브레인으로 구성되어 있기 때문에 일회용으로 사용할 수 있을 정도의 경제성을 가진다. 이는 약물전달, 미세유체제어 등을 통해 의료 및 환경 현장에 다양한 활용이 가능하다. 본 발표에서는 원리 및 성능에 대하여 논의한 후 다양한 응용 분야에 대하여 설명할 것이다. 문헌; (1) Shin, W.; Lee, J. M.; Nagarale, R. K.; Shin, S. J.; Heller, A. J. Am. Chem. Soc. 2011, 133, 2374. (2) Shin, W.; Zhu, E.; Nagarale, R. K.; Kim, C. H.; Lee, J. M.; Shin, S. J.; Heller, A. Anal. Chem. 2011, 83, 5023. (3) Shin, W.; Shin, S. J.; Lee, J. M.; Nagarale, R. K.; Heller, A. Drug Deliv. and

Transl. Res. 2011, 1, 342. (4) Nagarale R. K.; Heller, A.; Shin, W. J. Electrochem. Society, 2012, 159, P14.



일시: 2012년 4월 25~27일(수~금) 3일간

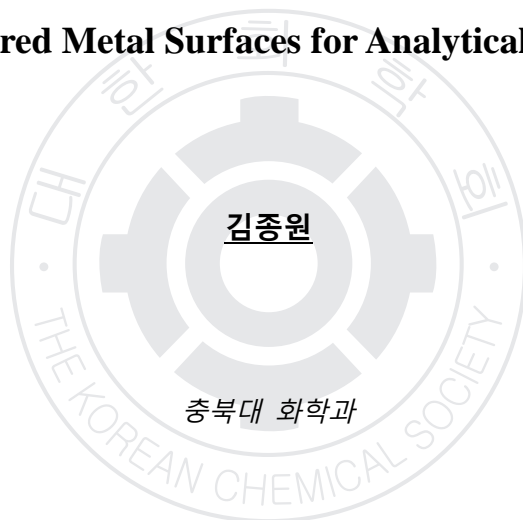
장소: 일산KINTEX

발표코드: ANAL1-7

발표분야: Recent Advances in Analytical Chemistry I

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 이광필

## Nanostructured Metal Surfaces for Analytical Applications



The fabrication of nanostructured metal surfaces has attracted intensive research interest due to their useful applications in heterogeneous catalysis, surface-enhanced Raman scattering (SERS)-based sensing, and electrocatalysis. Among various methods for the fabrication of nanostructured metal surfaces, electrochemical methods provide a simple route to construct well-defined and solid hierarchical metal nanostructures. Recently, a simple electrochemical deposition of nanostructured metal structures on a clean electrode surface in the absence of additives has received much attention. In this presentation, the simple electrochemical fabrication of various nanostructured metal surfaces such as nanoporous Au, dendritic Au rod, and highly faceted Pt structures and their analytical applications will be demonstrated. Nanoporous Au surfaces can be effectively used as substrates for laser desorption ionization-mass spectrometry (LDI-MS). Au and Pt nanostructures with faceted surface morphology exhibit high SERS activities and can be applied to electrochemical SERS systems. The structure dependent analytical activities and possible working mechanisms will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ANAL2-1

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 임재민

## Virus Outbreak in Biosensors and Bioelectronics



황인성 정택동

서울대 화학부

Bacteriophage fd is a filamentous virus whose coat proteins can be modified so that the virions can be accommodated to various materials, including proteins, nanoparticles, and electrodes. Multivalent phage display of antibody fragments or antibody binding domains can enhance the sensitivity of immunoassay by providing outstanding surface to volume ratio. However, multivalent display of fusion proteins either by minor or major coat proteins has limitations on the size of the guest proteins and requires laborious cloning procedure using phage vectors. Here, I will discuss about the new method on efficient multivalent display of proteins and demonstrate the effectiveness of the multivalent phage displaying system on biosensors.

일시: 2012년 4월 25~27일(수~금) 3일간

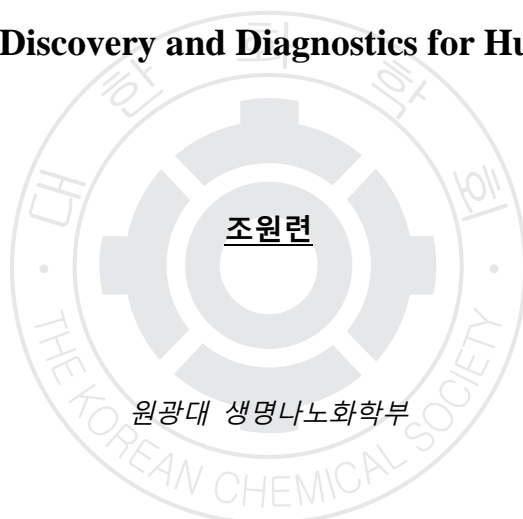
장소: 일산KINTEX

발표코드: ANAL2-2

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 임재민

## Biomarker Discovery and Diagnostics for Human Health



Targeted Glycoproteomics using affinity chromatography (AC) was used for identifying and quantifying cancer-related glycoproteins through cancer and normal plasma on breast cancer. AC has been used to isolate and identify potential cancer biomarker glycoproteins by targeting disease-associated glycans. Glycoproteins were selected from plasma of disease-free and breast cancer patients with narrow selectivity lectin AC column, an anti-Lewis x (Lex) AC column, and an anti-sialyl Lewis x (sLex) AC column. The captured protein fractions were identified and quantified through proteomics procedures. Some proteins were found to be potential breast cancer marker candidates based on their elevation in breast cancer patients. The potential of these candidates as cancer biomarkers remains to be validated in much larger, more diverse populations of breast cancer patients. Our ultimate goal is to develop simple and cheap diagnostics kits by discovering and quantifying disease-related glycoproteins through plasma samples. For this purpose/goal, the first step was to develop protein chips to select and compare proteins among disease samples and individual control ones using antibodies. The disease diagnostic kits have



several antibodies which should be immobilized on the inorganic surfaces with their native structures for their activities. Biocompatible polymer coatings were used to build up nanostructures on these chips and then applied to commercialized BioCD products.



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발표코드: ANAL2-3

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 임재민

## 고체시료의 신뢰성 있는 정량분석을 위한 광역조사 분광분석법

김재진 김재갑 정희일<sup>1</sup>

(재)전라남도생물산업진흥재단 천연자원연구원 <sup>1</sup>한양대 화학과

**Abstract** 물질의 구조 분석 및 정량분석 목적으로 널리 사용 되어지는 라만 분광법은, 시료의 전처리 과정을 거치지 않고 비파괴로 빠른 시간 안에 측정이 가능하다는 장점을 가지고 있다. 위와 같은 광역 조사 라만시스템의 성능을 평가하고 다양한 응용성을 제시하기 위하여 석유화학의 기초원료인 나프타의 조성분석, 캡슐 내 약효 성분 함량 비파괴 분석, 반도체 세정용액 조성의 온라인 실시간 분석, 분체 형태로 이동하고 있는 폴리에틸렌 펠렛의 온라인 밀도 분석을 시도하였다. 전체적으로 광역조사 라만시스템을 이용하여 정확도 및 재현성이 향상 된 정량분석이 가능하였다. 근적외선분광법 또한 다양한 고체시료들의 정량분석 목적으로 널리 이용되고 있다. 일반적으로 고체 시료를 측정 할 경우 간편하게 측정이 가능한 확산 반사 방법을 주로 사용하고 있다. 하지만 확산 반사 측정의 경우, 조사 된 빛이 시료 표면 근처에서만 확산 반사 되기 때문에 전체적인 시료의 조성을 대표하지 못 하는 경우가 자주 발생한다. 이런 문제점을 해결하기 위하여 광역조사

투과 근적외선 측정 시스템을 개발하였고, 폴리에틸렌 펠렛의 밀도 측정에 적용하였다. 본 연구를 통하여, 시료의 대표성을 높이면서 간단하게 측정 할 수 있는 광역조사 분광 시스템을 제안하였다. 특히 고체 시료 자체가 불균일 할 경우 광역조사 측정이 더욱 더 필요 할 것이다. 제안 된 시스템은 본 연구에서 제시 된 응용 분야 뿐만 아니라 농업, 제약, 고분자, 사료 등 다양한 분야에 응용이 가능 할 것으로 판단 된다.Acknowledgments 위 연구는 중소기업기술개발지원 사업의 하나인 연구장비활용기술개발 사업의 일환으로 진행하였습니다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ANAL2-4

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 팽기정

## 금속산화물을 활용한 고감도 바이오센서 적용 연구 (Study on highly sensitive biosensors based on metal oxides)

**최진섭**

인하대 화학공학과

본 발표에서는 나노구조를 가지고 있는 금속산화물을 전기화학적 전극으로 이용하고 DNA 및 immunosensor 적용하는 연구를 설명한다. 금속산화물을 제조하기 위한 방법으로는 금속을 전기화학적으로 산화시켜 다공성 구조의 산화물을 제조하는 양극산화 기법이 이용되었으며, 양극산화로 제조된 니오븀산화물, 아연산화물, 알루미늄 산화물에 10 nm 내외 두께의 gold 를 sputter 하여 전극을 형성시킨다. 합성 oligonucleotides (16S rDNA (E. Coli numbering: 190?208))의 probe 를 제조된 전극에 고정화하여 cyclic voltammogram 기법을 거쳐 DNA 센서 실험이 진행되었다. 이때 사용된 지시제는 methylene blue 가 이용되었다. immunosensor 센서 적용에 대한 실험으로는 sandwich type 의 연구가 진행되었다. biotinylated anti-mouse IgG 가 전극에 고정되었으며 target 물질인 mouse IgG 를 capture 하면 secondary antibody 인 ALP-conjugated anti-mouse IgG 의 alkalinephosphatase 가 4-Aminophenylphosphate 를

aminophenol 로 변화시켜 전기화학적 신호를 감지하는 기법이 이용되었다.본 연구에서 제시되는 방법의 장점은 저렴하며 대량생산이 가능한 양극산화 기법으로 나노구조를 제어하고 이를 활용하여 고감도 바이오센서에 적용하는 점이다.



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장소: 일산KINTEX

발표코드: ANAL2-5

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 팽기정

## **Nanoparticle-amplified SPR Biosensors for Biological and Environmental Applications**

이혜진

경북대 화학과

Surface plasmon resonance (SPR) measurements of biomolecular interactions on the surface of thin gold films have emerged as one of the leading techniques for the fast, in-situ detection of a wide spectrum of biological targets. In this talk, we will highlight our latest efforts to develop ultra-sensitive and selective SPR biosensors with different sizes and shapes of biofunctionalized nanoparticles for biomedical and environmental applications. For example, we compare the amplification performance of three different nanoparticle shapes (nanocages, nanorods and quasi-spherical nanoparticles) for the enhanced SPR detection of thrombin in conjunction with a thrombin specific aptamer chip created with a thiol-modified calix[4]arene derivative. In addition to increasing the nanoparticle size, with each type used here possessing at least one dimension at ~40?50 nm, changing the shape also introduces the possibility of adjusting the localized plasmon resonance properties of the nanoparticle over a much larger wavelength range. As a second example, we demonstrate a simple surface sandwich SPR analysis that uses a

combination of histidine coated quasi-spherical nanoparticles with a Ni(II) ion specific ligand, N-[5-(3'-maleimidopropylamido)-1-carboxypentyl]-iminodiacetic acid, coated SPR Au chip for the sub-ppb concentration range of Ni (II) ions.



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장소: 일산KINTEX

발표코드: ANAL2-6

발표분야: Recent Advances in Analytical Chemistry II

발표종류: 심포지엄, 발표일시: 금 11:50, 좌장: 팽기정

## **Development of LC/MS-based reference methods for food analysis: Combating matrix effects**

**김병주**

한국표준과학연구원 식품안전표준본부

LC/MS is more frequently used than before in food analysis field due to the high selectivity and sensitivity of this technique. However, analytical methods based on LC/MS usually suffer from matrix effects (ion suppression/enhancement), and ignoring these factors may cause sometimes strong biases in measurement results. Adopting isotope dilution techniques (using isotope labeled analogues of target analytes as internal standards) has been believed to be the solution for matrix effects. Our laboratory is developing reference methods for food analysis which can provide national standards to ensure reliability of food testing laboratories. Those reference methods are based on Isotope Dilution Mass Spectrometry (IDMS) in connection with chromatographic techniques such as LC because IDMS is known to provide accurate analytical results without systematic bias through the accurate correction of the recovery on target analytes along the sample clean up processes. However, we observed in many cases that matrix effects are not completely compensated when deuterated analogues are used as they have slightly different



chromatographic retention times from their corresponding target analytes and experience different ionization conditions. A few examples of those cases and solutions for these adverse effects will be presented. Solutions adopted were more rigorous sample clean-up and optimizing chromatographic separation. Recently, we adopted a standard addition method in combination with isotope dilution techniques for alternative solution when those strategies do not work



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO1-1

발표분야: Reactive oxygen species in age-related diseases

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 임태연

## Chemical 'omics' Approach for Understanding Protein Cysteine Oxidation by Reactive Oxygen Species (ROS)

서영호

계명대 약학대학

Oxidative cysteine modifications have emerged as a central mechanism for dynamic post-translational regulation of all major protein classes and correlate with many disease states. Elucidating the precise roles of cysteine oxidation in physiology and pathology presents a major challenge. Recent advances in chemical biology allow for the direct detection of specific cysteine oxoforms based on their distinct chemical attributes. In addition, new chemical reporters of cysteine oxidation have enabled in situ detection of labile modifications and improved proteomic analysis of redox-regulated proteins. Progress in the field of redox proteomics should advance our knowledge of regulatory mechanisms that involve oxidation of cysteine residues and lead to a better understanding of oxidative biochemistry in health and disease. Here we report on the development of chemical and immunochemical methods for detecting sulfenic acid, the initial oxidation product that results when a thiolate reacts with H<sub>2</sub>O<sub>2</sub>. Applying these approaches to several systems, including cancer cell lines, shows it can be used to monitor differences in

thiol redox status and reveals a diverse pattern of sulfenic acid modifications across different subtypes of breast tumors. These studies demonstrate the utility of these reagents for quantitatively profiling thiol oxidation associated with pathological conditions such as breast cancer and these strategies can be used as diagnostic tools for cancerous diseases.



일시: 2012년 4월 25~27일(수~금) 3일간

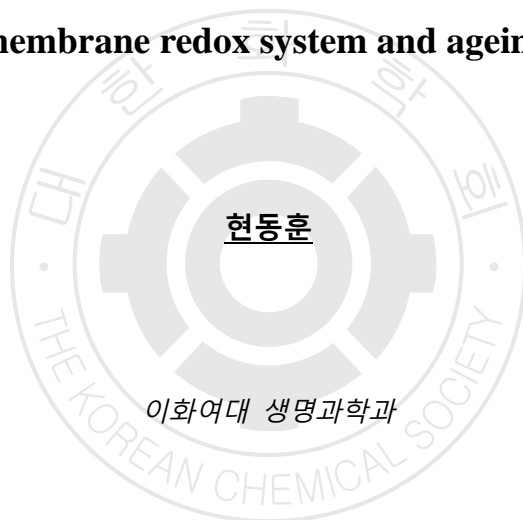
장소: 일산KINTEX

발표코드: BIO1-2

발표분야: Reactive oxygen species in age-related diseases

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 임태연

## The plasma membrane redox system and ageing intervention



Oxidative stress over time leads to the accumulation of damaged macromolecules and to profound physiological changes that are associated with age-related diseases including neurodegenerative diseases. The plasma membrane redox system (PMRS) appears to play a protective role during mitochondrial dysfunction to provide cells with a survival mechanism by lowering oxidative stress. The PMRS accomplishes this by producing more NAD(+) for glycolytic ATP production via transfer of electrons from intracellular reducing equivalents to extracellular acceptors. Activities of PMRS enzymes were selectively decreased in the PM from the hippocampus and cerebral cortex of 3xTgAD mice, an animal model of AD. However, they were elevated by caloric restriction (CR), a manipulation that protects the brain against aging and disease. A higher NAD(+)/NADH ratio and activation of adaptive stress response pathways are enhanced by the PMRS in neuroblastoma cells, enabling them to maintain redox homeostasis under conditions of energetic and proteotoxic stress. These findings have implications for the development of therapeutic interventions for neural tumors and neurodegenerative conditions.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO1-3

발표분야: Reactive oxygen species in age-related diseases

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 현동훈

## **Reduction of reactive oxygen speices by caloric restriction prevents the age-related thymic involution**

양현원

서울여대 생명환경공학과

Aging of thymus is characterized by reduction in naive T cell output together with progressive replacement of lymphostromal thymic zones with adipocytes. Determining how calorie restriction (CR), a prolongevity metabolic intervention, regulates thymic aging may allow identification of relevant mechanisms to prevent immunosenescence. Using a mouse model of chronic CR, we found that a reduction in age-related thymic adipogenic mechanism is coupled with maintenance of thymic function. The CR increased cellular density in the thymic cortex and medulla and preserved the epithelial signatures. Interestingly, CR prevented the age-related increase in epithelial-mesenchymal transition (EMT) regulators, FoxC2, and fibroblast-specific protein-1 (FSP-1), together with reduction in lipid-laden thymic fibroblasts. Additionally, CR specifically blocked the age-related elevation of thymic proadipogenic master regulator, peroxisome proliferator activated receptor gamma (PPARgamma), and its upstream activator xanthine-oxidoreductase (XOR). Furthermore, we found that specific inhibition of

PPARgamma in thymic stromal cells prevented their adipogenic transformation in an XOR-dependent mechanism. Furthermore, CR prevented the deterioration of the peripheral TCR repertoire diversity in older animals. Collectively, our findings demonstrate that reducing proadipogenic signaling in thymus via CR may promote thymopoiesis during aging.



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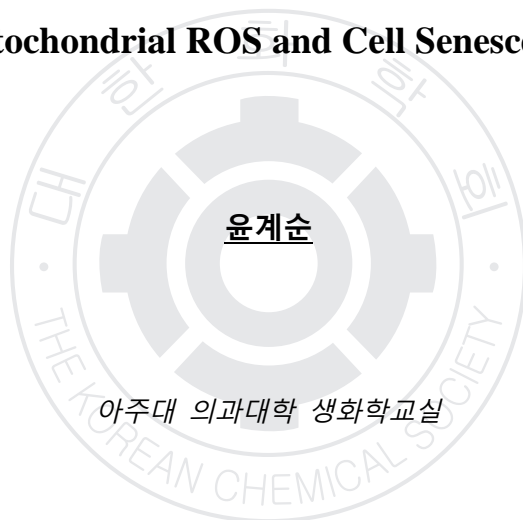
장소: 일산KINTEX

발표코드: BIO1-4

발표분야: Reactive oxygen species in age-related diseases

발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 현동훈

## Mitochondrial ROS and Cell Senescence



Functional defects of mitochondria have long been implicated in cellular aging process. However, its detailed underlying mechanism of how mitochondrial dysfunction is involved in cellular senescence remains unclear. Recently, we clearly demonstrated that respiratory defects are tightly linked with the prolonged generation of reactive oxygen species (ROS) by employing transforming growth factor  $\beta 1$  (TGF  $\beta 1$ ), a cytokine. TGF  $\beta 1$  induced senescence of Mv1Lu cell by persistently producing mitochondrial reactive oxygen species (ROS) through decreased complex IV activity. During the process glycogen synthase kinase 3 (GSK3) was progressively phosphorylated, corresponding well to the intracellular ROS generation profile. Unexpectedly, this GSK3 phosphorylation was found to be an upstream event of the ROS generation. Moreover, we found that GSK3 substantially exists in mitochondria of Mv1Lu cell and binds complex IV subunit 6b which has no electron carrier and is topologically located in the mitochondrial intermembrane space. Involvement of subunit 6b in controlling complex IV activity and overall respiration rate was proved with siRNA-mediated knockdown of subunit 6b. Finally, TGF  $\beta 1$

treatment decreased the binding of the subunit 6b to GSK3 and subunit 6b phosphorylation. Taken together, our results suggest that GSK3 inactivation is importantly involved in TGF  $\beta$ 1-induced complex IV defects through decreasing phosphorylation of the subunit 6b, thereby contributing to senescence-associated mitochondrial ROS generation.





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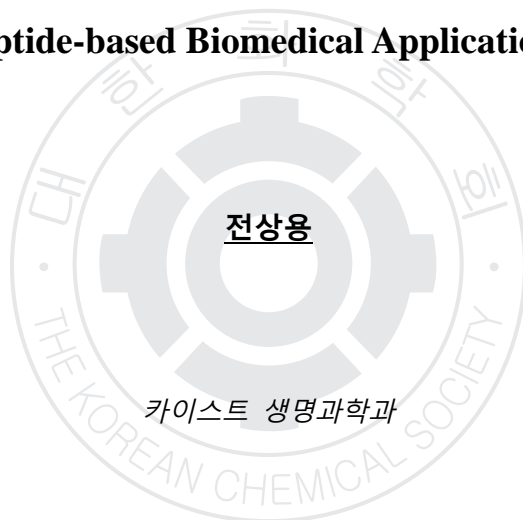
장소: 일산KINTEX

발표코드: BIO2-1

발표분야: Approaches of applied chemistry for translational research

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 최용두

## Aptide-based Biomedical Applications



Aptides, developed by us, are a novel class of high affinity and specificity peptides that offer the potential for use as diagnostic or drug candidates. In this lecture, I will show you a couple of aptide-based biomedical applications using cancer-specific aptides-nanoparticle conjugates. Two cancer-specific aptides (fibronectin EDB- and HER2-specific aptides, respectively) were conjugated with superparamagnetic iron oxide nanoparticles (SPIONs) with the aim of targeted cancer imaging by MRI. In vitro and in vivo experiments revealed that the aptide-SPION conjugates showed specific binding and/or accumulation to target cancer cells and tumors.

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장소: 일산KINTEX

발표코드: BIO2-2

발표분야: Approaches of applied chemistry for translational research

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 최용두

## Multi-direct Disease Metabolomics by TOF-SIMS: Gastric Cancer Case

이태걸

한국표준과학연구원 미래융합기술부

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) has been a useful tool to profile secondary ions from the near surface region of specimens with its high molecular specificity and submicron spatial resolution. However, the TOF-SIMS analysis of even a moderately large size of samples has been hampered due to the lack of tools for automatically analyzing the huge amount of TOF-SIMS data. Here, we present a computational platform to automatically identify and align peaks, find discriminatory ions, build a classifier, and construct networks describing differential metabolic pathways. To demonstrate the utility of the platform, we analyzed 43 datasets generated from seven gastric cancer and eight normal tissues using TOF-SIMS. A total of 87,138 ions were detected from the 43 datasets by TOF-SIMS. We selected and then aligned 1,286 ions. Among them, we found the 66 ions discriminating gastric cancer tissues from normal ones. Using these 66 ions, we then built a partial least square-discriminant analysis (PLS-DA) model resulting in a misclassification error rate of 0.024. Finally, network analysis of the 66

ions showed disregulation of amino acid metabolism in the gastric cancer tissues. The results show that the proposed framework was effective in analyzing TOF-SIMS data from a moderately large size of samples, resulting in discrimination of gastric cancer tissues from normal tissues and identification of biomarker candidates associated with the amino acid metabolism [1]. [1] Yun SJ, Park JW, Choi IJ, Kang B, Kim HK, Moon DW, Lee TG, Hwang D. TOFSIMS-P: A web-based platform for analysis of large-scale TOF-SIMS data. Anal. Chem., 2011, 83, 9298.



일시: 2012년 4월 25~27일(수~금) 3일간

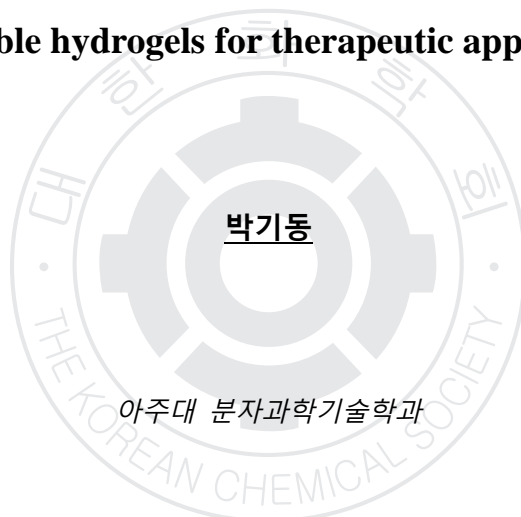
장소: 일산KINTEX

발표코드: BIO2-3

발표분야: Approaches of applied chemistry for translational research

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 최용두

## Injectable hydrogels for therapeutic applications



Injectable hydrogels have been paid much attention as an injectable matrix for therapeutic applications due to easy applications based on minimally invasive technique. Such a system makes cells, drugs and bioactive molecules easily incorporated in situ by a simply syringe injection of their aqueous solutions at target sites. Various types of hydrogels formed in situ through physical or chemical cross-linking reaction were reported. Among these reactions, enzymatic reaction using peroxidase has received much attention to fabricate in situ cross-linkable hydrogels due to biocompatibility and good controllability of the reaction rate. This cross-linking system enable hydrogels not only to be formed under mild conditions for short time period but also to be strengthened due to chemical cross-link, which are major issue in the development of in situ forming hydrogels. In addition, their physico-chemical properties can be controlled easily by varying the concentrations of catalysts. In this study, various kinds of in situ forming hydrogels via a peroxidase-mediated cross-linking reaction were developed as injectable matrices. To investigate the usefulness of the hydrogels as injectable materials for therapeutic applications, in vitro and in vivo studies

have been performed using various bioactive molecules, cells and animal models. Obtained results demonstrated that our enzyme-mediated injectable hydrogels are promising materials for therapeutic applications including tissue regeneration and drug delivery. Acknowledgements: This research was supported by grants from the Korea Science and Engineering Foundation, Ministry of Education, Science and Technology (MEST) (2011-0001805), and a National Research Foundation (NRF) grant funded by the Korea government (2010-0027776).



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO2-4

발표분야: Approaches of applied chemistry for translational research

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 최용두

## **Clinical use of near-infrared fluorescence: initial step in multimodal image-guided operation of cancer patient**

김석기

국립암센터 분자영상치료연구과

Although various 3D medical imaging techniques, such as CT, MRI, and ultrasound, have become available during the last few decades, surgeons primarily operate by the help of vision and touch. As these advanced imaging techniques could not be directly applied to the operation, other intra-operative/ real-time technology should be developed and applied. Radioisotope and fluorophore could be used for intra-operative guidance. At present, the most popular technique for intra-operative guidance is radio-guided method. Radio-guided method is the 'gold-standard' in clinical studies but has some drawbacks. It cannot offer visual information in the operation room. Whereas, fluorescence technique could give excellent visual information and it is suitable for the intra-operative usage. Although fluorescence has much potentiality, low energy photons associated with fluorescence imaging suffer significant attenuation by tissue absorption and scattering properties, as well as significant levels of auto-fluorescence. Near-infrared (NIR) fluorescence imaging, recently introduced, may have little or no auto-fluorescence as well

as significant tissue penetration. Breast cancer is one of the most important women cancers in Korea. It is clinically important and relatively easy to apply multimodal image-guided operation to the breast cancer. We developed multimodal approaches for sentinel lymph node mapping using dye, NIR fluorescence and radioisotope. We started clinical research for this multimodal sentinel lymph node mapping. We expect to disclose our method to be more surgeon-friendly and diagnostically better than conventional method.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO2-5

발표분야: Approaches of applied chemistry for translational research

발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: 최용두

## Smart nano-photomedicine for in vivo molecular imaging and photodynamic therapy of cancers



최용두

국립암센터 융합기술연구부 분자영상 치료연구과

Theranostic agents for simultaneous cancer diagnosis and therapy have received a great deal of attention. In particular, a variety of nanomedicines have been designed as theranostics due to their advantageous properties, which include a relatively large surface area for tagging targeting ligands and contrast agents, enhanced permeation and retention (EPR) in the circulatory system, and size- and shape-dependant optical and magnetic properties. Recently, gold nanorods (GNRs) have attracted attention for their interesting optical properties, including some which may have biomedical applications. Therefore, we have developed various types of gold nanorod-based theranostics for molecular imaging and subsequent photodynamic and/or photothermal therapy of cancers. We prepared photosensitizers and gold nanorod complex along with targeting ligands. Thereby we could detect tumors in vivo with high sensitivity and good signal-to-background ratio, and treat the detected tumors through photodynamic and photothermal therapy.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN1-1

발표분야: KCS-RSC joint symposium- Chemical Biology

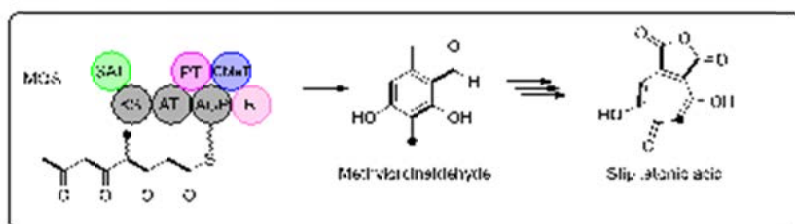
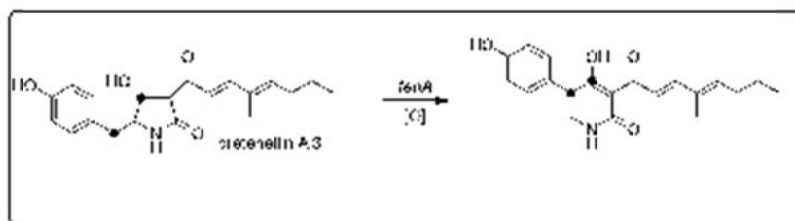
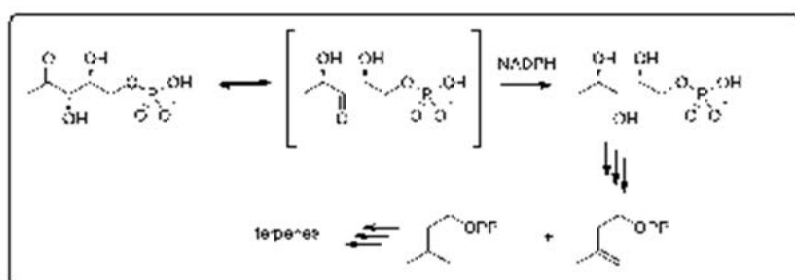
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 박승범

## Redox Rearrangements in Biosynthesis

Russell J. Cox

*School of Chemistry, University of Bristol.*

Redox rearrangements are remarkable reactions responsible for the construction of key structural motifs in natural products. Three examples will be discussed: The introduction of methyl branches by reductive rearrangement during the biosynthesis of the terpene precursors IPP and DMAPP; The oxidative rearrangement of tetramic acids to 2-pyridones; and the oxidative rearrangement responsible for tropolone biosynthesis in fungi. [Figure 1.] *Three redox rearrangements in biosynthesis.*



일시: 2012년 4월 25~27일(수~금) 3일간

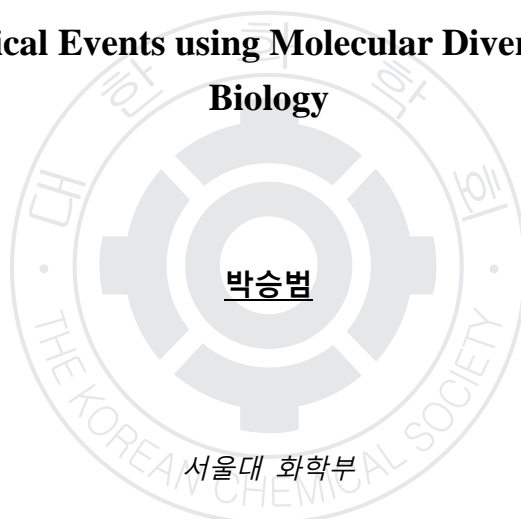
장소: 일산KINTEX

발표코드: ORGN1-2

발표분야: KCS-RSC joint symposium- Chemical Biology

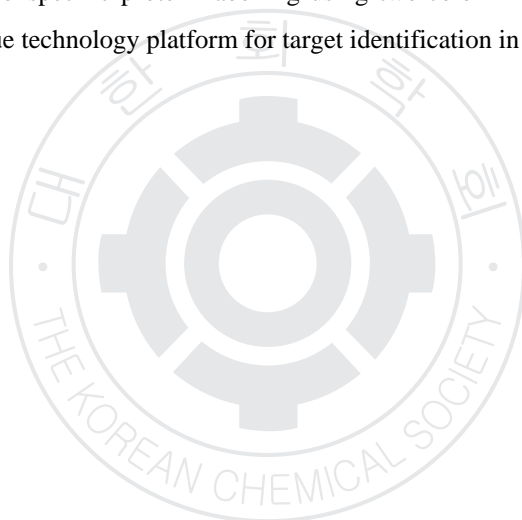
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 박승범

## Dissecting Biological Events using Molecular Diversity and Chemical Biology



A study of 9-aryl-1,2-dihydropyrrolo[3,4-b]indolizin-3-one, we name it Seoul-Fluor, were presented in this presentation. During our continuous efforts on the construction of drug-like small-molecule libraries using diversity-oriented synthesis (DOS) strategy, we identified a novel fluorescent core skeleton, 1,2-dihydropyrrolo[3,4-b]indolizin-3-one. Guiding with computational simulation, 24 fluorescent compounds library were constructed in combinatorial fashion, and which covers the full-color range. Further bioapplication of these fluorescent compounds was successfully demonstrated in the immunofluorescent staining. After discovery of Seoul-Fluor, we analyzed the fluorescent core skeleton more systematically and extensively. Using a concise and practical one-pot synthetic procedure, a 44-member library of new fluorescent compounds was synthesized. The systematic perturbation of electronic densities on the specific positions of Seoul-Fluor, guided with the Hammett constant, allows tuning the emission wavelength in full-color range. Furthermore, on the basis of these observations and a computational

analysis, we extracted a simple first-order correlation of emission wavelength with the theoretical calculation and accurately predicted the emission wavelength of Seoul-Fluors prior to their synthesis. Therefore, we clearly demonstrated that Seoul-Fluor could provide a powerful gateway for the generation of desired fluorescent probes without the need for tiresome synthesis and trial-and-error process. In addition, we developed a new technology platform, fluorescence difference in two-dimensional gel electrophoresis (FITGE), which aims to preserve protein-small molecule interactions under the intact cellular environment. We also demonstrated its application for the target identification of a new antitumor agent screened from our in-house small-molecule library. After a series of failures using conventional target ID methods, we successfully identified the protein target of anti-proliferative compound 1 with FITGE only under the live cell condition and observed the environment-dependent binding events of a functional small molecule by direct comparison between live cells and cell lysates. Even though it still requires the synthesis of bioactive probes with photo-crosslinker moiety, the FITGE strategy can address the current limitation of conventional target identification methods and significantly enhance the possibility of target ID via covalent capturing of target proteins under the intact cellular environment and the efficient exclusion of nonspecific protein labelling using two-color 2DGE. We believe our FITGE strategy can provide a unique technology platform for target identification in live cells.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN1-3

발표분야: KCS-RSC joint symposium- Chemical Biology

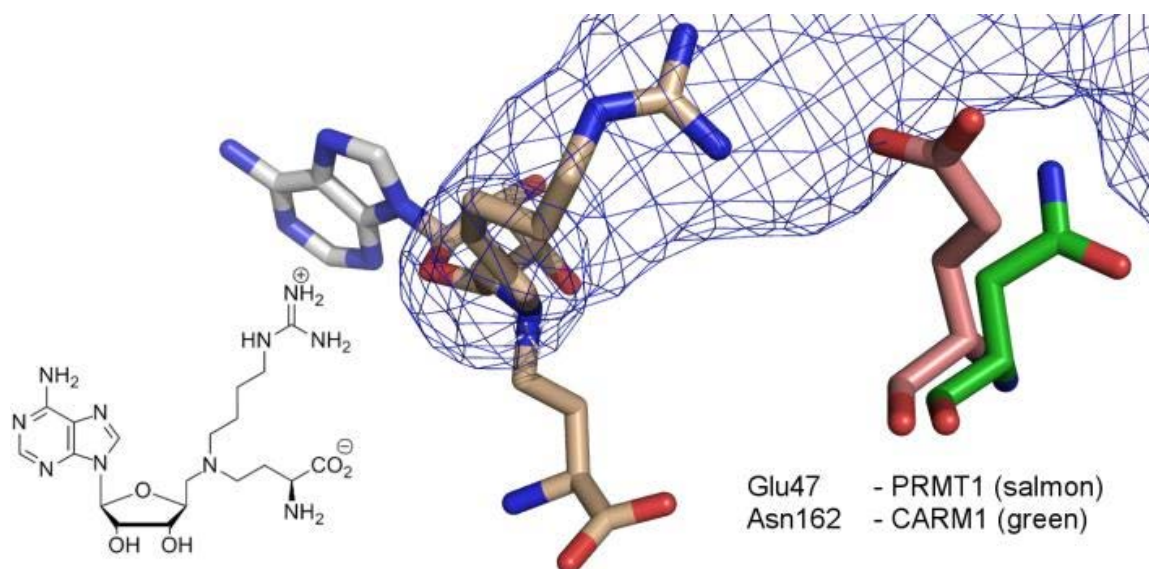
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박승범

## Chemical Probes inspired by cellular co-factors

James Dowden

School of Chemistry, University of Nottingham

Cellular co-factors provide a convenient, but challenging entry point for the design of small molecules that modulate the activity of novel biological targets. For example, we are currently focussed on developing modulators of protein arginine methyltransferases (PRMTs) since they may have a defining role in epigenetic regulation of cell status. This talk will outline our development of potential PRMT inhibitors designed to occupy binding sites for the co-factor AdoMet and the arginine protein substrate, some of which were found to discriminate between two PRMT enzyme family members, PRMT1 and CARM1. [Fig.] *That the molecule above inhibits PRMT1 but not CARM1 may be explained by a key difference in respective amino acids at the binding site, specifically an electrostatic interaction with Glu47 (PRMT1, salmon), but not Asn162 (CARM1, green). Docking and overlay reveals the inhibitor occupying both co-factor site and substrate channels (blue mesh) close to these divergent amino acids*



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN1-4

발표분야: KCS-RSC joint symposium- Chemical Biology

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 박승범

## Small Molecules That Regulate Biological Processes

Nur Elida M.Z 신인재<sup>1</sup> 김재호

아주대 분자과학기술학과 <sup>1</sup>연세대 화학과

Neurons are not regenerated effectively and their injury causes neurodegenerative diseases. These diseases may be treated by the transplantation of neurons derived from stem cells. However, ethical and technical issues restrict stem cell therapies. A more attractive approach is the use of small molecules with the capacity to induce neurogenesis from easily available cells or tissues. We discovered the first such molecule, neurodazine, identified by screening an imidazole library with C2C12 myoblasts. Further analyses show that neurodazine promotes the expression of neuron-specific markers in treated C2C12 cells. In addition, the use of neurodazines in conjunction with a microtubule-destabilizing agent allows neurogenic conversion of both differentiated immature myotubes and mature skeletal muscle. Apoptosis (or programmed cell death) is a fundamental biological process that regulates a variety of normal physiological processes. Since apoptosis is involved in both normal physiology and various human diseases, research on apoptosis has become a central area in basic biological studies and the development of therapeutic agents. We have identified a small molecule that interacts with Hsc70 and Hsp70. This

small molecule induces apoptosis in cells and holds considerable potential as a powerful cancer therapeutic in addition to aiding our understanding of the molecular basis of Hsp70-related apoptotic processes. We have also developed a new chemical modulator that can help gain more detailed insight into heart development. This compound induces abnormal heart development, including the formation of pipe-like heart structures and enlarged pericardiac sacs. In this presentation, I will discuss our current progress of small molecules that affect cell differentiation and development.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN1-5

발표분야: KCS-RSC joint symposium- Chemical Biology

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 박승범

## The Search for New Antibacterials Using Diversity-Oriented Synthesis

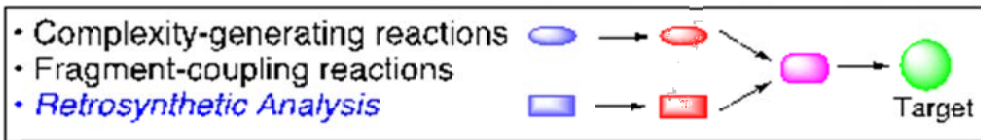
**David R Spring**

*Department of Chemistry, University of Cambridge*

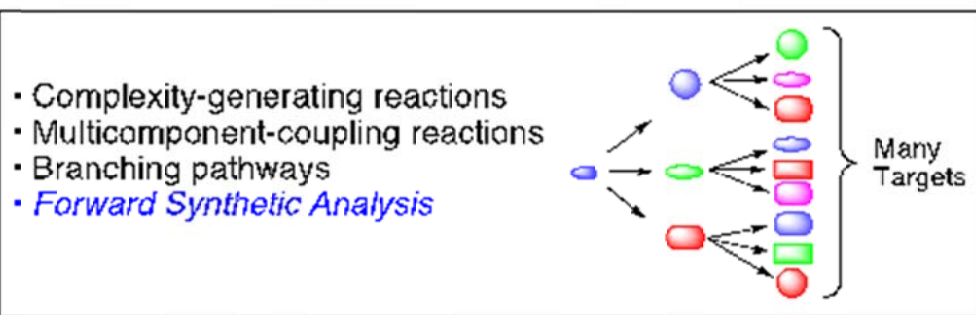
The synthesis of structurally diverse and structurally complex collections of small molecules remains a major challenge to synthetic chemists. We illustrate the diversity-oriented synthesis (DOS) of small molecule collections to directly address this need, directed towards the search for new antibacterials with novel modes of action.[1,2] Drug discovery programs use large collections of small molecules to look for lead structures from biological assays. The success of this approach depends upon the collection of compounds (and luck). Chemists are demanding the rapid preparation of collections of highly pure small molecules that are structurally diverse. Combinatorial chemistry has answered this need to an extent; however, most combinatorial libraries produce compounds of very limited structural diversity. Since only building block diversity has been employed the resulting compounds have the same stereochemistry, functional groups and scaffold. This is not desired if you want a diverse library, such as when you are looking for a phenotype in a biological screen, especially where there is no known small molecule hit. *Figure 1*. Comparison of Target-Oriented Synthesis versus Diversity-Oriented Synthesis. In contrast to target-oriented synthesis (TOS), DOS is not aimed at one particular target, and retrosynthetic analysis is

therefore not applicable directly (Figure 1). Instead we need to identify complexity-generating reactions and pathways that give structural diversity. In order to design a synthetic pathway leading to a collection of compounds with different scaffolds requires the use of branch points, where a common substrate is used in different reactions that give different skeletons.

### Target-Oriented Synthesis: **Convergent**



### Diversity-Oriented Synthesis: **Divergent**



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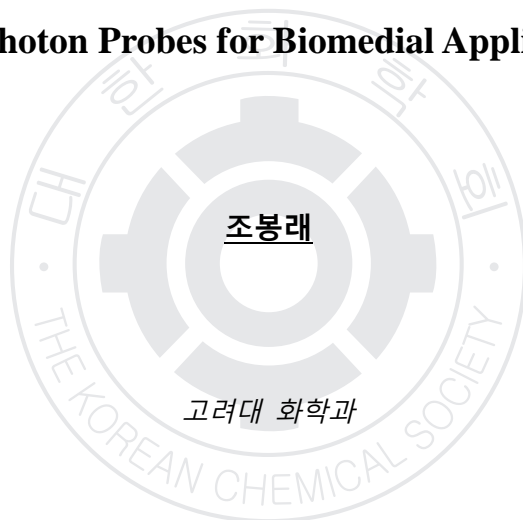
장소: 일산KINTEX

발표코드: ORGN1-6

발표분야: KCS-RSC joint symposium- Chemical Biology

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 박승범

## Two-Photon Probes for Biomedical Applications



Optical imaging with fluorescence microscopy is a vital tool in the study of living systems. The most common method for cell imaging, one-photon microscopy (OPM), uses a single photon of higher energy to excite the fluorophore. However, two-photon microscopy (TPM), which uses two photons of lower energy as the excitation source, is growing in popularity among biologists because of several distinct advantages. Using TPM, researchers can image intact tissue for a long period of time with minimum interference from tissue preparation artifacts, self-absorption, autofluorescence, photobleaching, and photodamage. However, to make TPM a more versatile tool in biology, researchers need a wider variety of two-photon probes for specific applications. In this context, we have developed a series of two-photon probes for the metal ions, acidic vesicles, membrane, and two-photon glucose tracers having 2-acetyl-6-aminonaphthalene and its derivatives as the fluorophore and receptors for the target ions or membrane or glucose, by considering following requirements: significant two-photon cross section for the bright image, receptors (sensing moiety) that trigger the emission of the two photon excited fluorescence upon binding

with the ions or membrane in the living system, sensitivity to the polarity of the environment for the selective detection of cytosolic and membrane-bound probes, appreciable water solubility to stain the cells and tissues, cell permeability, high photostability for a long term imaging. In this seminar, I will briefly describe our recent results on two-photon probes for metal ions, thiols, cancer cells, pH, and their applications in biology and medicine.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN2-1

발표분야: Current trends in Organic Chemistry: catalysis, structure and function

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 금교창

## Developing new flexibility-generating synthetic strategies using transition metal catalysis



이영호

포항공과대 화학과

Introducing molecular diversity in a controlled manner represents one of the most challenging goals in organic synthesis. Developing new chemoselective reactions is of crucial importance in this regard. In this presentation, our recent efforts in this area will be briefly summarized. New strategies as well as the synthetic application will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN2-2

발표분야: Current trends in Organic Chemistry: catalysis, structure and function

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 윤소원

## Functionalized Chiral Porous MOFs as a Mimic and Compilation of Enzyme Active Sites

정낙철

고려대 화학과

Chiral metal-organic frameworks (MOFs), which can be assembled using a modular approach with chiral organic links and metal ions, are of interest for applications in enantioselective separation and catalysis being especially important for the chemical and pharmaceutical industries. Conceptually, these materials are envisioned as a compilation of enzyme active sites if the pores bear the proper functionality. We have designed and synthesized a chiral metal-organic framework, (S)-KUMOF-1 ( $\text{Cu}_2(\text{S})-1)_2(\text{H}_2\text{O})_2 \cdot 1/4$  2,20-dihydroxy-6,60-dimethyl(1,10-biphenyl)-4,40-dicarboxylate) of which a non-interpenetrating NbO type framework provides a spacious pore ( $2 \times 2 \times 2 \text{ nm}^3$ ) and is equipped with potential catalytic sites exposed into the pore. With this in hand, we were able to delineate an underlying principle in building up a practically useful chiral MOF with reasonable size of cavities. And also, an unambiguous evidence for that the reactions took place inside the structure was obtained. More details of fundamental issues will be illustrated with a couple of reactions, the carbonyl-ene reaction and hetero Diles-Alder reaction.

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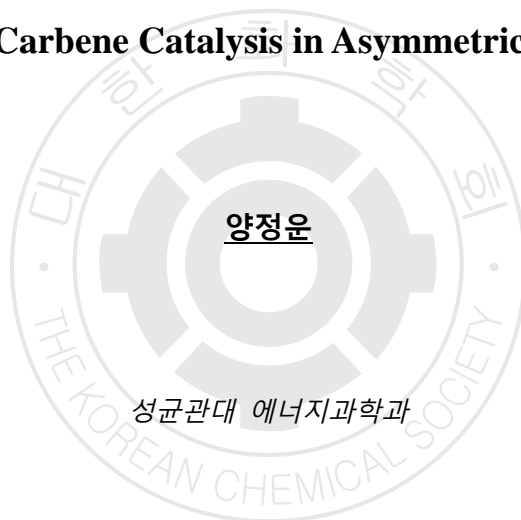
장소: 일산KINTEX

발표코드: ORGN2-3

발표분야: Current trends in Organic Chemistry: catalysis, structure and function

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 윤소원

## N-Heterocyclic Carbene Catalysis in Asymmetric Organocatalysis



N-Heterocyclic carbenes (NHCs) are one of the most promising classes of organocatalysts and can promote Umpolung reactivities of aldehydes. These strategies have been utilized in (asymmetric) benzoin condensation reactions and Stetter reactions. In this presentation, I'd like to introduce the first regioselective intermolecular crossed-acyloin condensation of acetaldehyde as a biomimetic acylanion source and asymmetric intermolecular Stetter reaction with *trans*-chalcone derivatives. An interesting domino reaction in the synthesis of carboxylic acids involving a combination of benzoin condensation reaction of aldehydes using NHC catalysts and oxidative cleavage reaction of benzoin using NaH-O<sub>2</sub> system will also be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN2-4

발표분야: Current trends in Organic Chemistry: catalysis, structure and function

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 민선준

## **Tandem reaction strategies using reactive intermediates in organic synthesis**

이희윤

KAIST 화학과

The concept of green chemistry emerged as the main focus of the 21st century chemistry. In total synthesis of target molecules, this concept was introduced as the aim of the synthesis, "ideal synthesis". One of the synthetic strategies toward the "ideal synthesis" in the organic synthesis is fulfilling the step economy of the synthesis which aims at the synthesis with as little synthetic operation as possible. To increase the complexity of the product from a starting material in one operation, many synthetic strategies have been developed. One of those strategies is the tandem reaction strategy which is designed to perform several reaction steps in a single operation. In this seminar, tandem reaction strategies using reactive intermediates such as free radicals or carbenes will be introduced and the application of such synthetic strategies to the total synthesis of natural products will be discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

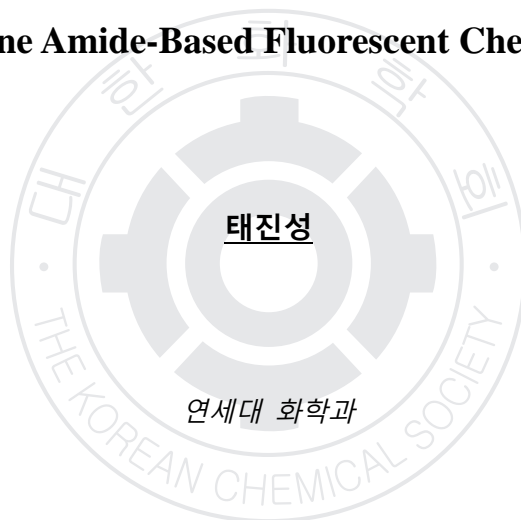
장소: 일산KINTEX

발표코드: ORGN2-5

발표분야: Current trends in Organic Chemistry: catalysis, structure and function

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 민선준

## Rhodamine Amide-Based Fluorescent Chemosensors



Fluorescent chemosensors are widely applied in the detection of many biologically relevant ions in recent years because they are simple to use and highly sensitive. Thus the demand for chemosensors that are selective for specific target materials is continuously increasing. Especially important in this regard are sensors that monitor toxic ions, toxic gases, and reactive oxygen species. Over the past few years, we have developed fluorescent sensing systems for selective detection of metal ions using rhodamine amide fluorophores. Whilst the ring-closed spirolactam form is nonfluorescent and colorless, the corresponding open form is strongly fluorescent and pink colored. An appropriate ligand attached to the spirolactam ring could selectively bind with a metal ion to induce ring opening and eventually turn on the fluorescence signal. We focused on developing chemosensors based on the rhodamine-hydrazide and hyroxamate binding units to increase the stability of the open form via chelation-controlled complex formation. We have also interested in the development of binding platforms utilizing biomimetic chelating units to

induce selective ring-opening of the rhodamine spiro-lactams. Developed chemosensors have been applied for biological imaging studies for practical applications.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MEDI-1**

발표분야: Drugs on the way for successful IND

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 안진희

## Discovery of novel B-Raf kinase inhibitor with potent orally anticancer activity

최남송

(주)유아이 신약개발연구소

The B-Raf, one of serine/threonine kinase, is related to the Ras-Raf-MEK-ERK (MAPK) signal transduction. The signaling pathway plays a key role in cell survival, growth and proliferation. The B-Raf mutants are found in various cancer patients, such as melanoma, papillary thyroid, cisplatin-refractory testicular cancer, colorectal, ovarian, and prostate cancer. Especially, over 90% of detected mutations in B-Raf are a V600E which leads to constitutive kinase activity 500-fold greater than B-Raf wild type and correlates with increased malignancy and decreased response the chemotherapy. There are currently numerous efforts to develop therapeutic agents to target B-Raf or its downstream kinases. The Raf inhibitors, sorafenib and vemurafenib, are now approved for the treatment of patients with advanced renal cell carcinoma. Recently, more selective Raf inhibitors have been disclosed, and chemical inhibition of B-Raf enzymatic activity using these compounds can result in diminished proliferation and survival of tumor cells. However, very limited drug candidates with in vivo data have been published for B-

Raf(V600E). In this study, some of rational-designed compounds were synthesized and carried out the in vitro and in vivo studies to investigate more efficient B-Raf(V600E) inhibitors. Our drug candidate, UAI-201, had good inhibition effect in malignant cells expressing B-Raf(V600E) mutant type of cell-line and xenograft mouse models. UAI-201 had no toxicity in normal cell-line(HS-27cell) and did not inhibit several CYP P450s and showed good oral bioavailability with an acceptable clearance and half-life pharmacokinetic properties. The in vitro and in vivo studies of UAI-201 indicate that it is safe and efficacious, and suggests that it may good drug candidate for the preclinical study. Preclinical study our candidate, UAI-201, was started and the results will be disclosed in the near future.



일시: 2012년 4월 25~27일(수~금) 3일간

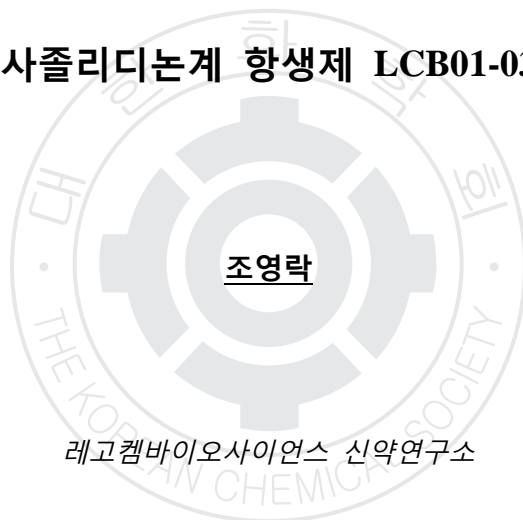
장소: 일산KINTEX

발표코드: **MEDI-2**

발표분야: Drugs on the way for successful IND

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 안진희

## 새로운 옥사졸리디논계 항생제 LCB01-0371의 개발



레고캠바이오사이언스 신약연구소

전세계적으로 슈퍼박테리아의 확산은 빠르게 진행되고 있어 이에대한 우려의 목소리가 높아지고 있다. 특히 메티실린 내성 황색포도상구균(MRSA)의 감염자수는 100 만명이 넘으며 이중 10 만명 정도가 매년 사망하여 HIV/AIDS 에 의한 사망자보다 더 많은 실정이나 이에 대한 대책은 여전히 미미하다. 최근 레고캠 바이오사이언스에서는 새로운 MRSA 치료제로 LCB01-0371 을 임상 개발 중이며 이 약물은 현재 사용되고 있는 자이복스보다 동물실험에서 약효 및 안전성에서 뛰어남이 입증되었다. 본 세미나에서는 이 약물의 프로파일과 임상 1 상까지의 개발과정에 대해 소개하고자 한다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MEDI-3**

발표분야: Drugs on the way for successful IND

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 안진희

## Development of a New Generation of Drug to Overcome NSCLC Resistance

서귀현

한미약품(주) 연구센터

Non-small cell lung cancer (NSCLC) associated with activating epidermal growth factor receptor (EGFR) mutations are initially responsive to EGFR-targeted tyrosine kinase inhibitor (TKI) such as Gefitinib and Erlotinib, but it appeared that most of patients fail to these drugs within one year because of several type of acquired resistance. Among these, the gatekeeper T790M point mutation accounts for about half of all resistance. While multiple clinical trials have studied therapies to overcome T790M resistance together with the development of new EGFR TKIs of pan-Her inhibitors, no therapy or drug being able to change clinical practice for T790M resistance has been developed until now. In this presentation, a novel EGFR TKI will be introduced as a next generation of drug to target acquired resistance of T790M as well as inherent activating EGFR mutations.

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장소: 일산KINTEX

발표코드: **MEDI-4**

발표분야: Drugs on the way for successful IND

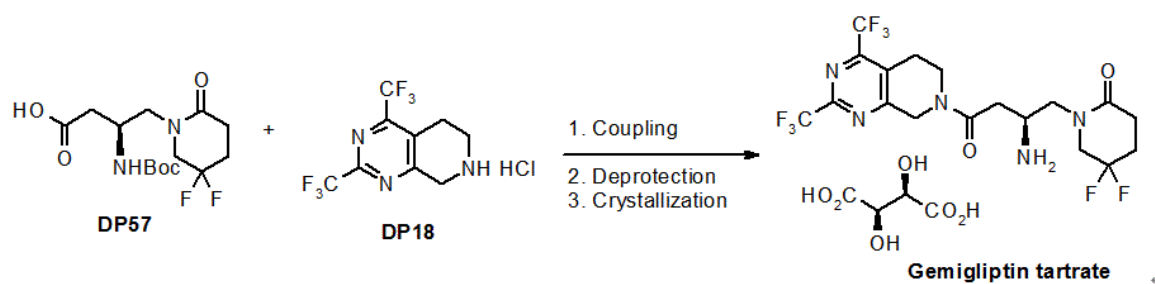
발표종류: 심포지엄, 발표일시: 금 11:50, 좌장: 남기엽

## Long road to the commercial production of Gemigliptin as a new DPP-IV inhibitor

이희봉

LG생명과학 공정연구소

Efficient synthesis of gemigliptin, a potent and selective DPP-4 inhibitor for the treatment of type 2 diabetes mellitus, has been developed. Gemigliptin were prepared from two key API starting materials, DP18 and DP57, in 75~80% yield and >99% purity over three steps under the GMP control: coupling, deprotection of N-Boc group, and final crystallization with L-tartaric acid. All steps were conducted in the same solvent system (i-PrOH) and the intermediates were isolated by simple filtration without distillation of solvent. The established process was validated obviously through the three consecutive batches for a commercial production.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MEDI-5**

발표분야: Drugs on the way for successful IND

발표종류: 심포지엄, 발표일시: 금 12:20, 좌장: 남기엽

**Pre-clinical and Clinical Development of Radotinib (Supect?) in  
Leukemia; identification of a next generation Bcr-Abl tyrosine kinase  
inhibitor**

**김동욱**

가톨릭대 암연구소

Imatinib mesylate (Glivec? or Gleevec?; Novartis co., Switzerland) has been preferentially used as 1st line therapy in chronic myeloid leukemia (CML) and has shown imposing responses in clinical practice. However imatinib resistance has observed in some patients and a majority of patients rapidly progressed to advanced disease resulting in fatal outcome. Based on the first successful development of imatinib and the mechanism of drug resistance, the development of more effective ATP-competitive BCR-ABL tyrosine kinase inhibitor (TKI) has been triggered and eventually second generation (2G) TKIs such as dasatinib (Sprycel?; Bristol Myers Squibb co., USA), nilotinib (Tasigna?; Novartis co., Switzerland), bosutinib (Pfizer co., USA), radotinib (Supect?; Ilyang co., Korea) have developed. In multicenter phase 2 and 3 clinical trials, 2G TKIs have been found to have superior cytogenetic and molecular responses. Radotinib was designed to be a potent, highly selective inhibitor of BCR-ABL kinase and we have

identified preclinical and clinical activities. In vitro potency is 35 to 50 times more potent than imatinib in various CML cell lines and at least 20 times more potent in suppressing CML tumor growth using xenograft mouse model. Except for T315I, it has sufficiently suppressed Y253H, E255K, F317L and M351T mutant clones. In phase 1 and 2 clinical studies, radotinib showed superior efficacy and good tolerability, and it was comparable to clinical results of other 2G TKIs. Radotinib is now approved for the treatment of patients with imatinib failure and a phase 3 clinical study to compare the efficacy and the tolerability with imatinib is currently ongoing in new patients. This presentation will summarize the detailed pre-clinical and clinical data of radotinib.



일시: 2012년 4월 25~27일(수~금) 3일간

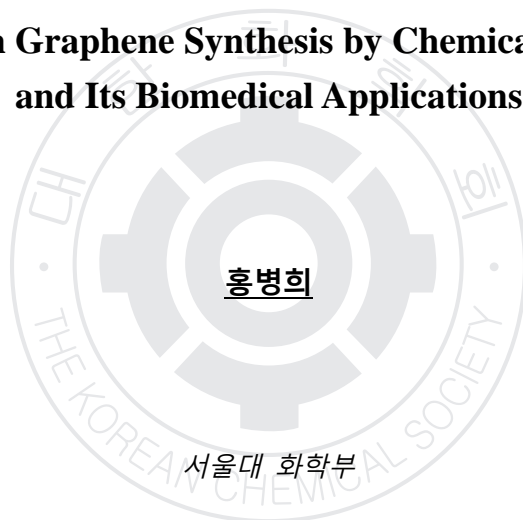
장소: 일산KINTEX

발표코드: MAT1-1

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 최성율

## Recent Progress in Graphene Synthesis by Chemical Vapor Deposition and Its Biomedical Applications



Graphene is a one-atom thick material with hexagonal carbon lattice that possesses outstanding electrical, optical and mechanical properties. Owing to its extreme flexibility and chemical stability, graphene has been widely used not only as flexible electrodes but also as various biological templates and scaffolds. The graphene has a unique surface property that is different from graphite including ultra-low friction and nano and microscale ripples, which are supposed to play an important role in the differentiation and growth of stem cells. In addition, graphene can be prepared as a few nm-sized quantum dots and soluble nanostructures that can be further functionalized and decorated with chemical/biological molecules using wet-chemistry. In this seminar, the recent biomedical applications of graphene including fluorescence cell imaging, bio-molecule sensing, and stem-cell differentiation/growth will be introduced.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT1-2

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 최성율

## Graphene Flakes and Their Possible Applications

**Hyoyoung Lee**

*Center for Smart Molecular Memory, Department of Chemistry, Samsung-SKKU Graphene Center,  
Sungkyunkwan University*

In recent, for the possible applications of graphene, graphene flakes prepared from direct exfoliation of natural graphite and/or from a reduction of graphene oxides (GOs) have been widely investigated in various fields such as 1) transparent/opaque electrodes for organic solar cells and organic light emitting devices, 2) conductive inks and electromagnetic interference filters, 3) energy storages for supercapacitors, batteries, fuel cells and hydrogen storages, 4) heat dissipaters, 5) bio-related works including bio sensors and growth of cells, 6) drug delivery and contrast agent with metal oxides. In order to prepare the device fabrication for the various applications, a development of many different mass-production methods of reduced graphene oxides (rGOs) and/or direct exfoliation from the natural graphite resources is necessary. Herein, we like to present novel synthetic scheme with new reduction condition of GO to rGO. For mass-production of graphene flakes, a chemical graphitization from graphene oxide (GO) to rGO was introduced at a room-temperature. New reducing reagent, hydroiodic acid in acetic acid (HI-AcOH) was introduced from GO to rGO, leading to one of best reduction method in solution- and vapor-

phase. Furthermore, it was possible to produce mass-production of rGOs at -10 degree celsius. We also like to introduce the device fabrication of field effect transistor (FET) using rGO as a channel and report the n- and p-type FET device with an electron donating and withdrawing functional molecules and quantum dots and non-volatile molecular memory device using rGO-Au nanoparticles and rGO. Finally, we like to introduce our on-going researches with graphene flakes and possible applications.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT1-3

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 최성율

## Strategies of Diagnostics and Drug Development Based on Graphene Oxide



Various nanomaterials are being harnessed as critical components of biosensing and diagnostics platforms such as gold nanoparticles for sensing of DNA-related biochemical changes. To design “good” biosensing systems using new nanomaterials, one should be able to understand and fully utilize chemical/physical properties to detect for changes in certain biochemical or biological status in a complex bio-system. Moreover, the new system should overcome some limitations of conventional assay methods?detection limits, cost issues, labors, efficiencies, quantitateness, reproducibility, etc. In this talk, I will introduce recent efforts to utilize “graphene oxide” for biosensing platforms and drug development tools, especially related to viral diseases including hepatitis C and SARS.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT1-4

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 최성율

## Graphene Oxide: Functionalization and Applications for Electronic Devices and Solar Cells



신현석

울산과학기술대 에너지공학부

Chemical approach like functionalization of graphene oxide (GO) and reduced graphene oxide (rGO) is crucial for various applications. In particular, tailor-made functionalization of graphene can supply physicochemical and electronic properties that we want to realize. In this talk, I introduce recent research results on functionalization and applications of GO and rGO. First, I demonstrate new approach for fabrication of GO and rGO multilayers which can be a building block for various hybrid films with 0 or 1 dimensional nanomaterials. This was achieved by using layer-by-layer (LbL) assembly of positively and negatively GO sheets which could provide highly controllable thin films in terms of thickness, transmittance, and sheet resistance. Another interesting thing is an integration of graphene and functional materials via covalent and non-covalent interaction. I introduce the assembly of rGO and fullerene (C60) into core/shell hybrid nanowires by employing the liquid-liquid interfacial precipitation (LLIP) method. C60 nanowires are first formed and then rGO sheets are coated on surfaces of them. The structural

characterization of the rGO/C60 nanowires and their applications for field-effect transistors and photovoltaic solar cells are introduced in this presentation. Lastly, I introduce functional hybrid films of rGO sheets with metal nanoparticles which are very promising for highly efficient and transparent counter electrodes of dye-sensitized solar cells.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT1-5

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 최성율

## Flexible organic light-emitting diodes using graphene anodes for solid-state lightings

이태우

포항공과대 신소재공학과

Graphene films have a strong potential to replace indium tin oxide anodes in organic light-emitting diodes (OLEDs), to date. However, the luminous efficiency of OLEDs with graphene anodes has been limited by a lack of efficient methods to improve the low work function and reduce the sheet resistance of graphene films to the levels required for electrodes. Here, we fabricate flexible OLEDs by modifying the graphene anode to have a high work function and low sheet resistance, and thus achieve extremely high luminous power efficiencies (37.2 lm/W in fluorescent OLEDs, 102.7 lm/W in phosphorescent OLEDs), which are significantly higher than those of optimized devices with an indium tin oxide anode (24.1 lm/W in fluorescent OLEDs, 85.6 lm/W in phosphorescent OLEDs). We also fabricate flexible white OLED lighting devices using the graphene anode. These remarkable device efficiencies increase the feasibility of using graphene anodes to make extremely high-performance flexible organic optoelectronic devices by overcoming the major drawbacks (low work function and trap formation due to diffusion of indium and

tin) of conventional ITO anodes. These results demonstrate the great potential of graphene anodes for use in a wide variety of high-performance flexible organic optoelectronics such as flexible, stretchable full-colour displays and solid-state lighting.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT1-6

발표분야: Graphene - Recent Advances and Future Outlook

발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 최성율

## Atomic layer field effect transistors with two-dimensional materials



**유영준**

한국전자통신연구원 그래핀소자 창의연구실

The next generation electronics need to not only be smaller but also be more flexible. To meet such demands, electronic devices using two dimensional (2D) atomic crystals like graphene, hexagonal boron nitride (h-BN), molybdenum disulfate (MoS<sub>2</sub>) and organic thin film have been studied intensely. In this talk, I will demonstrate the fabrication and the characterization of 2D atomic crystals and organic thin film field effect transistor (FET) toward performance enhancement by insulating h-BN substrate and graphene electrode.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-1

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박종남

## Single-Walled Carbon Nanotube/Polymer Hybrids for Near-Infrared Fluorescent Detection of Biological Molecules

김종호

한양대 화학공학과

A major challenge in the synthesis of nanotube or nanowire sensors is imparting selective analyte binding through means other than covalent linkages which compromise electronic and optical properties. We functionalized single-walled carbon nanotubes (SWNT) with synthetic polymers or proteins in non-covalent manner to selectively recognize the specific targets such as reactive oxygen and nitrogen species (ROS and RNS). First, we designed the SWNT-dextran hybrid (SWNT-dex) for selective detection of nitric oxide (NO). NO caused the nIR fluorescence change of SWNT-dex, but other reactive nitrogen and oxygen species didn't change its nIR fluorescence. Finally, SWNT-dex was successfully applied to in-vitro NO detection. Second, we designed the array of SWNT/collagen optical sensor for single molecule detection of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) that activates signal transduction pathways during angiogenesis. We utilized the SWNT/collagen sensor array to measure the single molecule efflux of H<sub>2</sub>O<sub>2</sub> from human umbilical vein endothelial cells (HUVEC) in response to angiogenic stimulation by vascular endothelial

growth factor A (VEGF-A) or the inorganic pro-angiogenic factor, europium (III) hydroxide nanorods. We found that the production of  $\text{H}_2\text{O}_2$  following VEGF stimulation was elevated outside of HUVEC, but not for stimulation via nanorods while increased generation was observed in the cytoplasm for both cases, suggesting two distinct signaling pathways.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-2

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 박종남

## Five Closely Related Li-Containing Rare-Earth Metal Germanides: Structural, Electronic and Magnetic Perspectives

유태수

충북대 화학과

Reported are the synthesis, crystal and electronic structures and magnetic properties of five different, but very closely related rare-earth metal-lithium germanides  $\text{RELiGe}_2$  ("1-1-2"),  $\text{RE}_2\text{Li}_2\text{Ge}_3$  ("2-2-3"),  $\text{RE}_3\text{Li}_4\text{Ge}_4$  ("3-4-4"),  $\text{RE}_7\text{Li}_8\text{Ge}_{10}$  ("7-8-10"), and  $\text{RE}_{11}\text{Li}_{12}\text{Ge}_{16}$  ("11-12-16") (RE = early to mid-early rare-earth metals). The "2-2-3" and "3-4-4" phases are crystallized in the orthorhombic  $\text{Ce}_2\text{Li}_2\text{Ge}_3$ -type and  $\text{Zr}_3\text{Cu}_4\text{Si}_4$ -type structures, respectively, whereas two other phases, "7-8-10" and "11-12-16", found to adopt two novel crystal structures with orthorhombic space groups  $Cmmm$  and  $Immm$ , respectively. Interestingly, crystal structures of two novel series of compounds can be described as a combination of "2-2-3" and "3-4-4" phases acting like structural building blocks. Therefore, the "7-8-10" phase can be viewed as a combination of two of the "2-2-3" and one of the "3-4-4" phase, and the formula is expressed as "7-8-10" =  $(2 \times \text{"2-2-3"}) + \text{"3-4-4"}$ . Along the same line, the formula of the "11-12-16" phase can be explained as either  $(4 \times \text{"2-2-3"}) + \text{"3-4-4"}$  or  $(2 \times \text{"2-2-3"}) + \text{"7-8-10"}$ . Structural transformation among

different phases containing various lithium contents has been examined at elevated temperatures, and temperature dependent magnetization measurements have been performed. Theoretical investigations by tight-binding muffin-tin orbital have been conducted to understand the correlation between electronic structures and structural stabilities.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-3

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 10:50, 좌장: 박종남

## Molecular Transport Junctions Created Using Self-Contacting Nanowires Prepared by On-Wire Lithography

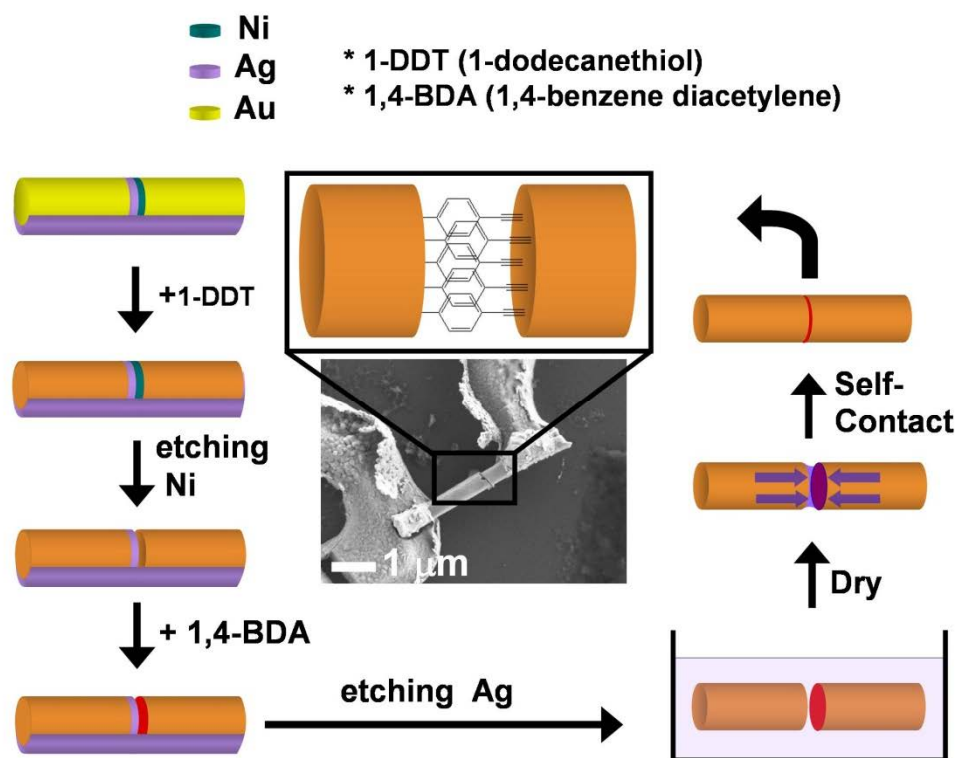
임종국

조선대 화학과

The straightforward and reproducible fabrication of molecular transport junctions (MTJs) is essential for realizing the promise of molecular electronic devices. A variety of techniques have been introduced to produce MTJs based on nanopores, scanning probes, liquid metals, wire crossings, electromigration, break junctions, and on-wire lithography (OWL). OWL is a particularly attractive method for fabricating MTJs because of the ability to regularly create sub-5 nm nanogaps along the long-axis of the wire, its high-throughput, and the ability to change the elemental composition and length of the segments during the fabrication of the nanowires. Although it is easy to control the gap size in OWL-generated nanostructures when the distance between segments is greater than 5 nm, creating gaps that are approximately the size of single-molecules (<2 nm), remains a considerable challenge. Herein, we introduce a new method to fabricate MTJs where molecules of different lengths can bridge the gaps of gapped nanowires without having to match the length of the sacrificial metal segment to the length of the



molecule during the fabrication of the nanowire. Moreover, the same sacrificial segment length can be used to create MTJs of molecular wires of different lengths, thereby overcoming a major challenge faced by researchers attempting to prepare MTJs with gapped nanowires.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-4

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 이재승

## **Tailored Design and Application of Hybrid Plasmonic and Carbonaceous Nanostructures**



김동하

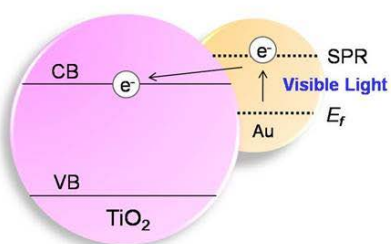
이화여대 화학나노과학과

In the Polymer Nanohybrid Materials at Ewha Womans University, a comprehensive approach for the design and synthesis of multifunctional hybrid nanomaterials has been systematically pursued 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 block copolymer self-assembly processes to construct well-defined hybrid nanoscopic features suitable for the 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 nanomaterials for highly selective/sensitive optical biosensing, visible

light active photocatalysis and dye-sensitized solar cells. References 1. 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, in press.

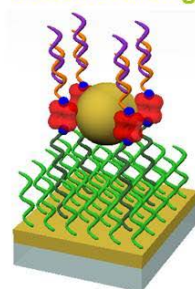
### Visible Light Active Photocatalysts

Au/TiO<sub>2</sub> (or ZnO)



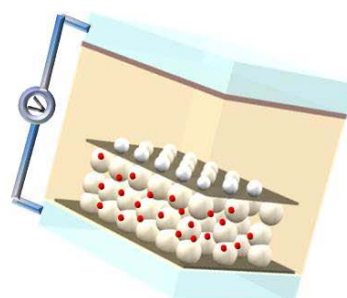
### Optical Biosensing

LSPR/PSPR-based Sensing



### Photovoltaics

Carbon-TiO<sub>2</sub> Nanostructures in Solar Cells



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-5

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 11:55, 좌장: 이재승

## Ordered Nanoporous Carbon as Noble Metal-Free Electrocatalysts for Energy Conversion Devices



주상훈

울산과학기술대 나노생명화학공학부

Pt-based noble metals have been predominantly used as electrocatalysts for energy conversion devices such as fuel cells and solar cells during the last several decades. Although Pt-based catalysts are highly efficient in electrocatalytic reactions, high costs and limited supplies of Pt have triggered a great deal of recent efforts toward seeking low-cost alternatives for Pt. In this talk, the preparation of new electroactive ordered nanoporous carbons, and their applications as noble metal-free electrocatalysts for cathode of polymer electrolyte membrane fuel cell as well as for counter electrode of dye sensitized solar cell will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT2-6

발표분야: Recent Trends in Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 12:20, 좌장: 이재승

## Active Modulation of Cells and Tissues with Engineered Materials for Therapeutic Purposes



김재윤

성균관대 화학공학부

By controlling their physical and chemical properties, diverse materials can exhibit unique characteristics which have high potentials to overcome various problems in current clinical approaches to treat diseases. Engineering of nanobiomaterials including diverse nanoparticles and three dimensional polymer scaffolds allow us to modulate cells and tissues on demand. These materials are used in diagnostics, drug delivery, cancer therapy, and tissue regeneration. In this talk, I will present some of the examples that explain how we are able to control the living systems through engineering materials for therapeutic purposes.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ELEC1-1

발표분야: Advances in electrochemistry

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김규원

## Polyaniline Nanofiber/Carbon Black Composite as Oxygen Reduction Catalyst for Air Cathode Microbial Fuel Cells

Ahmed Jalal 김성현 Yong Yuan<sup>1</sup>

건국대 생명공학과 <sup>1</sup>Guangdong Institute of Eco-environmental and Soil Sciences

Conductive polyaniline nanofibers (PANInf) have been synthesized by interfacial polymerization and used to prepare composite electrodes with carbon black. Thus prepared PANInf/carbon black composite (PANInf/C) has been employed as an oxygen reduction catalyst in a microbial fuel cell. Higher electrocatalytic activity for the oxygen reduction compared to pristine PANInf was resulted when the PANInf/C composite was used. Large enhancement in power density was observed when this composite cathode was used. The maximum power density of 185 mW m<sup>-2</sup> for the pristine PANInf increased to 496 mW m<sup>-2</sup> for the composite cathode. Although the power density is still lower than that of conventional Pt catalyst (604.3 mW m<sup>-2</sup>), a facile bulk synthesis and cheaper price would make PANInf/C an alternative to Pt when a large scale application comes to an issue.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ELEC1-2

발표분야: Advances in electrochemistry

발표종류: 심포지엄, 발표일시: 목 10:05, 좌장: 김규원

## Improved Electrochemical Performance of Nanocrystalline-Conductive Polymer Composite Cathodes

모선일

아주대 에너지시스템학부 화학

Composites composed of the nanosized electroactive inorganic crystal and conductive polymer are of great importance for rechargeable lithium ion batteries and are expected to exhibit synergistic effect for intercalation/deintercalation of lithium ions by the contribution from the durable inorganic crystals and flexible organic polymers. The composites as the cathodes for the rechargeable batteries could offer large capacity because of large surface area, easier lithium ion accessibility, mechanical flexibility, and improved conductivity. Nanodimensional crystals of  $V_2O_5$  and  $LiFePO_4$  were prepared by hydrothermal methods. Then, the crystals are imbedded into various composites electrochemically or chemically ( $V_2O_5/PANi$ ,  $V_2O_5/PPy$ ,  $V_2O_5/PEDOT$ , or  $LiFePO_4/PEDOT$ ) by incorporating conducting polymers. The electrochemical performance of the composite cathodes with an assembled coin-type (CR2032) Li cell was tested with a battery test system (Maccor 4000). Excellent stability of the  $V_2O_5/PEDOT$  and  $V_2O_5/PPy$  composite film cathodes under the repeated charge/discharge cycling was observed with almost

no fading for various amount of  $V_2O_5$  loading. For  $LiFePO_4$ /PEDOT composites, maximum theoretical capacity was obtained. The capacity retention was also excellent even at high 10C rate. Enhanced diffusion and increased accessibility of  $Li^+$  caused by the incorporation of conducting polymers in the composites result in the cycling stability of the rechargeable lithium ion battery. High capacities in addition to the cycle stability were achieved with the composite cathodes. The methods and explanations will be discussed in detail.





일시: 2012년 4월 25~27일(수~금) 3일간

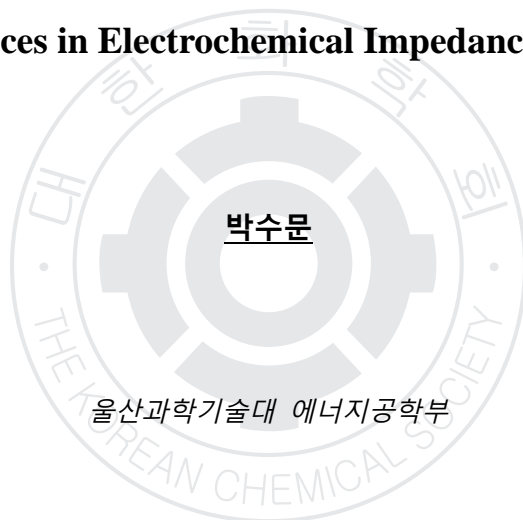
장소: 일산KINTEX

발표코드: **ELEC1-3**

발표분야: Advances in electrochemistry

발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 이영미

## Recent Advances in Electrochemical Impedance Spectroscopy



Recently, electrochemical impedance spectroscopy (EIS) has been enjoying an unprecedented popularity from the electrochemistry community. This is because it offers a viable way to completely describe the electrified interfaces when the EIS data are properly obtained and interpreted. One of its disadvantages is its measurement speed, however, which prohibits its real time measurements as a function of desired bias potentials so that the EIS data would be used for systematic analysis of the electrochemical reactions of interest. The dire needs for high speed have brought up numerous attempts to develop "fast" EIS measurements. In this presentation, we will review a few of these attempts and finally discuss the state-of-the-art technique for EIS measurements, which has recently been developed and allow real time measurements to be made during the potential sweep. A few examples demonstrating how useful the EIS data can be for the interpretation of problems related to the electrified interface will be presented as well.

일시: 2012년 4월 25~27일(수~금) 3일간

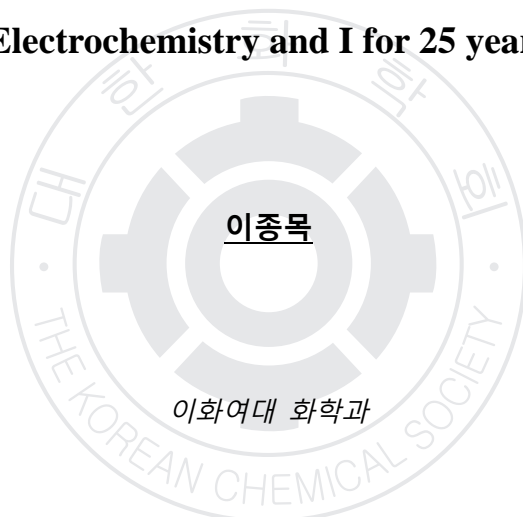
장소: 일산KINTEX

발표코드: **ELEC1-4**

발표분야: Advances in electrochemistry

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 이영미

## Electrochemistry and I for 25 years



This talk contains my brief history related to electrochemistry for twenty five years and is divided by following four parts: (1) The occasion to start to study electrochemistry; (2) What kind of electrochemistry for twenty five years with whom?; (3) What I have learned in electrochemistry for organometallic/organic compounds during latest ten years; (4) What I have been working for recently. For the topic (3), '18 electron rule versus redox reversibility', 'HOMO-LUMO level versus cyclic voltammetry', and 'charge and solubility versus redox chemistry' were considered. For the topic (4), applications of nano-structured materials focused on electrocatalytic reactions including electrochemical sensing. I appreciate all the coworkers' time and endeavors mentioned during this talk, especially Professor J. H. Shim and Y. Lee.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ELEC2-1

발표분야: New trends in electrochemistry

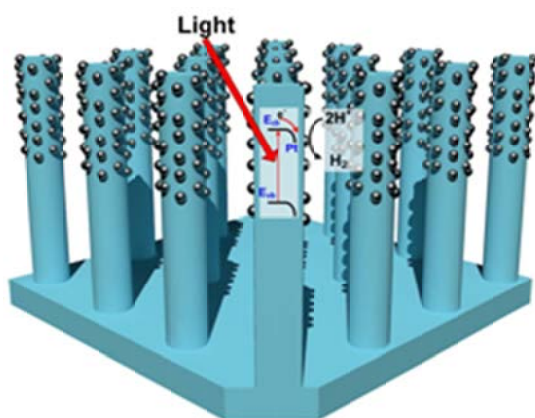
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 신재호

## Photoelectrochemical Hydrogen Production from Photocathodes Based on Silicon Nanostructures

오일환 황성필<sup>1</sup> 계주홍<sup>1</sup>

금오공과대 응용화학과 <sup>1</sup>명지대 화학과

Herein we report on photoelectrochemical hydrogen production using photocathodes based on nanostructured Si materials, including silicon nanowires (SiNWs) fabricated via metal-catalyzed electroless etching and porous silicon fabricated via anodic etching. It was found that a thin layer (<10um) of porous silicon can serve as anti-reflection layer for the underlying Si substrate, improving photocurrent by reducing photon reflection at the Si/liquid interface. On the other hand, the SiNW yielded a photoelectrochemical hydrogen generation performance superior to that of a planar Si, which is attributed to a lower kinetic overpotential due to a higher surface roughness, favorable shift in the flat-band potential, and light-trapping effects of the SiNW surface. The SiNW photocathode yielded a photovoltage of 0.42 V, one of the highest values ever reported for hydrogen generation on p-type Si/electrolyte interfaces.



일시: 2012년 4월 25~27일(수~금) 3일간

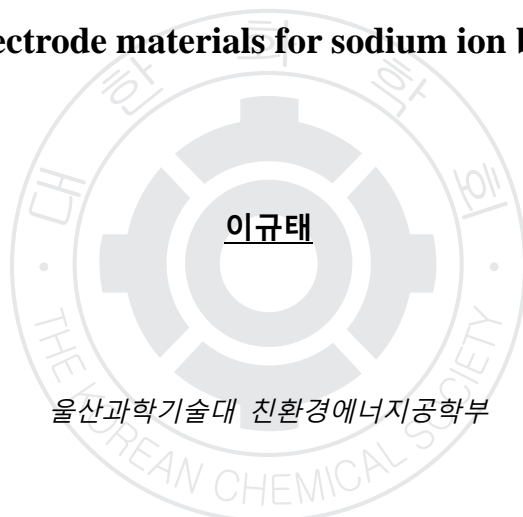
장소: 일산KINTEX

발표코드: **ELEC2-2**

발표분야: New trends in electrochemistry

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 신재호

## New electrode materials for sodium ion batteries



Over the last several decades, the major energy source has been fossil fuels, which are non-renewable, finite, and environmentally hazardous. To solve out these problems, clean and sustainable energy systems have been studied such as solar cells, fuel cells, and rechargeable batteries. While Li-ion rechargeable batteries are currently dominant energy storage systems in the market powering numerous portable electric devices, the commonly used electrode materials, such as  $\text{LiCoO}_2$  and  $\text{LiMn}_2\text{O}_4$ , are prepared from the limited mineral resources. Especially, the amount of lithium resources is not enough to supply a demand for the industry of electric vehicles. Therefore, recently, a sodium ion battery is regarded as an intriguing candidate of a next generation battery due to the non-toxicity and potential cost advantages coming from its natural abundance. Compared to wide attention on lithium intercalation to the layered compounds, limited studies have been reported on the sodium intercalation because of its slow kinetics by relatively large effective ionic radius (102 pm) compare to lithium ion (76 pm). Herein, we introduce

various new electrode materials for sodium ion batteries. The material characterization and electrochemical performance of those materials are examined.



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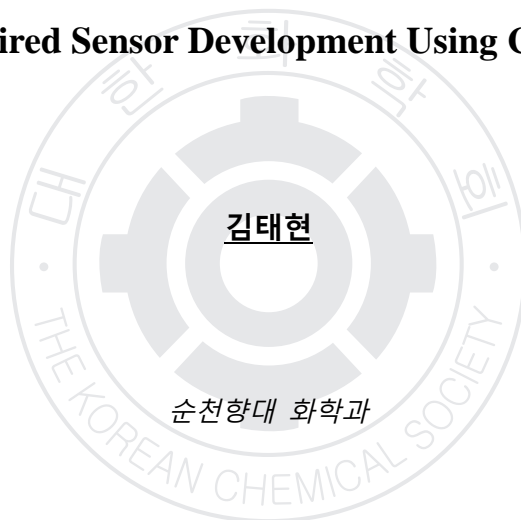
장소: 일산KINTEX

발표코드: **ELEC2-3**

발표분야: New trends in electrochemistry

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 신재호

## Biologically-Inspired Sensor Development Using Carbon Nanotubes



Biological receptors on the surface of cells function as sensors and mediators, which recognize molecules outside the cell and activate inside signal transduction pathways and, ultimately, cellular responses. These receptors have multivalent or cooperative binding sites, leading to highly specific molecular recognition through weak interactions based on hydrogen bonding, van der Waals interactions, etc. They are located in the cellular plasma membrane, the protective lipid bilayer that constitutes the critical barrier of the intracellular components to the extracellular environment. Cell membranes provide a unique platform to sense, respond to, and transduce signals and information. In these biological signaling processes, cooperativity is believed to play a crucial role, offering a mode of achieving selective recognition. The biochemical recognition processes that occur on the membrane surfaces form the basis of the most versatile and specific sensor systems known. By devising the capability of cellular membrane recognition systems, it may be possible to develop rapid, specific and biocompatible sensor systems. Furthermore, the intrinsic and unique functional plasticity of the specific receptor structures in the membrane suggests that

synthetic access to artificial receptor in the membrane could lead to the development of controllable nanoscale architecture. Recently, the employment of lipid membranes in electronics such as field-effect transistor (FET) has attracted much attention in the development of sensor system due to the potentiality of superior biosensing and diagnostics tools in nanostructured devices. Here, we reports nanoelectronic sensors based on lipid membrane/single walled carbon nanotube FET hybrids incoprated with biological receptors.





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장소: 일산KINTEX

발표코드: **ELEC2-4**

발표분야: New trends in electrochemistry

발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 이동일

## **A new trend of chemical instrumentation based on the smartphone: digitization of colorimetric measurements**

장병용

부경대 화학과

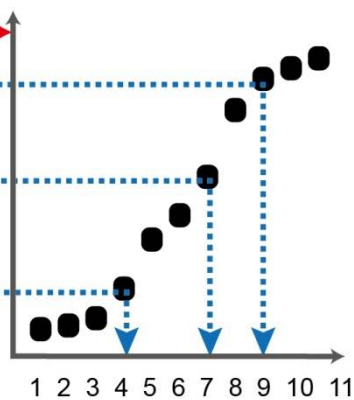
Here I present a new mobile instrumentation platform based on a smartphone using its built-in functions. Specifically a new colorimetric diagnosis is discussed. The color change as a result of chemical reaction is taken on a picture through a CCD camera built in the smartphone, and results in values to give the well-defined relationship between the color and the concentration. To prove the concept in this new strategy, proton concentration measurements are demonstrated using pH paper and a smartphone. Even though this work is not directly related to electrochemistry, but is believed to show the possibility of adapting a smartphone to a mobile analytical transducer including electrochemical sensors as many colorimetric methods have already been known to use faradaic reactions. Also, this smartphone-base instrumentation will make a new trend in chemical applications using combinations of other built-in functions of the smartphone.

① snapshot taking



② calibration from the reference

③ evaluation of samples



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장소: 일산KINTEX

발표코드: ELEC2-5

발표분야: New trends in electrochemistry

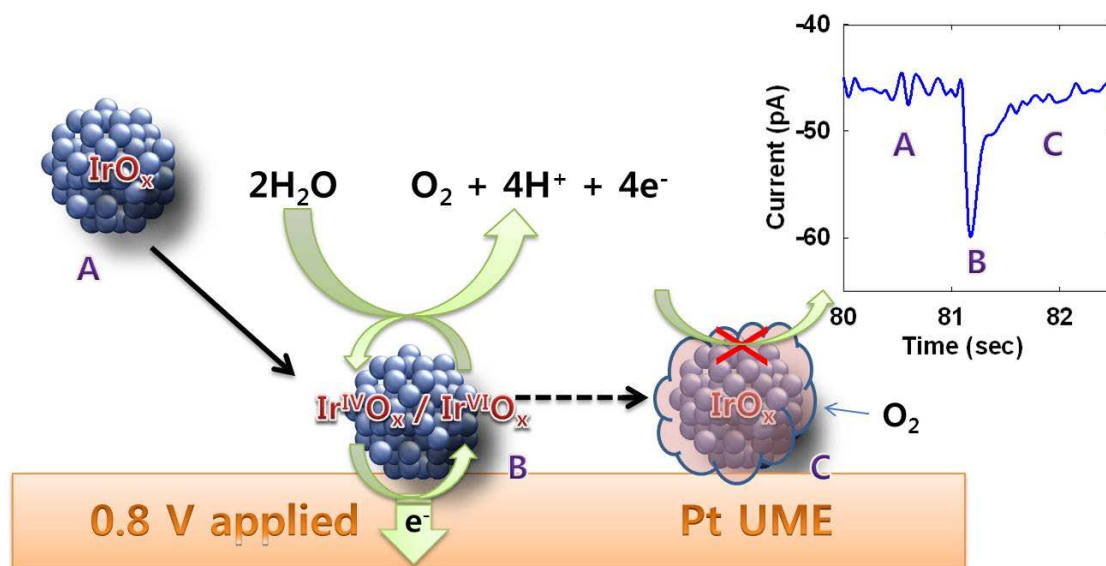
발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 이동일

## Observation and Analysis of Stochastic Iridium Oxide (IrOx) Single Nanoparticle Collisions at ultramicroelectrode

권성중 Allen J. Bard<sup>1</sup>

건국대 화학과 <sup>1</sup>University of Texas at Austin

We describe the electrochemical detection of single iridium oxide nanoparticle (IrOx NP) collision at a less catalytic electrode surface such as the NaBH<sub>4</sub>-treated Pt or the bare Au. We could observe the single NP collision through the enhanced current by electrocatalytic redox recycling. The overall current transient consists of repeated current spikes, superimposed on a current decay to reach a steady-state value. The current responses were caused by random individual events as a function of time rather than the usual continuous current caused by an ensemble of a large number of events. The treatment of stochastic electrochemistry like single NP collisions is different from the usual model for ensemble-based electrochemical behavior. Models for the observed responses are discussed, including simulations, and the height and frequency of the peak current are investigated.



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발표코드: ENVR1-1

발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 백민훈

## 지하미생물에 의한 산화우라늄의 환원 및 거동

이승엽

한국원자력연구원 방사성폐기물처분연구부

토양 및 지표면 하부에 많은 종류의 혐기성 미생물들이 생존하고 있으며, 특히 철, 망간, 그리고 황산염 등을 환원시키는 금속환원미생물들이 다양하게 분포하고 있다. 이 미생물들은 일반 금속원소 등을 환원시킬 뿐만 아니라 물에 용존된 산화핵종들까지도 환원시킬 수 있다. 대표적인 방사성 핵종인 우라늄의 경우 박테리아에 의해 6 가 우라늄(산화상태)이 4 가 우라늄(환원상태)으로 환원될 수 있으며, 이 과정에서 불용성의 우라늄 광물이 생성된다. 지하수를 따라 이동 가능한 우라늄의 경우 용해도가 높은 6 가 우라늄이 대부분을 차지하고 있을 것으로 예측되나, 최근 연구 결과에 의하면 생지화학적으로 환원된 4 가 우라늄이 나노 크기의 콜로이드로 밝혀짐에 따라 실제 지하수 내 우라늄의 이동 형태에 논란이 되고 있다. 즉, 심부 지하수에는 용존가능한 6 가 우라늄 뿐만 아니라 콜로이드 형태의 4 가 우라늄이 같이 공존할 가능성도 배제할 수 없다. 본 연구에서는 용액상의 6 가 우라늄이 금속환원미생물에 의해 4 가 우라늄으로 변환되는

생지화학적 과정을 밝히고 있으며, 박테리아에 의해 생성되는 황화광물의 이차적인 역할에 대해서도 논의하고 있다. 본 실험결과에 의하면, 지하수 내 용존 핵종들은 지하미생물들의 직접적인 환원작용의 영향을 받을 뿐만 아니라 이차적으로 생합성되는 황화광물과 같은 생합성 무기물질에 의해서도 환원되고 있고, 이러한 복합적인 지화학반응 과정은 용존우라늄의 지하 거동 및 이동에 상당한 영향을 미칠 것으로 판단된다.



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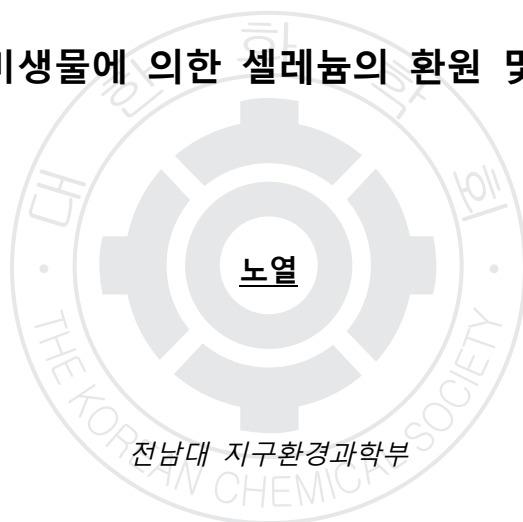
장소: 일산KINTEX

발표코드: ENVR1-2

발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 백민훈

## 지구미생물에 의한 셀레늄의 환원 및 침전



셀레늄은 selenide [Se(-II)], elemental selenium [Se(0)], selenite [Se(IV)], selenate [Se(VI)]로 존재한다. 이 중 selenide, elemental selenium 은 침전물 상태로 존재하나, 고체형태가 아닌 selenate 은 용해성이 크며 이동도가 높은 이온이다. 금속환원 지구미생물의 이화적대사작용에 의해 발생한 전자가 금속의 환원에 관여하여 산화상태로 존재하는 Se(VI)가 안정한 Se(0) 결정형태로 침전 될 수 있다. 이 연구에서는 국내 갯벌퇴적물 및 지하수에서 농화배양한 금속환원 지구미생물의 selenate 환원 및 침전으로 selenate 의 고정화(immobilization)에 대해 연구하고자 한다. 실험에 이용된 지구미생물은 금속 환원 능력이 있다고 보고된 전남 무안군 해제면 갯벌퇴적물에서 농화배양된 Haejae-1 과 한국원자력연구원 지하연구터널 지하심부(약 140 m)에서 채취한 지하수에서 농화배양된 KURT-1 이다. 각각의 미생물 성장배지에 전자공여체 유기산 5 종(acetate, formate, glucose, lactate, pyruvate) 10 mM 와 전자수용체인 sodium selenate 15 mM 을 1 mM 씩 주입한 후, Haejae-

1 과 KURT-1 배양액 1 mL씩 주입하여 농화배양하고 성장배지 내 변화양상을 관찰하였다. 미생물 성장배지에 주입된 금속이온 selenate 의 농도 변화 관찰, 금속환원 지구미생물의 활동에 의해 형성된 침전물 관찰과 성분분석 및 입도분석, 광물종류 및 결정 형태 분석을 위해 ICP-AES, SEM/TEM-EDS, DLS 및 zeta-PSA, XRD 를 실시하였다. Haejae-1 과 KURT-1 은 주입당시 전자공여체별 852 mg/L 범위를 보이는 selenate 를 주입 5 일 이내에 18.2 mg/L 로 감소시켰다. 지구미생물 활동에 의해 감소된 selenate 는 미생물 표면 및 체 외에 2 가지 결정구조(Hexagonal, Cubic)를 갖는 약 200 nm 의 구형 elemental selenium 결정으로 바뀌었다. 국내 갯벌퇴적물과 지하수에 존재하는 지구미생물은 유독한 수용성이온 selenate 의 환원시킴으로서 유독성이온을 고정화할 수 있으며 이 때 형성된 elemental selenium 는 나노크기의 결정으로 존재하기 때문에 이 결과는 지구미생물을 이용한 금속 환원 방법이 자연수 내의 selenate 의 안정화 방법으로 사용될 수 있으며 부가적으로 나노산업에 이용이 가능할 것으로 사료된다.





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발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 백민훈

## 산화 조건에서 우라늄(VI)과 대수층 퇴적물의 무생물적 반응



현성필

한국지질자원연구원 지구환경연구본부 지하수연구실

함우라늄 광미에 의해 오염된 미국 콜로라도 라이플 사이트에서 무생물적 반응에 의한 우라늄(VI)의 이동 지연 인자를 평가하기 위해 대수층 퇴적물에 의한 우라늄(VI) 흡착을 연구하였다. 사이트의 지화학 조건을 재현하기 위해 산화 조건에서 인공 지하수 용액의 조성을 변화시키며 흡착 실험을 수행하였다. 비정전기적 두자리-두반응 흡착 모델을 개발하였고 이를 흡착 실험 데이터를 사용하여 검증하였다. 이 모델은 전 실험 조건에서 우라늄 흡착을 잘 모사하였다. 그리고 우라늄 흡착량이 퇴적물의 비표면적에 의해 표준화될 수 있음을 보여주었다. 또한 현장 관측공에서 측정한 우라늄 농도를 잘 예측하였다. 유사한 지질 특성을 가지는 나투리타 사이트에서 보고된 데이터에 이 모델을 적용한 결과는 두 사이트에서 보고되는 우라늄 흡착의 차이가 용존 칼슘 농도 차에 기인함을 제안하였다. 이 연구는 우라늄 이동을 장기적으로 예측하는 모델이 오염 지역 지하수 조성의 전 범위 하에서 얻어지는 데이터를 바탕으로 개발/검정되어야함을 보여준다. 이 모델은 앞으로 산화-

환원 반응과 미생물적 과정을 고려한 우라늄 반응/이동 모델 개발에 기여할 것으로  
기대된다.



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발표코드: ENVR1-4

발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 백민훈

## 분광기술을 이용한 수용액 내 우라늄 화학종 정량분석

**정의창 조혜륜 차완식**

한국원자력연구원 원자력화학연구부

수용액 매질에 미량 존재하는 우라늄(U) 화학종 정량분석 방법에 대해 논의한다. 대표적인 U 화학종은 U(VI)와 U(IV)이다. U(VI) 화학종은 형광을 측정함으로써 나노 몰 농도의 극미량까지 분석이 가능하다. 형광 특성이 없는 U(IV) 화학종은 광흡수를 측정함으로써 마이크로 몰 농도의 정량분석이 가능하다. 제품으로 구입이 가능한 KPA(Kinetic Phosphorescence Analyzer)와 우리 실험실에서 구축한 TRLFS(Time-Resolved Laser Fluorescence Spectroscopy) 시스템을 이용하여 U(VI) 형광을 측정한 경우의 특징적인 양상을 비교한다. 물의 라만산란 세기와 U(VI) 형광 세기의 비를 이용하여 U 화학종을 정량할 수 있는 새로운 분광기술을 소개한다. U(IV) 화학종의 검출한계를 높이기 위해 LWCC(Liquid Waveguide Capillary Cell)을 이용하여 흡수분광학을 시도한 사례를 소개한다. 형광과 흡수분광기술을 이용하여 자연수 시료를 분석할 때 자연수 속에 포함된 다양한 금속이온들이 U 정량분석에 미치는 영향에 대해 논의한다.

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장소: 일산KINTEX

발표코드: ENVR1-5

발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 백민훈

## Formation of ternary uranyl(VI)-calcium-carbonate complexes studied by TRLFS

이준엽 윤종일

KAIST 원자력 및 양자공학과

TRLFS providing a nano-scale quantitative and qualitative analysis has been applied for characterizing the chemical behaviors and spectroscopic properties of uranyl(VI)-calcium-carbonate complexes. The two distinctive  $\text{UO}_2^{2+}/\text{Ca}^{2+}/\text{CO}_3^{2-}$  complexes,  $\text{Ca}(\text{UO}_2)(\text{CO}_3)_3^{2-}$  and  $\text{Ca}_2(\text{UO}_2)(\text{CO}_3)_3(\text{aq})$ , show similar spectrum shapes and peak positions whereas the fluorescence lifetimes are determined discrepantly to be  $11 \pm 2$  ns for  $\text{Ca}(\text{UO}_2)(\text{CO}_3)_3^{2-}$  species and  $22 \pm 1$  ns for  $\text{Ca}_2(\text{UO}_2)(\text{CO}_3)_3(\text{aq})$  species at  $10^{-2}$  M and  $10^{-5}$  M aqueous calcium concentrations, respectively. Furthermore, the  $\text{UO}_2(\text{CO}_3)_2^{2-}$  complex is observed at low calcium concentration while the  $\text{Ca}_2(\text{UO}_2)(\text{CO}_3)_3(\text{aq})$  species exist predominantly at higher calcium concentration. Under more alkaline conditions, the hydrolyzed uranyl species of  $\text{UO}_2(\text{OH})_3^-$  are formed regardless of the calcium concentration. The uranyl(VI) complexes omnipresent in aerobic natural groundwaters from the Daejeon area are spectroscopically very similar to the  $\text{UO}_2^{2+}/\text{Ca}^{2+}/\text{CO}_3^{2-}$  complexes. For confirming the precise nature of those ternary uranyl(VI)-calcium-carbonate complexes,

the slope analysis using EDTA- $\text{Ca}^{2+}$  complexation and the anion exchange method are utilized complementarily.

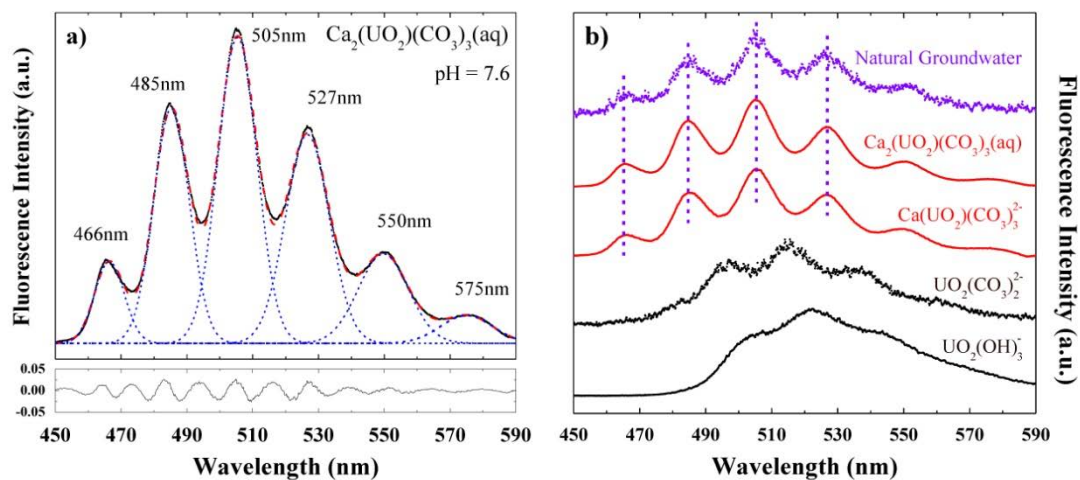


Figure 1: (a) Individual fluorescence peak positions of  $\text{Ca}_2(\text{UO}_2)(\text{CO}_3)_3(\text{aq})$  at  $[\text{Ca}^{2+}] = 10^{-2} \text{ M}$  and pH 7.6. (b) Fluorescence spectra of  $\text{Ca}_p(\text{UO}_2)_q(\text{OH})_r(\text{CO}_3)_s^{2p+2q-r-2s}$  complexes in the neutral to alkaline pH range at  $I = 0.5 \text{ M Na/HCl}$



일시: 2012년 4월 25~27일(수~금) 3일간

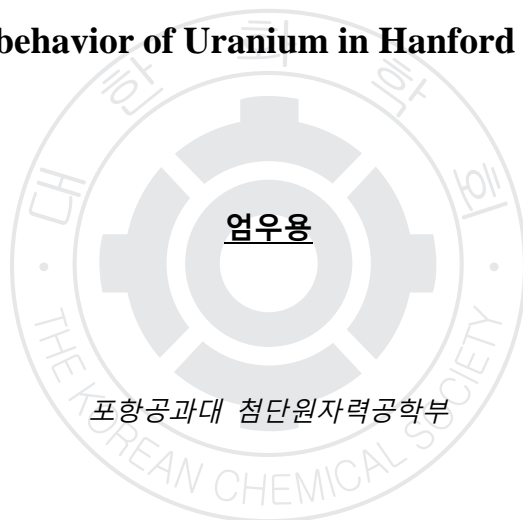
장소: 일산KINTEX

발표코드: ENVR1-6

발표분야: The behavior of radioactive chemical species and heavy metals in subsurface environments

발표종류: 심포지엄, 발표일시: 목 11:50, 좌장: 백민훈

## Transport behavior of Uranium in Hanford vadose zone



Different uranium solid phases were determined using macroscopic and spectroscopic investigations (XAFS, XRF, and TRLIF) using Hanford contaminated vadose zone sediments. Hexavalent uranium, U(VI) exists as different surface phases at different depths below ground surface (bgs). Secondary precipitates of U(VI) silicate precipitates (boltwoodite and uranophane) were present dominantly in shallow-depth sediments (15-16 m bgs), while adsorbed U(VI) phases and polynuclear U(VI) surface precipitates were considered to dominate in intermediate-depth sediments (20-25 m bgs). Because U(VI) silicate precipitates dominate in the shallow-depth sediments, the released U(VI) concentrations result from both desorption and dissolution processes. However, U(VI) located in the deep vadose zone is believed to discharge to the Columbia River by desorption. The U(VI) desorption reaction was best described as an equilibrium surface complexation reaction. The noted differences in desorption behavior appear to result from U(VI) contamination and hydrologic history as well as sediment carbonate content.

Insights are provided on the dynamic adsorption/desorption behavior of uranium contaminant in linked groundwater/river systems in vadose zone environment.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ENVR2-1

발표분야: Biomass-based energy and biomaterials

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 한종인

## **The Current Challenges and Solutions to Algal Biofuels and Bioproducts Research and Development: A Perspective from the National Alliance of Advanced Biofuels and Bioproducts (NAABB)**

박민성

Los Alamos 국립연구소 Bioscience Division

Recently biomass-derived fuels have received increasing attention as a solution to US's continued and growing dependence in imported oil, which exposes US to the risk of critical disruption in fuel supply, creates economic and social uncertainties for individuals, businesses, and national security. By the establishment of The Energy Independence and Security Act of 2007, US recently revived investment in algal biofuels. Through appropriate dollars and the American Recovery and Reinvestment Act of 2009, US has been investing in a variety of research, development, and demonstration (RD&D) projects that seek to identify key technical and engineering hurdles associated with commercializing algal biofuels. Within this context National Alliance of Advanced Biofuels and Bioproducts (NAABB) was created to identify key challenges and propose solutions to produce algal biofuels and bioproducts that are economically viable and environmentally sound. The overall goal of the NAABB is to produce new



technologies that can be implemented by our commercial partners and others developing the algal biofuel industry. In order to achieve this goal, NAABB program incorporates major objectives in Algal Biology, Cultivation, Harvesting/Extraction, and Conversion to fuels, Co-product development, and Economic/energy-balance modeling and resource management components that will establish the technologies' viability for overall sustainability. As the original organizer and a lead research institute of NAABB, Los Alamos National Laboratory (LANL) has been developing algae growth enhancer technology, algal systems biology pipeline that includes the algal genomics resource, stable-isotopes assisted MS/NMR-based metabolomics, and algal genetic transformation technology. LANL also developed technologies for low-energy algal harvest and extraction, CO<sub>2</sub> capture and storage, fuel conversion and water quality control technologies. In this presentation the membership, technical highlights of NAABB and the current algal biofuels and bioproducts researches at LANL will be discussed. Additionally, the talk will review other major RD&D and investment activities in algal biofuels and bioproducts in U.S. (This work is supported by US-DOE grant DE-EE003046 awarded to NAABB).



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ENVR2-2

발표분야: Biomass-based energy and biomaterials

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 한종인

## Application of wastewater and carbon dioxide for cost-effective microalgae cultivation in biodiesel production

이태호

부산대 사회환경시스템공학부 환경공학전공

Modern society demands new energy sources which are sustainable, environment-friendly, and bioenergy has the potential because photosynthetic plants produce biomass using light energy from carbon dioxide. Therefore, mass cultivation of microalgae expects to mitigate greenhouse gas (GHG) emissions by enabling the direct utilization of fossil-fuel originated CO<sub>2</sub>. By the way, photosynthetic organisms essentially demand nutrients such as nitrogen and phosphorus for their living, so they should be supplemented externally. For economic cultivation of microalgae, several wastewaters sampled from a WWTP in Busan were tested for a nutrient source and carbon dioxide was applied to promote algal growth and lipid production. To get effective microalgae having high lipid productivity, but the strains should utilize nutrients in wastewaters as well as high concentration of CO<sub>2</sub> in flue gases as a carbon source, several domestic microalgae tolerant to high concentration of CO<sub>2</sub> (to 30%) were isolated from the water stream of Nak-dong river, and analyzed of their growth and lipid production. Considering

complain about the expensive production cost when it is compared with fossil-based fuels, it will be a reducing way of the production cost to realize biodiesel production from microalgae.



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장소: 일산KINTEX

발표코드: ENVR2-3

발표분야: Biomass-based energy and biomaterials

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 이태호

## **Optimal design of scalable photo-bioreactor and strain improvement for photoautotrophic culture of *Haematococcus pluvialis***

최승필

고려대 화공생명공학과

In photoautotrophic culture of *Haematococcus pluvialis*, both a development of photobioreactor and a strain improvement are important for the economic astaxanthin production. An low-energy multi-tubular photobioreactor were optimized in terms of performance factors, such as a slope of a V-shaped bottom design, a volumetric flow rate of air, a ratio of height/diameter and diameter of an air sparger. Consequently, through the optimization of photobioreactor, 2.62 g/L of the biomass density and 78.37 mg/L of astaxanthin concentration were obtained. In order to shorten the astaxanthin induction time, highly photoinducible mutant in photoautotrophic condition was made by enhancing inherent photosensitivity of *Haematococcus* cells using conventional random mutagenesis and well-defined isolation method (PS-PP). It was observed that the enhanced light-sensitive phenotype was associated with a partial lesion in photosystem II and elicited an improved astaxanthin production from an effective encystment and carotenogenesis. As a result, the concentrations of cell biomass and astaxanthin were

dramatically increased by 19% and 64% under strong light and 40% and 126% under moderate light, respectively. These two developments will improve the yields of astaxanthin in photoautotrophic culture system and lead to economic production of astaxanthin using *H. pluvialis*.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ENVR2-4

발표분야: Biomass-based energy and biomaterials

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 이태호

## Climate change and microalgae

안치용

한국생명공학연구원 환경바이오연구센터

Recently, microalgae are attracting global attention, as the most probable solution to both of climate change and alternative energy source. Throughout the history of the earth, microalgae have been representative determinants of climate change. Cyanobacteria, the first oxygenic photosynthesizers, started to provide oxygen to the primeval atmosphere of the earth 3.5 billion years ago, reducing carbon dioxide. Microalgae made not only the atmosphere, but also the ocean's chemistry. Particularly, the equatorial and subarctic Pacific Ocean was observed to be relatively low in phytoplankton growth, in spite of rich macronutrients (nitrate and phosphate). These regions were named as "high-nutrient, low-chlorophyll (HNLC)" areas. Iron is a micronutrient for microalgae, but indispensable to photosynthesis and nitrogen fixation. Iron addition to these regions promoted algal growth, increasing CO<sub>2</sub> uptake. Some species of phytoplankton also produced dimethyl sulfide (DMS) that acts as nuclei for cloud formation, which in turn reflects more sunlight from the earth, ultimately cooling the atmosphere. Although such large scale manipulation is expected to give an actual and prompt impact on climate change, its practical

efficacy and safety on aquatic ecosystems are still in controversy. Besides their effects on climate, microalgae are the most promising bioenergy source. Microalgal lipid productivity is incomparably higher than those of plants. Furthermore, microalgae can be cultivated in freshwater or seawater, evading competition with crops for limited lands. If a large-scale cultivation could attain the productivity of lab experiments and defend against contamination, algae-derived bioenergy would be able to substitute fossil fuels in the near future.



일시: 2012년 4월 25~27일(수~금) 3일간

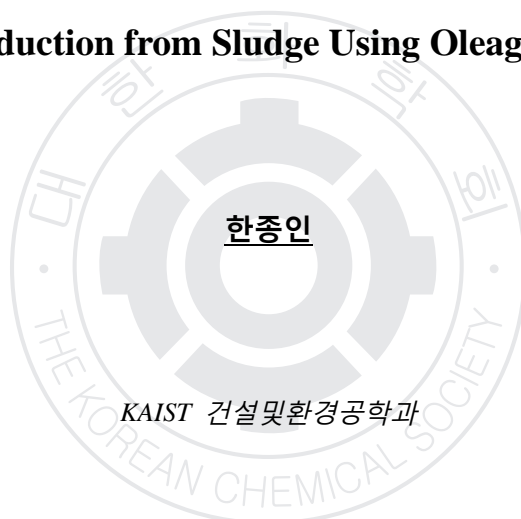
장소: 일산KINTEX

발표코드: ENVR2-5

발표분야: Biomass-based energy and biomaterials

발표종류: 심포지엄, 발표일시: 목 16:35, 좌장: 이태호

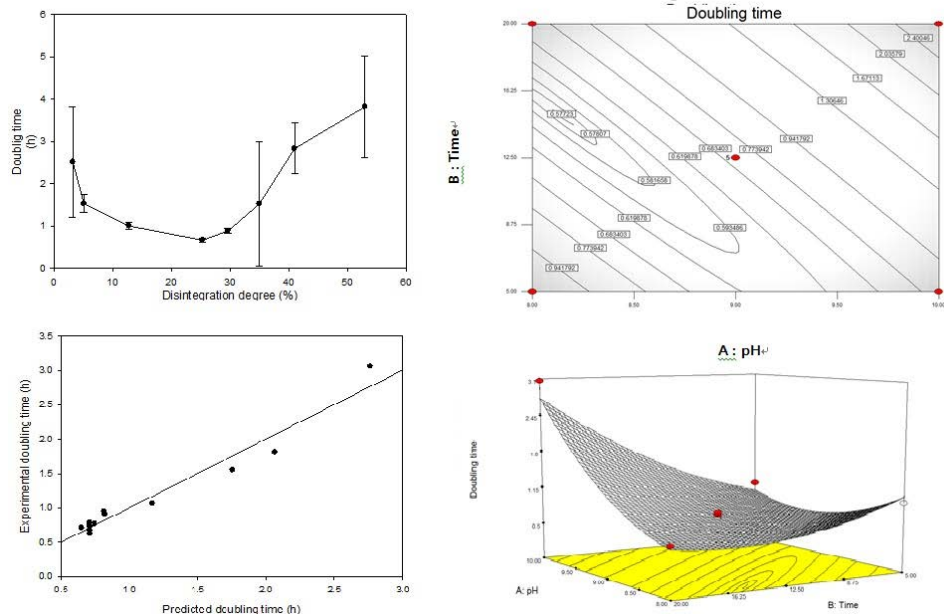
## Bio-oil Production from Sludge Using Oleaginous Yeasts



Recently, biodiesel, especially produced via microbes, has received wide attention as a renewable, biodegradable, and environmentally friendly fuel. There have been a meaningful amount of reports on oil-producing microorganisms, collectively called oleaginous microbes, but these studies have mainly focused on photoautotrophic cells. While the phototrophic oil production certainly has advantages such as the use of free energy and the consumption of a greenhouse gas, it requires much more intensive research to be even considered for its commercial commercialization. This is true, because the phototrophs, such as microalgae, grow slowly and only to the limited density. Heterotrophs, on the other hand, grow sufficiently fast and to high enough cell density. Cultivation can also be relatively easily done, as it is almost identical to the well-established fermentation (Miao and Wu, 2006). Nevertheless, the application of heterotrophic culture to biodiesel production has been questioned, as feedstock, instead of free energy and carbon, must be supplied for their cultivation and in general it is economically unviable. In fact, approximately 50% of expense for the heterotrophic cultivation results from the medium. Caron source,



such glucose, is estimated to account for around 80% of total medium cost (Li et al., 2007). In order to attain the economic feasibility, therefore, there is absolute need of the reduction of the cost of medium cost, particularly carbon sources. To this end, this study explored if activated sludge could support the growth and oil-accumulation of well-known oleaginous yeasts, *Cryptococcus curvatus*.



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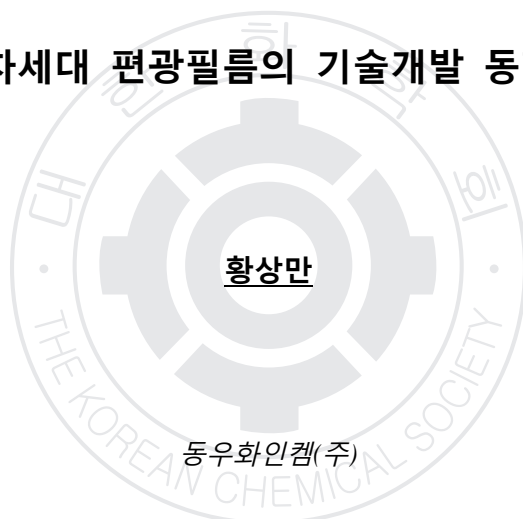
장소: 일산KINTEX

발표코드: KCS1-1

발표분야: Current Trends in Display Materials with 동우화인켐㈜

발표종류: 심포지엄, 발표일시: 목 14:45

## 차세대 편광필름의 기술개발 동향



최근 급변하고 있는 디스플레이 시장에서 디스플레이의 메가 트렌드에 따른 편광필름의 개발동향을 짚어보고 차세대 편광필름에 요구되는 특성 및 이를 극복하기 위한 핵심기술을 소개하고자 한다. 편광필름의 기술동향과 차세대 핵심기술을 설명하기 앞서 Multi Layer 필름으로 구성된 편광필름의 각 Layer 별 기능과 특성, 특히 표면처리 필름 기술, 위상차 보상필름 기술, PVA 편광자 연신기술에 대한 원리 소개와 더불어서 휴대폰, 노트북, 태블릿 PC 및 TV 에 사용되는 편광필름의 종류 및 요구 특성에 대하여 기술하였다. 이와 같은 기술을 바탕으로 차세대 편광필름이 갖추어야 할 특성 및 이를 구현하기 위한 핵심기술에 대한 소개 및 방향성을 논하였다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS1-2

발표분야: Current Trends in Display Materials with 동우화인켐㈜

발표종류: 심포지엄, 발표일시: 목 15:40

## 터치패널용 차세대 투명전극 소재 기술 현황

김한기

경희대 정보전자신소재공학과

투명 전극 소재는 저항막 방식/정전용량 방식의 터치패널 (TSP)의 핵심 소재로 다양한 투명 전극 소재를 응용하기 위한 연구가 진행되고 있다. 저항막 방식에서는 ITO 투명 전극의 접촉에 의한 전기적 신호를 발생시키기 때문에 500 Ohm/square 이상의 면저항의 투명 전극이 사용되나, 정전용량 방식의 경우 사람의 손과 TSP 간에 발생하는 정전용량의 변화를 인식하는 전극으로 사용되기 때문에 200-300 Ohm/square 영역의 면저항을 갖는 투명 전극을 적용하고 있다. 특히 TSP의 사이즈가 증가함에 따라 더욱 낮은 면저항을 갖는 투명 전극의 개발이 필요한 상황이다. 이에 본 발표에서는 현재 TSP에 사용되는 ITO 투명 전극 소재의 연구 동향과 PEDOT:PSS, CNT, Graphene, Ag Nanowire와 같은 차세대 투명 전극 소재의 기술현황을 소개한다. 인듐의 가격 상승으로 다양한 저가형 투명 전극 소재가 ITO를 대체하기 위해 국내외 적으로 개발중에 있으며 ITO의 단점을 개선할 수 있는 다양한 투명 전극 기술이 제안되고 있다. 그러나 아직까지 각 투명 전극 소재가 가진 문제점으로 인해

ITO 의 장벽을 넘지 못하고 있는 실정이다. 이러한 문제점을 해결하기 위해 연구진이 개발하고 있는 다양한 투명 전극 소재와 고이동도 투명 전극 소재, 산화물-금속-산화물 다층 투명 전극의 장단점과 터치패널 응용가능성을 제시하고 ITO 대체 가능성에 대해 논한다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS1-3

발표분야: Current Trends in Display Materials with 동우화인켐㈜

발표종류: 심포지엄, 발표일시: 목 16:30

## Color Photo Resist for White OLED



“기능성 칼라린트(Functional Colorants)”는 섬유 및 고분자 착색제(염료)로서의 단순기능에서 차별화 된 특정 광학적 특성과 성능 발현이 가능한 색소를 의미하며, 구체적으로는 디스플레이 (LCD, PDP, OLED, e-paper), 광 기록 매체 (BD-R, DVD), 특수 광학용 부품 (NIR Film, Security 및 Agricultural Film)의 핵심 소재로 응용할 수 있는 p 전자 공액계 유기 소재를 지칭한다. 착색이라는 고전적 의미와 기능에서 벗어나서 외부의 에너지 자극(전기 및 광학)에 의해 가시광선 및 근적외선 영역의 에너지를 흡수 또는 방출하는 기능적 역할로 인해 정보·전자매체의 핵심 소재로 응용 및 활용되고 있다. 본 발표에서는 -chromophore 의 분자 화학적인 해석과 이론적 지식을 기초로 하여 정보재료 및 소재로서의 응용과 활용에 대해 소개하고자 한다. 특히, Polyacrylate 의 합성과정에서 부산물로 얻어지는 HCN 의 4 량체(tetramer)인 Diaminomaleonitrile(DAMN)로 부터 합성 가능한 Dicyanopyrazine 유도체는 형광모체나 전자 수용체로서의 매우 유용한 결과를 얻을 수 있었고, 또한 차세대 기능성 화합물로서 다양한 연구 결과를 소개하고자 한다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-1

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김성진

## Development and Biological Applications of Electrochemical Microsensors

이영미

이화여대 화학나노과학과

There have been many research efforts for developing sensing methods to monitor various important biological species within confined area. As one of these efforts, in this presentation, we demonstrate the development of electrochemical microsensors and their applications for detecting one or two different biological molecules simultaneously in living biological samples. The analytical performances (i.e., sensitivity, selectivity, detection limit, response time, stability, etc.) of these microsensors are characterized. Our target analytes include nitric oxide (NO), carbon monoxide (CO), well known for its crucial functions as a vasodilator, a neurotransmitter; oxygen ( $O_2$ ) essential for sustaining the lives of most living organisms; glucose main indicative factor in diabetes . In fact, blood flow/volume, i.e., oxygen supply, is regulated carefully by vasodilation/vasoconstriction where NO and CO are important signaling molecules. Therefore, it is of great interest to measure these gases simultaneously in biological

environments. The simultaneous measurements of NO/CO or NO/O<sub>2</sub> in living biological tissues are also presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-2

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 김성진

## Design and Synthesis of Inorganic Functional Materials for Energy Applications



문회리

울산과학기술대 친환경에너지공학부

One of the biggest issues in today's global economy is energy, and thereby enormous efforts have been devoted to the developments of novel materials for energy applications. Especially, in conjunction with pressing needs for the "environmentally benign" clean energy that can replace fossil fuel, the development of hydrogen storage and carbon dioxide capture materials have emerged as today's edge-cutting research. This talk will introduce the synthetic strategies of high-performance alkaline earth metal hydrogen storage materials. The magnesium nanoparticles, which is one of the most promising hydrogen storage materials, can be prepared by the well-designed synthetic methods to be air-stable and highly efficient hydrogen storage materials.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-3

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 김성진

## Nanobiotechnology for Drug Development and Drug Delivery



Recently, various nanomaterials are being harnessed as critical components of bioanalytical systems such as gold nanoparticles for sensing DNA-related biochemical changes. 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 some limitations of conventional assay methods?detection limits, cost issues, labors, efficiencies, quantitateness, reproducibility, etc. In this talk, I will introduce recent efforts to utilize “graphene oxide” for the development of bioanalytical systems and biotechnological tools. In addition, I will discuss on the efforts towards successful interfacing of graphene for biosystems.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-4

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 민달희

## Size-Controlled Self-Assembly of Magneto-Polymersomes

**So-Jung Park Rob Hickey**

*Department of Chemistry, University of Pennsylvania, USA*

Here, we present the size-controlled self-assembly of nanoparticles and amphiphilic block-copolymers. Three distinct structures were fabricated by controlling the solvent-nanoparticle and polymer-nanoparticle interactions: 1) polymersomes densely packed with magnetic nanoparticles (magneto-polymersomes), 2) core-shell type polymer assemblies where nanoparticles are radially arranged at the interface between the polymer core and the shell (magneto-core shell), and 3) polymer micelles where nanoparticles are homogeneously incorporated (magneto-micelles). We show that the incorporation of nanoparticles drastically affects the self-assembly structure of block-copolymers by modifying the relative volume ratio between the hydrophobic block and the hydrophilic block. The size of polymersomes was effectively controlled by varying the size of incorporated nanoparticles. Furthermore, we demonstrated that the morphology of nanoparticle-encapsulating polymer assemblies significantly affects their magnetic relaxation properties, emphasizing the importance of the self-assembly structure and nanoparticle arrangement as well as the size of the assemblies.

일시: 2012년 4월 25~27일(수~금) 3일간

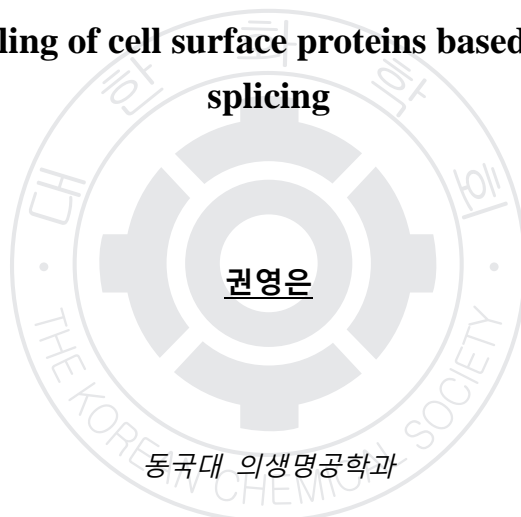
장소: 일산KINTEX

발표코드: KCS2-5

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 민달희

## Site-specific labeling of cell surface proteins based on protein trans-splicing



It is important to visualize movement of proteins in live cell without interfering their original function. Here we describe a highly specific and robust method for labeling cell surface proteins with synthetic probes. The method uses the trans-splicing reaction of *Nostoc punctiforme* (Npu) DnaE split-intein. The trans-splicing reaction is a self-processing reaction and can be used for introduction of various synthetic probes to target proteins with a minimal size linker. In this work, we utilized cell surface proteins fused to N-terminal fragment of Npu. DnaE Intein and C-terminal fragment of Npu. DnaE Intein fused to a fluorescent probe. The expressed model proteins were successfully labeled with synthetic fluorescent probes through specific interaction between N- and C-fragment of inteins within 30 mins. No external energy was required for the labeling reaction. This improved labeling method will provide a useful tool for studying functions and mobilities of proteins in live cells.

일시: 2012년 4월 25~27일(수~금) 3일간

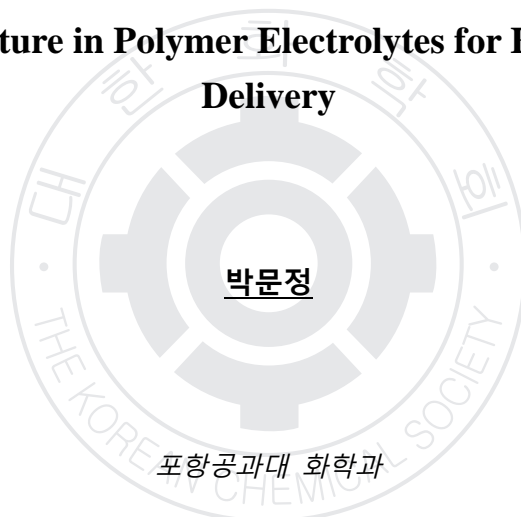
장소: 일산KINTEX

발표코드: KCS2-6

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 민달희

## Role of Nanostructure in Polymer Electrolytes for Energy Storage and Delivery



The growing threat of an energy crisis is drawing major public attention in recent days. There are rising demands for developing more efficient energy materials to stem the depletion of fossil fuels. This has prompted significant research efforts on proton exchange fuel cells and lithium batteries. 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. How parameters such as self-assembled nanostructures, domain sizes, and domain orientations affect conductivities of PEMs will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-7

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 박소정

## DEVELOPING A MOLECULAR FRAMEWORK FOR UNDERSTANDING MOLECULAR ASSEMBLY AT COMPLEX INTERFACES

**Geraldine L. Richmond**

*Department of Chemistry, University of Oregon, USA*

Over the past decade we have witnessed many exciting advances in the laboratory towards the development of new materials, in the area of molecular architecture and nanoscience, as well as in the development of new “bio-inspired” materials that seek to emulate materials that have evolved in nature. Many of these new materials are being made in more complex and reactive environments than in the past where vacuum or clean-room conditions were traditionally used. The assembly of thin films at liquid/solid and liquid/liquid interfaces fall into this category as well the multitude of unique nanostructured materials that assemble in solvents and at surfaces. We have also begun to see advances in moving the synthesis and assembly of these materials to more environmentally benign solvents, such as in aqueous solutions, where complex interactions between the water solvent and the largely hydrophobic material can play a controlling role. This increased complexity of the materials growth environment is usually accompanied by less predictability, often because of our limited knowledge of the fundamental

molecular interactions that lead to the assembly and stability of molecules at these interfaces. This presentation gives an overview of ongoing research in my laboratory that is aimed at obtaining a molecular level picture of the adsorption and assembly of surfactants, nanoparticles and macromolecules from aqueous solution to both solid and fluid surfaces. We employ both experimental and computational methods to unravel the complex structural, reactive and bonding interactions present at these interfaces. These fundamental studies have direct relevance to many important areas of technological interest including environmental remediation, waste water treatment, green chemistry, materials growth, surface wetting and hydrophobicity, and macromolecular assembly.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: KCS2-8

발표분야: Developing Bonds Between Women Chemists in the U.S. and Korea

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 박소정

## Developing Bonds Between Women Chemists in the U.S. and Korea

**Geraldine L. Richmond**

*Department of Chemistry, University of Oregon, USA*

In nearly every country around the world women face higher barriers to success in science and engineering relative to their male colleagues; barriers that deprive the world of an important source of talent. In 1997 a group of women chemists in the United States formed an organization called “COACH” (Committee on the Advancement of Women Chemists) with the goal of reducing these barriers and to also providing important mentoring, friendships and networking to help women chemists in their career advancement. This presentation will describe COACH, its programs, its successes in advancing the careers of women chemists in the U.S. and its growing international programs to help develop similar supportive networks for women scientists in developing countries.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.O-1

발표분야: General Oral Presentation

발표종류: 분과기념강연, 발표일시: 금 10:00, 좌장: 이인수

## Synthetic Methods of Preparing Composite Silica Nanoparticles and Quantitative Modification of Their Surfaces



이진규

서울대 화학부

We have developed various synthetic methods to prepare fluorescent/magnetic silica nanoparticles. Size-controllable fluorescent/magnetic silica nanoparticles having various fluorescent colors were successfully synthesized by the modified Stober method from TEOS and derivatized fluorescent organic dye molecules in the presence of magnetic nanoparticles. They are highly dispersible in alcohol and water at a wide range of pH from acidic to basic, along with good thermal and photochemical stabilities. The continuous monitoring experiments with several cell types clearly showed that our fluorescent nanoparticles did not affect the proliferation of cells and they could be used for long-term and multiple-times bio-imaging systems. The surface modification technique was also very important to utilize silica nanoparticles into various applications such as biological specific targeting purposes and polymer/nanoparticle composites. We have recently found the easy and simple modification method of nanosilica surfaces with amino-functional trialkoxysilanes such as aminopropyltrimethoxysilane (APTMS)



and (3-trimethoxysilylpropyl)diethylenetriamine (DETAS) to generate monolayer modification. We were able to quantitatively analyze the number of amine functional groups on the modified SiO<sub>2</sub> nanoparticles by acid-base back-titration method, and determine the effective number of amine functional groups for the successive chemical reaction by the fluorescence-tagging method. We believe that our method to generate monolayer modification and analyze the number of amine sites on nanoparticle surface will be useful in nano-bio research applications, such as sensors, diagnosis, and drug or gene deliveries, where reliable and reproducible modification and quantitative analysis are very critical.



일시: 2012년 4월 25~27일(수~금) 3일간

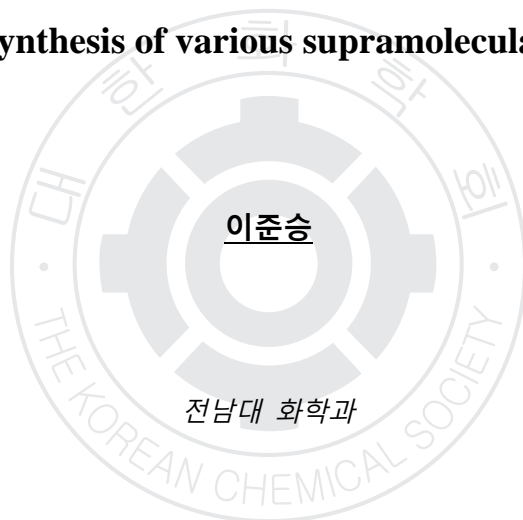
장소: 일산KINTEX

발표코드: INOR.O-2

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 이인수

## Selective synthesis of various supramolecular polygons



We present a general strategy for the synthesis of stable, multicomponent fused polygon complexes in which coordination-driven self-assembly allows for single supramolecular species to be formed from multicomponent self-assembly and the shape of the obtained polygons can be controlled simply by changing the ratio of individual components. If the vertex or edge of polygons shares, fused polygons can be prepared easily. From this simple idea, we made the edge-shared double triangle and rectangle polygons. Also, the vertex-shared double hexagon system and edge-shared double and triple hexagon systems have been prepared. The shape and size of supramolecules have been controlled by the stoichiometric control of multiple different donors and accepters.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-3**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 이인수

## **Porous Metal-adeninate Crystalline Materials: Design, Synthesis and Emerging Properties**

안지현

서울대 화학교육학과

Porous materials constructed from bio-compatible and environmentally-friendly constituents could potentially be useful for a variety of applications in areas such as environmental clean-up, greenhouse gas sequestration, the food industry, and medicine. We are developing a coordination-chemistry based approach for designing and constructing crystalline porous materials using biocompatible metal-ions and biomolecules. Here, we describe several representative examples of such materials: a macrocyclic zinc-adeninate species, and biomolecular metal-organic frameworks (bioMOF-1, bioMOF-11, and bioMOF-100). We examine their porosity through gas sorption studies, and we show that their intrinsic porosity leads to new and unusual properties that will render these materials useful for a range of biological and environmental applications.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.O-4

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이인수

**Redox-active Metal-organic Framework Supported Palladium  
Nanoparticles for CO Oxidation: In situ Generated Active Species  
during Catalytic Reaction**

문회리

울산과학기술대 친환경에너지공학부

MOF-based catalysis has recently emerged as a burgeoning subfield of heterogeneous catalysis. The catalytic functions of MOFs are endowed by active metal sites and/or reactive organic groups that constitute the frameworks of MOFs. In addition, the incorporation of catalytic metal nanoparticles (NPs) into the cavities of MOFs can also impart catalytic function. Herein we will present the preparation of redox active MOFs supported Pd nanocatalysts via the redox-couple-driven method, and their catalytic applications toward CO oxidation. We prepared Pd NPs on the redox-active Ni-carboxylate-based MOF (Pd@ra-MOF) for CO oxidation. The Pd@ra-MOF was found to be a highly active catalyst for CO oxidation. Significantly, Pd@ra-MOF is transformed during the catalytic reaction into a PdOx-NiOy/C nanocomposite to generate catalytically superior species in situ, and the resultant nanocatalyst shows sustainable activity through synergistic stabilization.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.O-5

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 이인수

## Theoretical investigation of magnetic structure and optical properties on Cs<sub>2</sub>AgF<sub>4</sub>

**이창훈** Jianwei Tong<sup>1</sup> Juergen Koehler<sup>1</sup> Arndt Simon<sup>1</sup> Myung-Hwan Whangbo<sup>2</sup> **심지훈**

포항공과대 화학과 <sup>1</sup>MPI for Solid State Research, Stuttgart <sup>2</sup>North Carolina State University

Cs<sub>2</sub>AgF<sub>4</sub> [1] containing the unusual Ag<sup>2+</sup> (d<sup>9</sup>) ions occurs in the tetragonal K<sub>2</sub>NiF<sub>4</sub> layered perovskite structure and is isotopic to La<sub>2</sub>CuO<sub>4</sub>, the parent of the high-temperature superconducting cuprates. Cs<sub>2</sub>AgF<sub>4</sub> has attracted much attention, because it undergoes a phase transition into a ferromagnetic state at low temperature [2], whereas the isostructural homologues K<sub>2</sub>AgF<sub>4</sub> and Na<sub>2</sub>AgF<sub>4</sub> undergo a phase transition into an AFM state at low temperatures. A number of theoretical studies [3,4] on the magnetic properties of Cs<sub>2</sub>AgF<sub>4</sub> have been carried out to show that the orbital order takes place in each AgF<sub>4</sub> layer such that the magnetic orbitals of adjacent Ag<sup>2+</sup> ions become orthogonal to each other, thereby leading to no overlap between them and hence a FM spin exchange between nearest-neighbor Ag<sup>2+</sup> ions [6]. The optical properties of Cs<sub>2</sub>AgF<sub>4</sub> have not been well studied. In connection with the question of possible superconductivity, the optical-conductivity of Cs<sub>2</sub>AgF<sub>4</sub> was recently calculated based on density functional theory (DFT). In the present work we examine the optical spectra of the modena colored

Cs<sub>2</sub>AgF<sub>4</sub> by UV-vis spectroscopy and interpret the results on the basis of DFT electronic structure calculations for Cs<sub>2</sub>AgF<sub>4</sub>[1] R. H. Odenthal, D. Paus, Z. Anorg. Allg. Chem. 1974, 407, 144. [2] S. E. McLain, M. R. Dolgos, D. A. Tennant, J. F. C. Turner, T. Barnes, T. Proffen, B. C. Sales, R. I. Bewley, Nature Materials 2006, 5, 561.[3] D. Dai, M.-H. Whangbo, J. Kähler, C. Hoch, A. Villesuzanne, Chem. Mater. 2006, 18, 3281.[4] a) D. Kasinathan, H. Rosner, Phys. Rev. Lett. 2007, 99, 247210. b) X. Hao, D. Zhou, X. Liu, J. Meng, Phys. Rev. B 2007, 76, 054426. c) H. Wu, D. I. Khomskii, Phys. Rev. B 2007, 76, 155115.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-6**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 문회리

## **Inorganic Porous Nanohybrids for Advanced Electrochemical and Catalytic Applications**

백승민

경북대 화학과

Recently, heterostructured nanomaterials have attracted considerable research interest, due to their unique physicochemical properties, which cannot be obtained by conventional solid-state reactions. The fabrication of layered nanomaterials has been demonstrated through controlled synthetic techniques including intercalation, exfoliation-reassembling, and pillaring reactions. Such soft-chemical methods give rise to an almost unlimited set of new nanoporous hybrid compounds with a large spectrum of desirable properties. Due to the unique two-dimensional structures and properties, various kinds of functional nanohybrid materials can be utilized as photocatalysts and electrode materials. For instance, the electrochemical performance of layered molybdenum oxide and graphene nanosheet as electrode materials for lithium rechargeable batteries, would be improved by the introduction of porosity through the hybridization method. In addition, the physicochemical properties of the fabricated nanohybrids could

be finely tailored at a molecular level to optimize their applicability as photocatalysts and dye-sensitized solar cells.





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장소: 일산KINTEX

발표코드: INOR.O-7

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:15, 좌장: 문회리

## Europium-doped Gadolinium Sulfide Nanoparticles as a Dual-Mode Imaging Agent for T1-weighted MR and Photoluminescence Imaging

정종진 김미애 이승재<sup>1</sup> 양일승<sup>2</sup> 김성근<sup>2</sup> 박정규<sup>3</sup>

한국화학연구원 나노기술융합연구단 <sup>1</sup>연세대 화학과 <sup>2</sup>서울대 화학부 <sup>3</sup>한국화학연구원 형광물질연구팀

We present a facile synthesis of europium-doped gadolinium sulfide (GdS:Eu<sup>3+</sup>) opto-magnetic nanoparticles (NPs) via sonochemistry. Their photoluminescence and strong paramagnetic properties enable these NPs to be utilized as an in vitro cell imaging and in vivo T1-weighted MR imaging probe. The GdS:Eu<sup>3+</sup> NPs have a prominent longitudinal (r<sub>1</sub>) relaxivity value, which is a critical parameter for T1-weighted MR imaging. Here, we showed not only their strong positive contrast effect to blood vessels and organs of mice, but also blood half-life and biodistribution including clearance from organs, in order to assess the GdS:Eu<sup>3+</sup> NPs as a competent nanocrystal-based T1 contrast agent. We further showed confocal images of breast cancer cells containing GdS:Eu<sup>3+</sup> NPs to evaluate as a photoluminescence probe. Dual-mode imaging capability obtained from the GdS:Eu<sup>3+</sup> NPs will allow target-oriented cellular imaging as well as the resulting disease-specific MR imaging.

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장소: 일산KINTEX

발표코드: INOR.O-8

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 문회리

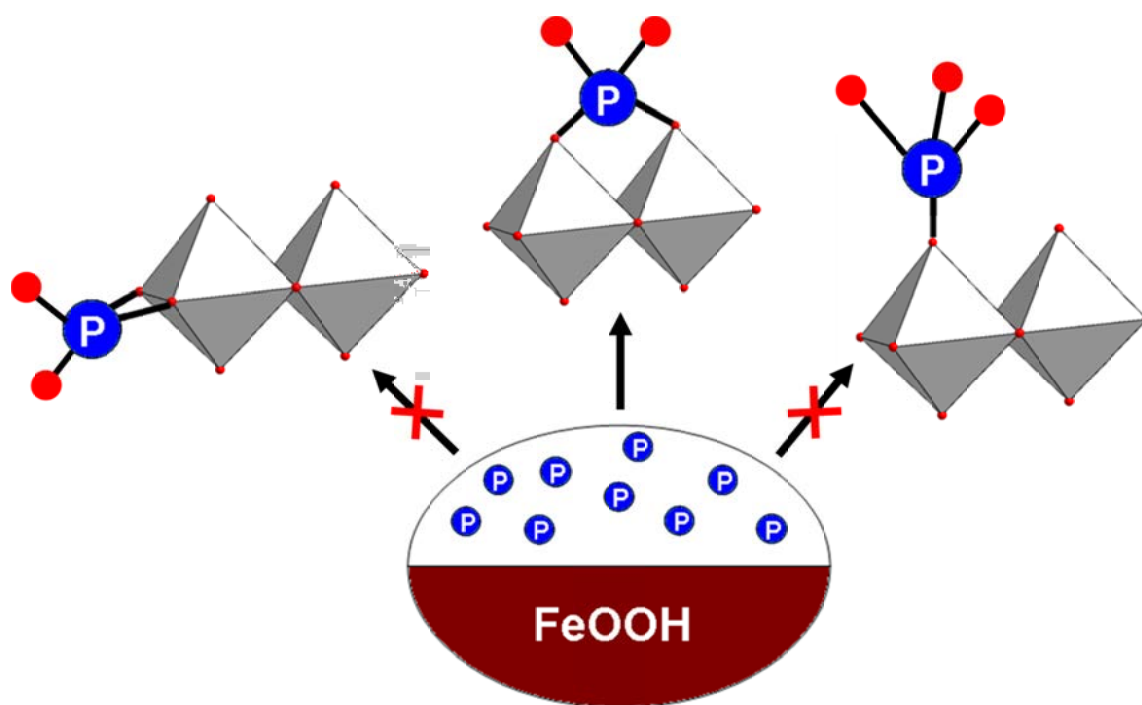
## Phosphate adsorption on the iron oxyhydroxides goethite ( $\alpha$ -FeOOH), akaganeite ( $\beta$ -FeOOH), and lepidocrocite ( $\gamma$ -FeOOH): a $^{31}\text{P}$ NMR Study

김종식 Wei Li<sup>1</sup> Brian L. Phillips<sup>2</sup> Clare P. Grey<sup>3</sup>

동아대 화학과 <sup>1</sup>Delaware Environmental Institute, University of Delaware <sup>2</sup>Department of Geosciences, Stony Brook University <sup>3</sup>Chemistry Department, University of Cambridge

Phosphate adsorption on the surfaces of the iron oxyhydroxide polymorphs goethite, akaganeite, and lepidocrocite were studied by using  $^{31}\text{P}$  static spin-echo mapping NMR experiments to determine how this environmentally-important anion binds to common soil minerals. The large  $^{31}\text{P}$  hyperfine shifts confirm the formation of inner-sphere complexes between the phosphate anion and the iron oxyhydroxide surface, the large shifts indicating the presence of  $\text{Fe}^{3+}\text{O?P}$  covalent bonds. Binding was explored as a function of pH and phosphate concentrations, the phosphate ion binding via two oxygen ions to the oxyhydroxide surface under all conditions and for all the surfaces. To support our analysis of the NMR spectra, adsorption of dimethyl phosphinic acid (DPA) on iron oxyhydroxides was also investigated, since this ion can only bond via one  $\text{Fe?O?P}$  interaction to the surface. The  $^{31}\text{P}$  hyperfine shifts observed for

this anion were 50% of those seen for the phosphate anions, confirming that the phosphate ions bind to the surface via two P=O/Fe linkages.



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장소: 일산KINTEX

발표코드: INOR.O-9

발표분야: General Oral Presentation

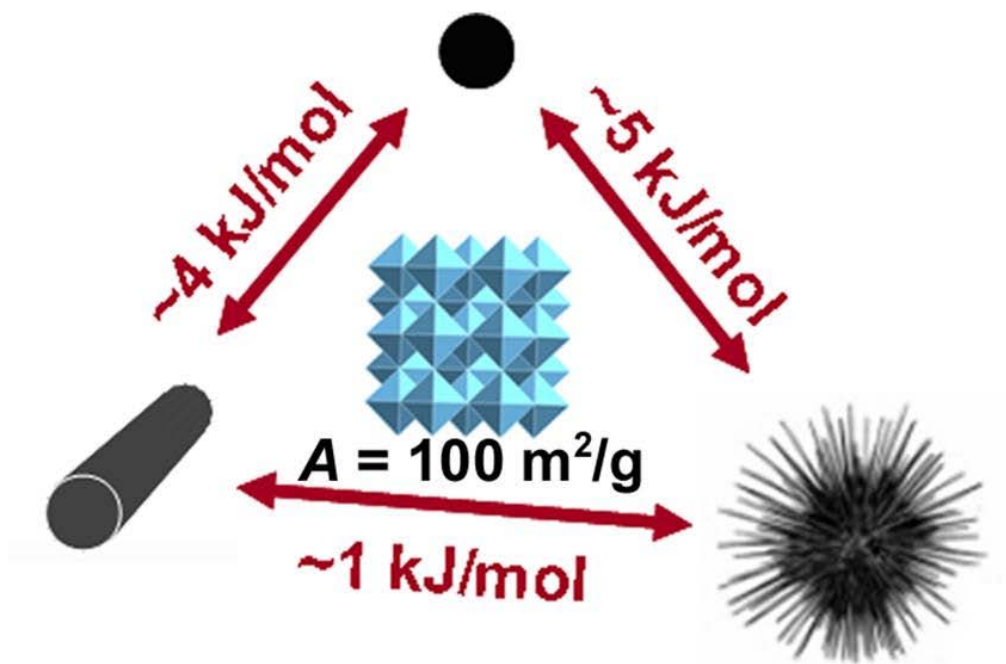
발표종류: 구두발표, 발표일시: 금 12:45, 좌장: 문회리

## Shape-dependent surface energetics of nanocrystalline TiO<sub>2</sub>

박태진 Alexandra Navrotsky<sup>1</sup> Stanislaus S. Wong<sup>2</sup>

한국원자력연구원 방사성폐기물처분연구부 <sup>1</sup>UC Davis <sup>2</sup>SUNY Stony Brook

We report the direct determination of surface enthalpies for nanophase TiO<sub>2</sub> anatase with different morphologies derived from drop solution calorimetry in a molten sodium molybdate solvent at 702 °C. The energetics of surface hydration has been measured using a Calvet microcalorimeter coupled with a gas dosing system. The surface enthalpies of hydrated surfaces for anatase TiO<sub>2</sub> nanoparticles, nanowires and sea-urchin-like assemblies are  $0.51 \pm 0.05$ ,  $1.07 \pm 0.28$ , and  $1.29 \pm 0.16$  J m<sup>-2</sup>, respectively, whereas those of anhydrous surfaces are  $0.74 \pm 0.04$ ,  $1.24 \pm 0.28$ , and  $1.41 \pm 0.16$  J m<sup>-2</sup>, respectively. The trend in TiO<sub>2</sub>, which shows higher surface enthalpies for more complex nanostructures, is consistent with that reported in ZnO. The shape-dependent surface enthalpy at the nanoscale level is discussed in terms of exposed surface structures. The enthalpies of hydration appear to be similar for all morphologies.



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장소: 일산KINTEX

발표코드: **PHYS.O-1**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 석차옥

## Constructing Polarizable Force Fields for Chlorophylls



김현우 이영민

포항공과대 화학과

Protein-ligand interaction is important in investigating the association of various biomolecules and is often studied with the molecular dynamics technique. Polarizable force fields enable us to consider the induction effect in molecular dynamics, which is ignored with conventional force fields. Because the induction effect becomes important when molecules are exposed to various electrostatic environments, detailed dynamics of a ligand embedded in a protein will likely be strongly affected by the induction. In addition, excited state molecules are generally more polarizable than ground state molecules. Thus, polarizable force field will be potentially crucial in performing molecular dynamics simulations in the excited state. Here, as a preliminary effort to simulate photosynthetic pigment-protein complexes with of chlorophylls, we will report a way of constructing polarizable force fields for the chlorophyll molecules in both electronically ground and excited states. Because the electrostatic parameters such as atomic polarizabilities are essential elements for polarizable force fields, we will lay a stress on explaining how

the optimizations of these parameters are performed. Derivations of other parameters will also be explained in a brief way.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.O-2**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 석차욱

## Finding Density Functionals with Machine Learning

**John Snyder Matthias Rupp<sup>1</sup> Katja Hansen<sup>2</sup> Klaus-Robert Muller<sup>2</sup> Kieron Burke**

*Department of Chemistry, University of California, Irvine <sup>1</sup>Machine Learning Group, Technical  
University of Berlin and Institute of Pharmaceutical Sciences <sup>2</sup>Machine Learning Group, Technical  
University of Berlin*

Machine learning is used to approximate density functionals. For the model problem of the kinetic energy of non-interacting fermions in 1d, mean absolute errors below 1 kcal/mol on test densities similar to the training set are reached with fewer than 100 training densities. A predictor identifies if a test density is within the interpolation region. Via principal component analysis, a projected functional derivative finds highly accurate self-consistent densities. Challenges for application of our method to real electronic structure problems are discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.O-3**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 석차욱

## Internal Cavity Control of Tubule Transformed from Surface Grafted Sheet Polymer

한민우 심은지

연세대 화학과

We investigate internal cavity controlled tubular formation through simple modification of tether coils that are grafted on the surface of 2D polymer sheet. Dissipative particle dynamics simulations show that coarse-grained 2D sheets transform to various cylindrical structures including tubular and filled scrolls in the presence of broken volume and chemical symmetries of tether coils: volume (chemical) asymmetry arises when coils on one side have different number of beads (solvent affinity) from those on the other side. It is clear from a phase diagram that the scroll formation is governed by the balance between hydrophobicity and entropy of coils. The density profiles show that a wide range of interior cavity diameter can be obtained by employing volume asymmetry on coils with weak chemical asymmetry. Also we found that the sheet asymmetry arises from discrepancy in graft configuration on the two surfaces and results in spontaneous scroll formation. We believe this work provides a framework for further research of surface grafted sheet polymers.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 석차옥

## **GalaxyDock: A Flexible Protein-Ligand Docking Program for High-accuracy Binding Mode Prediction**

신윙희 석차옥

서울대 화학부

Protein-ligand docking techniques are one of the essential tools for structure-based drug design. Although conformational changes of protein receptor frequently occur in the binding process, a large fraction of contemporary docking programs ignore receptor flexibility. Consideration of protein flexibility efficiently and accurately in docking studies is challenging due to difficulties in developing accurate scoring function and in sampling conformations efficiently. Previously we developed a docking program called LigDockCSA which incorporates LigDock scoring function that combines AutoDock3 and PLP scoring function and conformational space annealing (CSA) as a sampling method. However, the program treats protein rigid. Here, we present GalaxyDock, an extension of LigDockCSA that accounts for flexibility of pre-selected side-chains of receptor protein in the binding site. To test the performance of the new docking method, 3 proteins that show side-chain conformational changes upon ligand docking were

selected as test sets: HIV-PR, LXR $\beta$  and cAPK. The cross-docking results show that the accuracy of binding pose prediction is increased about 20% when compared with our previous rigid-receptor results.



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발표코드: **PHYS.O-5**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 석차욱

## Molecular dynamics of synthetic chromophore derivatives of green fluorescent protein (GFP)

이정화 Pi-Tai Chou<sup>1</sup> 주태하

포항공과대 화학과 <sup>1</sup>National Taiwan University

The green fluorescence protein (GFP) has been widely used as biological markers in living cells, since it is noninvasive and does not need any substrate or coenzyme to fluoresce. The cyclization and oxidation reaction among three amino acids yield the fluorophore of GFP (p-HBDI). The chromophore without protein matrix shows low quantum yield of fluorescence which can be understood as conformational relaxation leading to radiationless deactivation. For suppression of conformational relaxation, o-HBDI was synthesized as an ortho isomer of p-HBDI. Earlier study revealed that o-HBDI undergoes ESIPT reaction with ultrafast rate. Various derivatives of o-HBDI, which have different functional groups like -Br, -NO<sub>2</sub>, -OMe and -phenyl, are synthesized to clarify the effect of the electronic property to ESIPT reaction. Also the photophysical property results in a wide spectral range of fluorescence, which gives feasibility of application like OLED. The time-resolved fluorescence measurement with high time resolution will unveil the ESIPT dynamics of derivatives of o-HBDI, about 30 fs. The ultrafast proton

transfer can initiate coherent nuclear wavepacket motion in the product keto isomer, which is manifested by the oscillations of the time-resolved signals. Since there are dissimilarity of the vibrational frequencies in spite of the similarity of skeletal geometry, these TRF results are remarkable. We have performed quantum mechanical calculations to understand the origin of oscillatory components appeared in time resolved signals. This theoretical verification can figure out the proper structural change during the reaction and prove the possibility of TRF spectroscopy as an observer which collects the geometrical information of reaction dynamics.



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장소: 일산KINTEX

발표코드: **PHYS.O-6**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 송재규

## **Ultrathin TiO<sub>2</sub> films on ZnO electron-collecting layers of inverted organic solar cell**

**김영독 서현욱**

성균관대 화학과

Nanostructured ZnO thin films were fabricated on Indium Tin Oxide (ITO) as hole-blocking and electron-collecting layers of inverted organic solar cells. In addition, TiO<sub>2</sub> thin films were deposited on ZnO surfaces using atomic layer deposition. Ultrathin TiO<sub>2</sub> layers with a mean thickness of less than 3 nm could enhance photovoltaic performance of the inverted organic solar cell; in particular, short-circuit current (J<sub>sc</sub>) and power conversion efficiency (PCE) were increased by deposition of TiO<sub>2</sub> layers. A higher thickness of TiO<sub>2</sub> resulted in reduced photovoltaic performance. Studies on electronic structure using photoelectron spectroscopy showed that the TiO<sub>2</sub> layers should act as barrier for the electron-collection on ZnO. However, recombination of electrons and holes on the surface of ZnO can be quenched by TiO<sub>2</sub>, resulting in an improved efficiency of the IOSCs. It is demonstrated that atomic layer deposition with a precise control of film thickness can be of potential application for fabrication of energy devices.

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장소: 일산KINTEX

발표코드: **PHYS.O-7**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 송재규

## Novel 3D Hierarchical Gold Templates Based on Networks of Carbon Nanotubes as Substrates for Biosensing Applications

이문근 조석진 조용덕<sup>1</sup> 서정은 김선애 박태정<sup>2</sup> 이해원

한양대 화학과 <sup>1</sup>한양대 나노융합과학과 <sup>2</sup>KAIST 나노종합팹센터 나노바이오융합연구센터

Three-dimensionally (3D) structured gold were directly synthesized on the 3D networks of carbon nanotubes (CNTs) by using electrochemical deposition (ECD). In the line with an issue of the difficulty in 3D mass transfer during ECD process, pulsed DC plating was adopted to assist mass transfer from the outer of 3D structure. The topography of gold nanomaterials constituting a hierarchical structure was varied from nanoparticles to nanowires by ECD conditions. The feasibility of 3D gold templates to biosensing applications was electrochemically and optically investigated. A variety of data were acquired by localized surface plasmon resonance, surface-enhanced Raman scattering, cyclic voltammetry and chronoamperometry. The results indicated the synthetic advantages of 3D hierarchical gold templates in biosensing applications, that originate from the dimensionally lofty structures combined with the inherent talents of gold.

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장소: 일산KINTEX

발표코드: **PHYS.O-8**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 송재규

**Intramolecular charge transfer (ICT) dynamics of 4-(dimethylamino)benzonitrile and its planarized analogue by using highly time-resolved fluorescence**

박명기 주태하

포항공과대 화학과

4-(dimethylamino)benzonitrile is well-known for its dual fluorescence. Since Lippert's work, several models have been proposed such as twisted ICT (TICT) and planar ICT (PICT). Initially, the TICT model, where fully twist of the dimethylamino group is required to undergo the ICT reaction, was widely accepted. However, recent advances on time-resolved techniques including femtosecond transient absorption (TA) and time-resolved fluorescence (TRF) have found evidences for somewhat complicated ICT reaction dynamics of DMABN. In addition, our recent time-resolved fluorescence (TRF) and time-resolved fluorescence spectra (TRFS) of DMABN proposed a multi-faceted ICT process controlled in part by the conformational distribution of the ground state. 1-tert-butyl-6-cyano-1, 2, 3, 4-tetrahydroquinoline (NTC6), a planarized analogue of DMABN, also shows dual fluorescence and it has been considered to be an important evidence for the PICT model. Theoretically, Gomez et al. showed that



the PICT concept cannot be excluded in the ICT reaction, although a recent work by Hüttig et al. indicated that the ICT reaction of the planarized NTC6 proceeds along the twisting coordinate because of the flexibility of the amino group to some extent. We employed highly time-resolved fluorescence measurements at several different wavelengths, and compared those of NTC6 and DMABN. In contrast to those of DMABN, TRFs of NTC6 do not exhibit the ultrafast rise components, and they display essentially the same ICT reaction rates regardless of the solvents used. So, the ICT dynamics of NTC6 is found to be homogeneous rather than the dispersive dynamics found in flexible DMABN.



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장소: 일산KINTEX

발표코드: **PHYS.O-9**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 송재규

## High aspect ratio front silver grid line in crystalline silicon solar cells by controlling rheological properties of silver paste

홍준의 김상호

공주대 화학과

Traditional screen printing is still a dominant process for electrode formation on c-Si solar cells. Therefore, the study of silver paste for high efficiency solar cells has been one of the key issues in c-Si solar cells. Since front electrodes block the incoming light onto the solar cells, resulting in shadowing loss, it is important to construct fine electrode lines with high aspect ratio. In this study, we have studied the rheology of silver paste to achieve fine printing and high aspect ratio. The rheological properties of Ag paste were studied by controlling organic vehicle, and the shape and size of silver particles. Silver paste with high thixotropic index values(Thixotropic index as the ratio of the viscosity at 1s<sup>-1</sup> and viscosity at 100s<sup>-1</sup> at 25°C) and fast recovery behavior(Three stages were created to simulate the paste behavior during printing: I?pre-print, II-print, III-post-print. The first stage represents the paste in the rest on screen, but slightly prestressed from stirring and flooding, in which a minor shear rate of 0.1s<sup>-1</sup>. In the next stage, the shear rate is 1000s<sup>-1</sup>. Under such high shear rate the paste structure was destroyed to reach it

minimum viscosity. In third stage the shear rate returns back to the initial of  $0.1\text{s}^{-1}$ ) are realized and the electrode showed  $\sim 80\text{ }\mu\text{m}$  width and  $>25\text{ }\mu\text{m}$  height. The solar cell made with this silver paste showed improved cell efficiency.

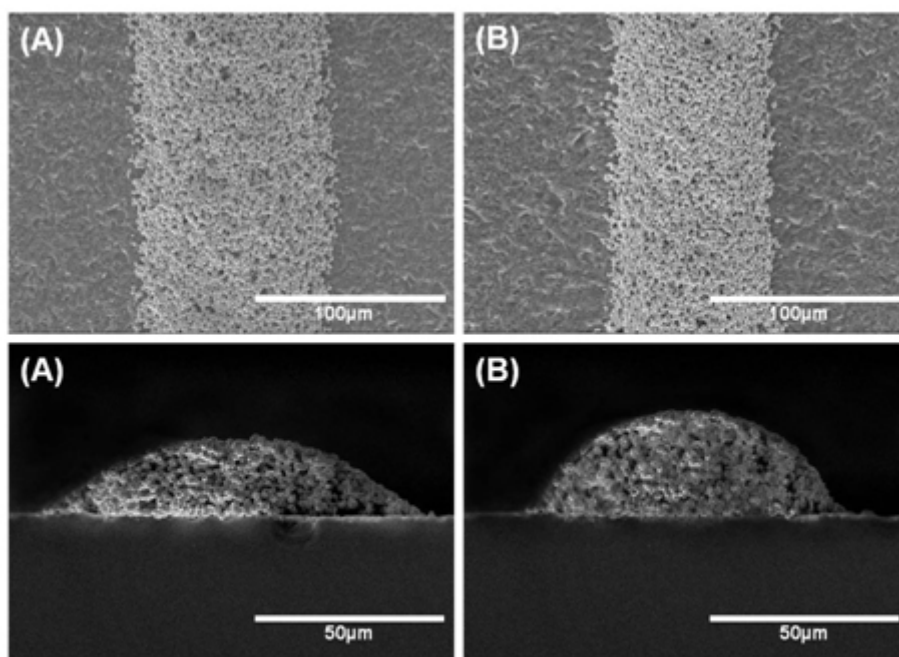


Figure 1. Comparison of conventional electrode (A) and rheology controlled electrode (B)



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발표코드: **PHYS.O-10**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 송재규

## Highly Conductive Flexible Transparent Electrode using Silver Nanowires & Conducting Polymer

서동민

공주대 화학과

As displays become larger and solar cells become cheaper, there is an increasing need for low-cost transparent electrodes. Intensive effort has been made to replace ITO (Indium Tin Oxide) based transparent electrode with cheap and flexible ones. Among those, silver nanowires have got limelight because of its great conductivity and flexibility. Even though the electric property of the Ag nanowire based transparent electrode surpassed ITO, the optical property needs to be improved (lower transmittance, higher haze). Here, we reported transparent electrode based on Ag nanowires and conducting polymer to improve optical properties. The Ag nanowires are coated onto PET films and the resulting transparent electrode film shows 200 ohm/□ resistance and > 90% optical transmittance.



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발표코드: **PHYS.O-11**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 송재규

## **Single-shot Characterization of Electronic Optical Activity Field by Heterodyne detection technique**

**엄인태 안성현 이한주**

한국기초과학지원연구원

Chiroptical spectroscopy such as circular dichroism (CD), optical rotatory dispersion (ORD), Raman optical activity (ROA), etc., has been widely used as structural probe in stereo-chemistry. In the conventional approach, these quantities are characterized by measuring the difference between optical responses of chiral molecule for left- and right- circularly (or elliptically) polarized lights. Because of the weakness of the corresponding signal, however, the measurement is significantly affected by light intensity fluctuation as well as imperfect polarization control. In this regard, we developed a new chiroptical method to overcome such difficulties. A simultaneous heterodyne detection of chiral and achiral free induction decay (FID) signals enables us to realize a self-referenced single-shot characterization of CD and ORD. Combined with proper initiation strategies, this technique will be extended to time-domain OA spectroscopy to investigate structural dynamics of biomolecules and chemical species in real time.

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장소: 일산KINTEX

발표코드: **PHYS.O-12**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 송재규

## **Ultrasensitive and Label-free Detection of Annexin A3 Based on Quartz Crystal Microbalance**

**Md. Mahbubur Rahman**

건국대 신기술융합학과

A detection method for the lung cancer and prostate biomarker protein annexin 3 (ANXA3) was developed using simple label-free ultrasensitive quartz crystal microbalance (QCM) immunosensor based on a quantum dots (QDs) nanoprobe. The QDs nanoprobe was fabricated by covalently attaching carboxylic acid group functionalized cadmium sulfide (CdS) quantum dots on the mixed cystamine (CYS) and mercaptoethanol (MCE) self-assembled monolayer (SAM). Anti-ANXA3 antibody was covalently immobilized on the carboxylic acid group functionalized QDs through the formation of amide bond. The resultant CYS-SAM/QDs/Anti-ANXA3 immunosensor probe was used to detect ANXA3 by monitoring the frequency change. Under the optimized condition, the ANXA3 immunosensor showed a dynamic range between 0.075 and 50 ng/mL with a detection limit of  $0.075 \pm 0.01$  ng/mL ( $75 \pm 10$  pg/mL). The immunosensor could detect ANXA3 as low as 0.1 ng/mL in spiked human blood and urine samples in 15 min without any interference from other proteins.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.O-1

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 신승훈

## Breathing Tubules from Self-Assembly of Non-Covalent Macrocycles

황철강 이명수

서울대 화학과

We have shown that a bent-shaped aromatic amphiphile which can self-assemble into hexameric macrocycles in aqueous solution. The non-covalent macrocycles were observed spontaneously stack on top of each other with mutual rotation in the same direction to form chiral tubes. Within aromatic macrocycles, the adjacent aromatic segments could slide with each other in response to external triggers to reversibly produce expanded and contracted helical tubes. Notably, chiral inversion is accompanied with reversible structure transformation. This structural transition arises from reversible hydrogen bonding between pyridine and water molecules. In addition, the tubules reversibly encapsulate hydrophobic C<sub>60</sub> molecules through hydrophobic interactions. Such one-dimensional aggregates with dynamic structural changes may provide a new strategy for creating intelligent nanomaterials with internal channels. References[1] H.-J. Kim, S.-K. Kang, Y.-K. Lee, C. Seok, J.-K. Lee, W.-C. Zin, M. Lee, *Angew. Chem. Int. Ed.* 2010, 139, 8471.[2] H.-J. Kim, T. Kim, M. Lee, *Acc. Chem. Res.* 2011, 44, 72.



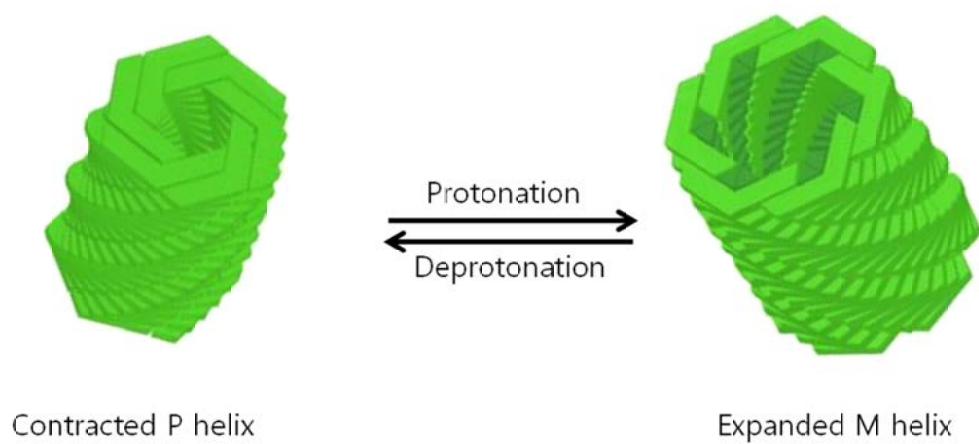


Figure 1; Reversible helical tubular stacking.



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장소: 일산KINTEX

발표코드: ORGN.O-2

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:12, 좌장: 신승훈

## Molecular Basis for the Chiral Recognition of Lipase with Molecular Dynamics

엄희성 하현준 이원구<sup>1</sup>

한국외국어대 화학과 <sup>1</sup>서강대 화학과

Lipase-mediated reactions have been widely used obtaining the enantiomerically enriched products where molecular basis were studied with molecular dynamics (MD). Specifically two cases were studied; 1) BCL-mediated hydrolysis of  $\beta$ -substituted  $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactones 2) desymmetrization of 3-alkylpentanedioates. The favored substrates for hydrolytic reactions mediated by BCL in aqueous media has R configuration of  $\gamma$ -position near the reaction site for  $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactones, trans- $\beta$ -methyl- and  $\beta$ -ethyl- $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactones. However, enantiomeric preference was reversed for the substrates cis- $\beta$ -methyl- and  $\beta$ -ethyl- $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactones, i.e. S configuration of  $\gamma$ -position near the reaction site was favored for the reaction. It may be an evidence that enantioselectivity of enzymic hydrolysis can be controlled and depends on remote stereogenic center. The origin of this reversal stereoselectivity on the BCL mediated enantioselective hydrolysis of  $\beta$ -substituted  $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactones was investigated. Only “Umbrella-like inversion”

model can account for the experimental results. CALB-catalyzed desymmetrization of prochiral 3-alkylpentanedioic acid diesters was succeeded for the preparation of optically active 3-alkylpentanedioic acid monoesters bearing various alkyl substituents including methyl, ethyl, propyl and allyl. Allyl esters among many alkyl esters showed far better stereoselectivity implying the possible pi-pi interaction between the olefin of substrate and the side chains of Trp104 at the active site. This interaction called 'allyl effect' was investigated.



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장소: 일산KINTEX

발표코드: ORGN.O-3

발표분야: Oral Presentation for Young Organic Chemists

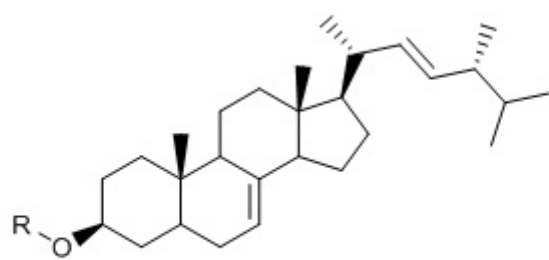
발표종류: 구두발표, 발표일시: 금 10:24, 좌장: 신승훈

## Synthesis and anti-inflammatory activity of glycosyl 5,6-dihydroergosterol derivatives

박훈규 민지은<sup>1</sup> 오세한<sup>2</sup> 김학원<sup>2</sup>

경희대 화학과 <sup>1</sup>경희대 응용과학대학 응용화학과 <sup>2</sup>경희대 응용화학과

Glucosyl spinasterol 과 Glucosyl ergosterol 같은 glycosyl steroid 화합물들은 anti-photoaging activity 와 anti-inflammatory activity 등 흥미로운 생화학적 활성을 보인다. 특히 강력한 anti-inflammatory activity 를 갖는 것으로 알려진 glucosyl spinasterol 은 추출과 합성이 어려운 단점을 갖고 있다. 본 연구진에서는 glucosyl spinasterol 을 대체할 수 있는 glycosyl 5,6-dihydroergosterol 유도체를 제안하였고, 이의 합성법을 연구하였다. Target molecule 의 key intermediate 인 5,6-dihydroergosterol 은 쉽게 구입 가능한 ergosterol 의 선택적인 이중결합의 환원반응을 통하여 얻을 수 있다. 5,6-dihydroergosterol 과 glycosyl trichloroacetimidate 의 Lewis acid 를 사용한 glycosylation 반응을 통하여 target molecule 을 합성하였으며, 합성된 화합물들의 anti-inflammatory activity 를 시험하였다.



R= glucosyl, galactosyl, etc



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발표코드: ORGN.O-4

발표분야: Oral Presentation for Young Organic Chemists

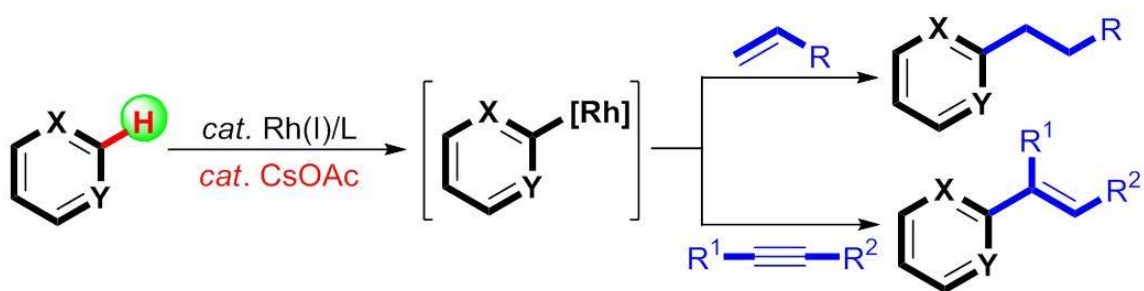
발표종류: 구두발표, 발표일시: 금 10:36, 좌장: 신승훈

## **A Versatile Rh(I) Catalyst System Enabling the Addition of Heteroarenes to both Alkenes and Alkynes via C-H Bond Activation Pathway**

**유재윤 장석복**

KAIST 화학과

A highly efficient and convenient rhodium catalyst system was developed for the direct hydroheteroarylation of unsaturated compounds with heteroarenes. A base cocatalyst was found to facilitate the key arene C-H bond activation step which is believed to proceed via a base-assisted pathway. Substrate scope was very broad to include both electron-deficient pyridine N-oxides and electron-rich azoles. The identical catalytic system was successfully applied to the hydroheteroarylation of both alkenes and alkynes with excellent regio- and stereoselectivity.



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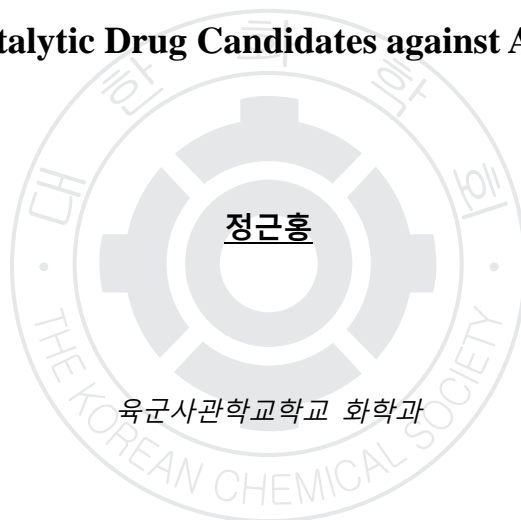
장소: 일산KINTEX

발표코드: ORGN.O-5

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:48, 좌장: 신승훈

## Synthesis of Catalytic Drug Candidates against Amyloid Diseases



The association of  $\beta$ -sheets, amyloidoses, has been implicated in the formation of protein aggregates and fibrils observed in many human diseases such as Alzheimer's disease (AD), Parkinson's disease (PD), type 2 diabetes (T2DM), spongiform encephalopathies, Huntington's disease, and familial British dementia (FBD). Drug candidates for amyloidogenic peptides such as  $\beta$ -amyloid 42-mer,  $\alpha$ -synuclein, and human islet amyloid polypeptide (h-IAPP) have been recently reported as new therapeutic option by Suh group. Subsequently, we have synthesized more drug candidates on h-IAPP and performed cell tests on INS-1. Recently, those compounds showed cleavage activity against ABri 34-mer which is the major component of the insoluble amyloid deposits that are likely to be involved in familial British dementia. Accordingly, on this research topic, we will continue to synthesize other catalytic drug candidates against amyloid diseases.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.O-6

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 신승훈

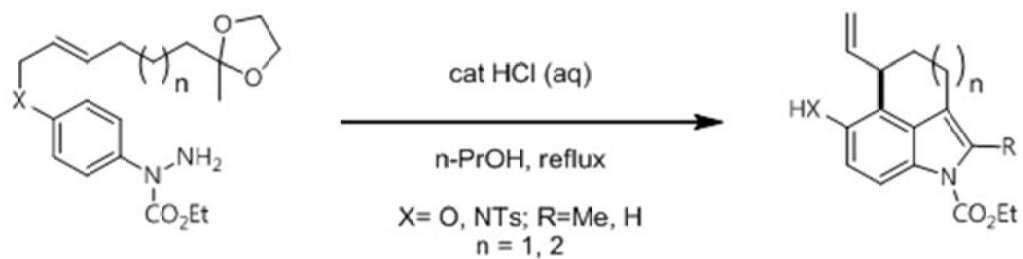
**The first intramolecular Fischer indolization and its combination with  
aromatic Claisen rearrangement for the synthesis of tricyclic  
benzo[cd]indole**

**박인걸 박준 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. In addition, 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.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.O-7

발표분야: Oral Presentation for Young Organic Chemists

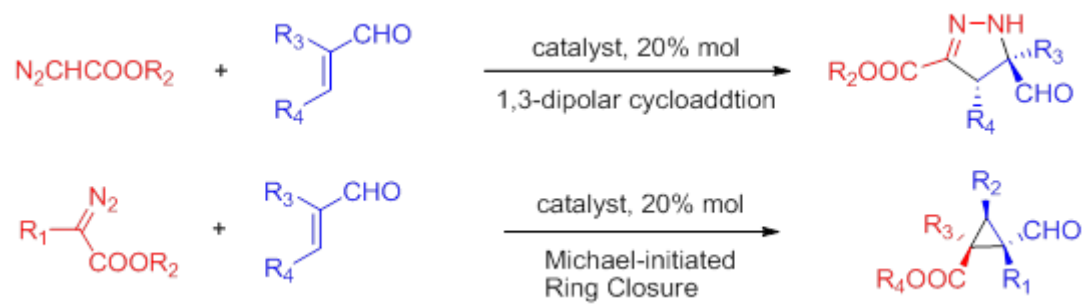
발표종류: 구두발표, 발표일시: 금 11:32, 좌장: 신승훈

## Catalytic Enantioselective Cyclic Reactions of Diazoacetates

gaolizhu 류도현

성균관대 화학과

1, 3- Dipolar cycloadditions between diazocompounds and activated olefins or acetylenes have been extensively investigated and are presently well understood but, there has been little work reported on 1, 3-dipolar additions with substituted acroleins. Catalytic synthetic approach to get the highly functionalized pyrazolines was investigated. In the presence of chiral (S)-oxazaborolidinium ion as catalyst, the reaction proceeded with high to excellent enantioselectivities (up to 99 % ee). Enantioselective cyclopropanation reactions via Michael- initiated ring closure between diazoacetates and  $\alpha,\beta$ -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 (up to 93%) with high to excellent diastereoselectivity (up to 98% de) and enantioselectivity (up to 95% ee).



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장소: 일산KINTEX

발표코드: ORGN.O-8

발표분야: Oral Presentation for Young Organic Chemists

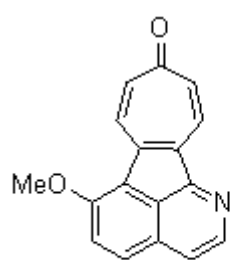
발표종류: 구두발표, 발표일시: 금 11:44, 좌장: 신승훈

## Total synthesis of pareitropone and its analogs via intramolecular radical coupling

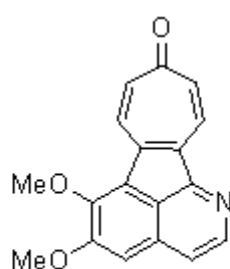
김현정 김영규 신나라

서울대 화학생명공학부

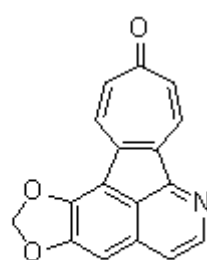
Tropoloisoquinoline alkaloids have been attractive synthetic targets due to their unique architecture and potent cytotoxicity. Pareitropone, the most effective tropoloisoquinoline against the leukemia P388 cell line ( $IC_{50} = 2.7$  nM), was first chemically synthesized via alkynyliodonium chemistry by Feldman and coworkers in 2002. We have completed the second total synthesis of pareitropone via intramolecular radical coupling of phenolic nitronate. Starting from vanillins, properly substituted biaryl aldehydes were prepared by Suzuki coupling and introduction of nitroalkyl(or nitroalkenyl) group afforded the cyclization precursors. To investigate how the methoxy substituents affect the biological activities, several analogs of pareitropone have been prepared and all the compounds were synthesized by the intramolecular radical coupling as a key reaction.



**4-demethoxy  
pareitropone**



**pareitropone**



**4,5-methylenedioxy  
pareitropone**



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.O-9

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:56, 좌장: 신승훈

## Reversible self-crosslinked polymer nanogels for stable delivery vehicles

유자형

서울대 화학과

Research concerning drug delivery vehicles has attracted tremendous interest due to the potential for encapsulating insoluble and toxic hydrophobic drugs, inducing controlled release through relevant biomarkers and achieving selective delivery to target sites. Self-assembled systems such as polymeric micelles, dendrimers and liposomes have been widely studied because of their encapsulation capacity for water-insoluble guests and ability for simple modification through molecular design. Nanoscale vehicles for delivery have been of interest and extensively studied for two decades. However, the encapsulation stability of hydrophobic drug molecules in delivery vehicles and selective delivery into targeting disease cells is a potential hurdle for efficient delivery systems. Here, we demonstrate a simple and fast synthetic protocol of nanogels that shows high encapsulation stabilities. These nanogels can also be modified various targeting ligands for active targeting. We show that the targeting nanogels (T-NGs), which are prepared within 2 hours by a one-pot synthesis, exhibit very narrow size distributions and have the

versatility of surface modification with cysteine-modified ligands including folic acid, cyclic arginine-glycine-aspartic acid (cRGD) peptide, and cell-penetrating peptide. T-NGs hold their payloads, undergo facilitated cell internalization by receptor-mediated uptake, and release their drug content inside cells due to the reducing intracellular environment. Selective cytotoxicity to cells, which have complementary receptors, is also demonstrated.





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장소: 일산KINTEX

발표코드: ORGN.O-10

발표분야: Oral Presentation for Young Organic Chemists

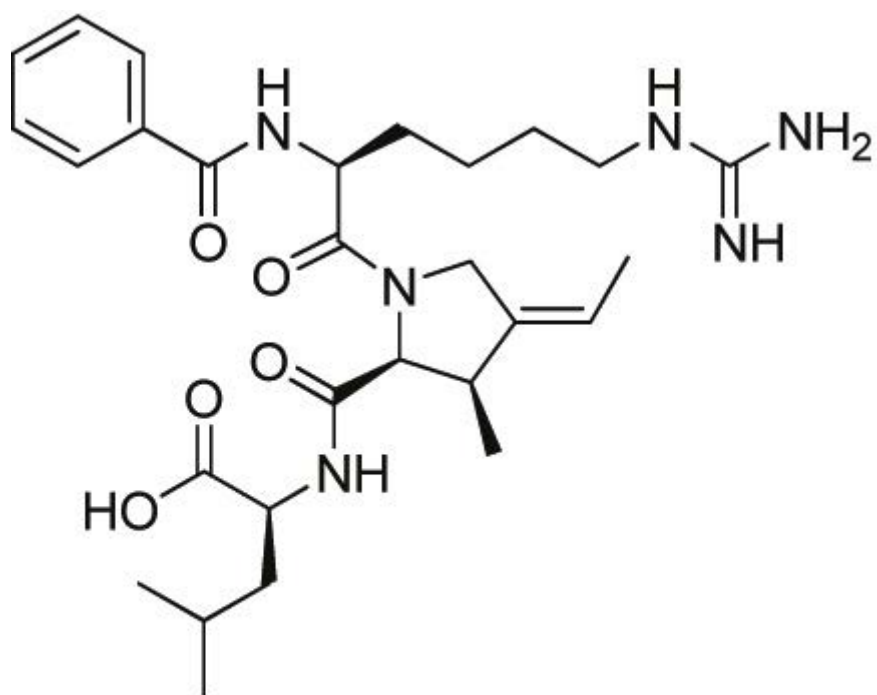
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## Chemical Elucidation of Lucentamycin A

이백경 이원구<sup>1</sup> 심태보<sup>2</sup>

서강대 화학과, KIST 화학키노믹스연구본부 <sup>1</sup>서강대 화학과 <sup>2</sup>KIST 화학키노믹스연구본부

Lucentamycins A-D are natural products isolated from the marine-derived actinomycete *Nocardiopsis lucentensis* by Fenical in 2007. Lucentamycin A exhibited a significant in vitro cytotoxicity against HCT-116 human colon carcinoma with an IC<sub>50</sub> value of 200 nM. The structures of Lucentamycins were analyzed by the spectroscopic 1D and 2D NMR analysis. However, the proposed structure of Lucentamycins turned out to be wrong by our group and others. We have been trying to do chemical elucidation of Lucentamycins. The core structure of Lucentamycin was synthesized by Rh-catalyzed, stereoselective reductive cyclization mediated by hydrogen from optically active 1,6-enynes using chiral BINAPs. It could furnish four stereoisomers of the proposed structure of lucentamycin A. Our results reveal that the proposed core structure of lucentamycin A needs revision. We have therefore been trying to revise core structure of lucentamycin A and these our efforts will be presented in this talk.



lucentamycin A



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장소: 일산KINTEX

발표코드: ORGN.O-11

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 신승훈

## Atom-economical synthesis of stereodefined 1,3-dienes via Gold catalyzed intramolecular enyne metathesis

박현설 구재영 신승훈

한양대 화학과

Intramolecular enyne metathesis are mediated by electrophilic metal catalysts, such as Pt, Au, Pd as well as Grubbs and Fischer carbene complexes. Compared to the latter catalytic systems, the electrophilic metal-catalyzed processes have received fewer attention in terms of synthetic applications. We recently discovered intermolecular cross metathesis reaction between acceptor-substituted alkynes and various alkenes under Au(I) catalysis. This protocol provides for an atom-economical route to stereodefined 1,3-dienes. Herein, we extend this stereospecific intramolecular enyne metathesis between a propiolamide and tethered alkenes. We noted that E or Z-alkenes gave E, or Z-dienes respectively in a stereospecific fashion.

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장소: 일산KINTEX

발표코드: ORGN.O-12

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 12:32, 좌장: 신승훈

## Polydiacetylene Based Electrospun Fibers for Detection of HCl Gas

이송이 김명화<sup>1</sup> 윤주영<sup>2</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 화학 나노과학과 <sup>2</sup>이화여대 화학-나노과학과

Conjugated polymer based sensors have been intensively studied because their absorption, emission, and redox characteristics are sensitive to environmental perturbations. Among them, polydiacetylenes (PDAs), a family of conjugated polymers, are very intriguing materials in several respects. PDAs display an intense blue color and the blue PDAs can undergo a color shift to a red phase upon environmental stimulation. Accordingly, colorimetric detection of biologically, chemically, and environmentally important target molecules such as DNAs, viruses, anions, metal ions, and surfactants, etc. have been reported. In the current work, we synthesized PDA monomers bearing dimethyl amine (PCDA-DMEDA) and incorporated them with PEO into electrospun fibers. For the first time, we successfully demonstrated that PDA based electrospun fibers can be used for the naked-eye detection of HCl gas by simple color change (blue to red). A HCl concentration as low as 2.0 ppm could be detected by the naked eye and the HCl gas could be detected within 1 second. Furthermore, this change can be monitored via fluorescence enhancement.

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장소: 일산KINTEX

발표코드: ORGN.O-13

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 12:48, 좌장: 신승훈

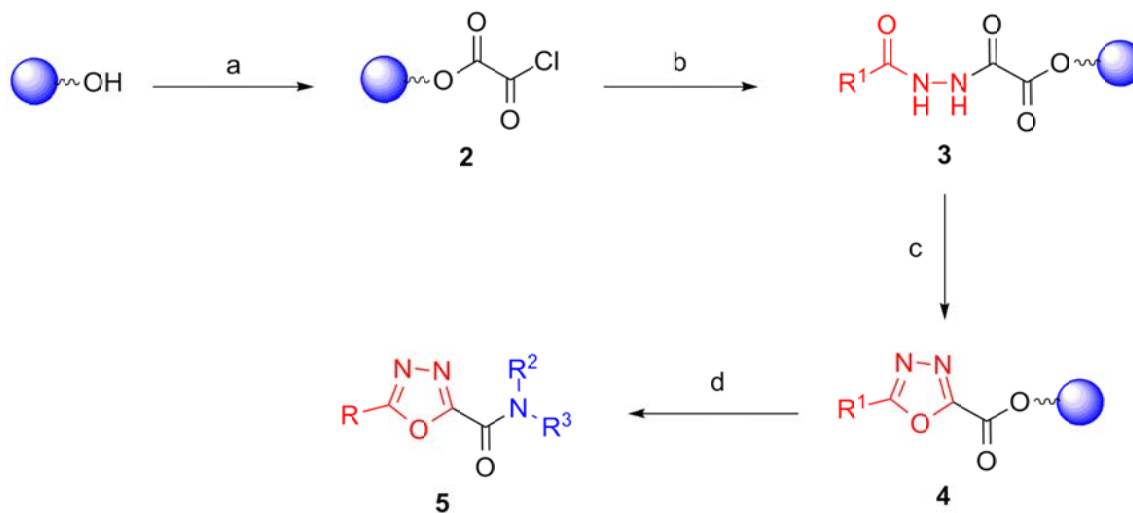
## Solid Phase approach for the synthesis of 2-amido oxadiazole

이상협 BALAJI<sup>1</sup>

대구가톨릭대 생명화학과 <sup>1</sup>대구가톨릭대 화학과

New synthetic methods for solid-phase synthesis are the powerful technique in generating combinatorial libraries of small molecules. Parallel solid phase synthesis is a valuable alternative to traditional synthesis. Solid phase synthesis is the technique where molecules are temporarily bound by solid support in order to streamline the synthesis process. Advantages include easy removal of excess of reactants and by products via washing and filtration. Heterocycles are the single most important class of organic compounds which possess the wide range of biological and industrial applications. Pharmaceutical, agrochemicals and cosmetic industries are using the different heterocyclic compounds by changing the structural features. The wide spread use of 1,3,4-oxadiazole as a core of the large number of therapeutic area, such as anti-bacterial, anti-fungal, anti-miotic, anti-inflammatory, anti-hypertensive, HIV integrase inhibitor and the angiogenesis inhibitors. They also used as intermediate for preparation of various biologically active compounds. As a part of our ongoing work in the development novel polymer supported catalyst, reagents and polymer supported synthesis of small drug molecules. Therefore, herein we developed the new

procedure for the synthesis of 1,3,4-oxadiazole using hydroxyl methyl Janda Jel linker. In the present investigation we introduced the use of polymer bound benzyolhydrazinecarboxylate, from which the respective targets were generated by cyclo-dehydration and smart cleavage reaction to increase the diversity of the scaffold.



일시: 2012년 4월 25~27일(수~금) 3일간

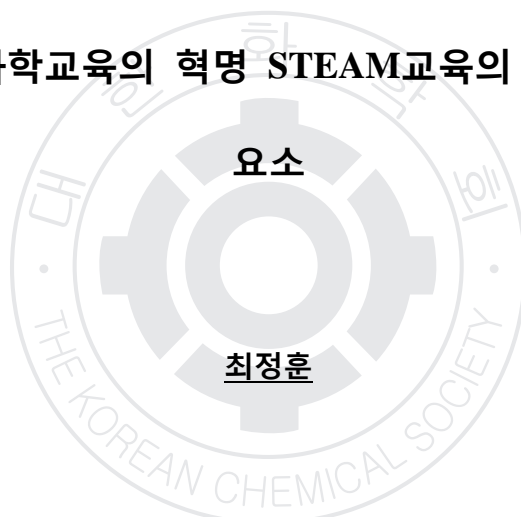
장소: 일산KINTEX

발표코드: EDEC.O-1

발표분야: STEAM Based on Chemistry

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 여상인

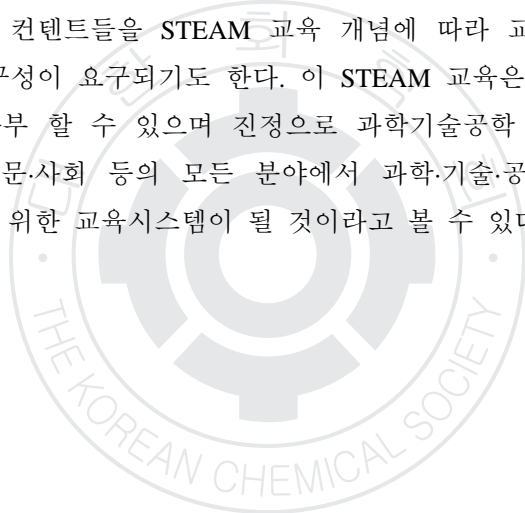
## 새로운 초중등 과학교육의 혁명 STEAM교육의 특징과 주요 구현



한양대 화학과

교육과학기술부는 2011년 창의적인 융합인재 양성을 위한 초·중등 STEAM 교육을 강화하겠다고 발표와 함께 이에 따른 교육과정의 개발, 교사·학생 현장연수 체험 프로그램을 제공하고 미래형 과학기술 교실과 수업모델을 개발을 추진한다고 발표하였다. 즉, 창의적인 과학교육을 위해서는 과학, 기술, 공학 및 예술이 연계된, 통합 및 융합을 기반으로 하는 교육으로 전환되어야 한다는 것이다. 근래에 들어 과학·기술·공학에 대한 발전은 그야말로 엄청난 변화가 일어나고 있다. 그런데 과학교육에서 이런 변화를 따라가지 못하고 수십 년간 같은 내용과 개념으로 일관되어 왔다. 따라서, 최근 다양한 첨단과학기술 제품들에 익숙한 청소년들이 이런 진부한 과학교육 내용에 흥미를 잃는다는 것은 당연한 것이라 할 수 있다. 특히 기업은 최근에 글로벌 융합기술 사회로 바뀌고 있는데, 초·중등학교에서는

현실성이 없는 과학교육만을 하고 있다는 불만을 터트리고 있는 것이다. 이에 각국은 초·중·고등학교에 대개혁을 실시하고 있다. 그런데 우리의 융합을 기반으로 하는 창의적인 과학교육 모델은 과학·기술·공학적인 지식과 인문사회학적인 지식 및 예술적 감각으로 대중으로부터 공감대를 이끌어낼 수 있도록 하는 창의적인 교육을 강조하고 있다. 이것이 미국 등 선진국이 추구하는 STEM 교육과는 다르게 예술과 인문·사회 분야를 아우를 줄 아는, 특히 사회시스템과도 연계할 능력을 가진 과학기술공학인재 양성을 위한 STEAM 교육 개념으로 확장하게 된 것이다. 우리의 STEAM 교육 콘텐츠는 과학·기술·공학에 종합적인 지식 이해 능력을 바탕으로, 융합시대의 빠른 지식변화에 맞는 새로운 과학·기술·공학 지식을 빠르게 습득하여, 이에 대한 구체성과 정확성을 바탕으로, 초·중·고 지식수준과 눈높이에 맞추어 쉽고 재미있게 그리고 흥미롭게 전달할 수 있어야 하기 때문에 기존과는 달리 고도의 전문개발자가 요구되고 있는 것이다. 따라서 성공적인 STEAM 교육을 위한 고려되어야 할 중요한 14 가지 과학교육 콘텐츠 구성 요소를 제시하고 이것을 기초로한 STEAM 교육 모델을 제시하게 되었다. 그런데 STEAM 교육이 성공적으로 정착하기 위해서는 교사들에게 적시에 과학기술변화에 따라 효율적이고 체계적으로 이에 대한 STEAM 교육 수업자료 및 도구를 제공하여 줄 수 있는 시스템 구축이 매우 중요하다. 이와 동시에 이런 교육 콘텐츠들을 STEAM 교육 개념에 따라 교과과정의 내용과 수준에 따른 수직적 체계의 재구성이 요구되기도 한다. 이 STEAM 교육은 세계에서 가장 선도적인 과학교육 시스템이라 자부 할 수 있으며 진정으로 과학기술공학 인재양성을 위한 것만이 아닌 예술, 경영 및 인문·사회 등의 모든 분야에서 과학·기술·공학적 개념으로 창의적인 글로벌 인재를 양성하기 위한 교육시스템이 될 것이라고 볼 수 있다.





일시: 2012년 4월 25~27일(수~금) 3일간

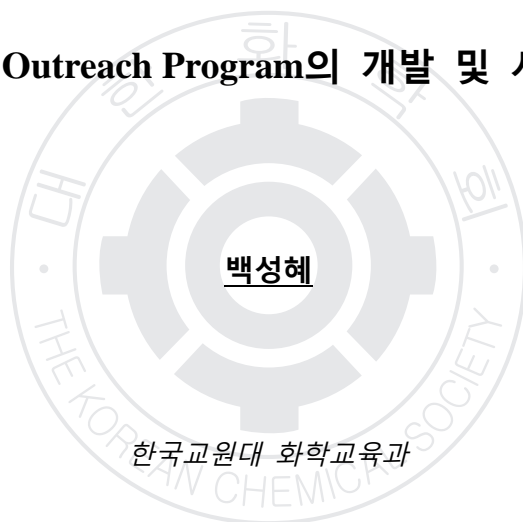
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발표분야: STEAM Based on Chemistry

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 여상인

## STEAM Outreach Program의 개발 및 시범 적용



2011 년 11 월부터 시작하여 2012 년 4 월에 마감하는 한국과학창의재단의 STEAM Outreach Program 사업의 진행 및 개발 프로그램의 시범 적용 사례 등에 대한 내용을 소개하고자 한다. 건국대학교 충주캠퍼스의 생명공학, 컴퓨터공학, 신소재공학 등 전공 교수들이 참여하여 충주고등학교 학생들과 함께 1 박 2 일로 진행한 융합콘서트, 대전서암초등학교와 한밭대학교 HCL 전공 김수경 교수 및 대학원생들이 함께 진행한 3 일 과정의 로봇 개발 프로그램, 경남 사천 한국우주항공산업체와 충남고등학교 학생들이 함께 진행한 1 일 체험 교육 등 다양한 교육기부 프로그램과 이에 대한 학생들의 반응을 제시하고, STEAM outreach program 에 참여한 전문가 운영단, 참여 대학원생 봉사단 등의 효율적인 운영 방안 및 체계적 정착을 위한 제안 등을 제시한다.

일시: 2012년 4월 25~27일(수~금) 3일간

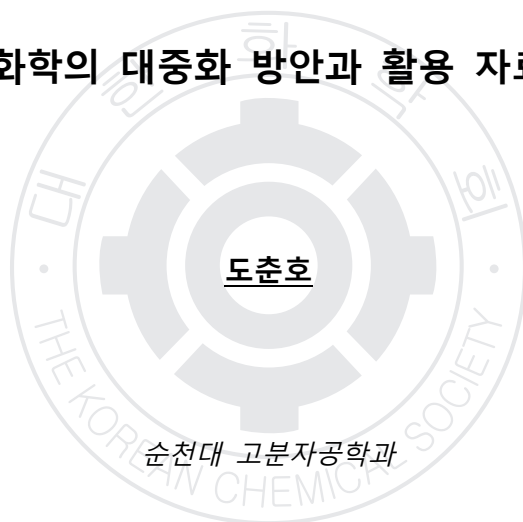
장소: 일산KINTEX

발표코드: EDEC.O-3

발표분야: STEAM Based on Chemistry

발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 유미현

## 화학의 대중화 방안과 활용 자료



화학은 인류 문화와 문명의 발달에 크게 기여해 왔고 앞으로도 그런 역할을 할 것으로 화학 교육자들은 학생들을 교육하고 있다. 그러나 학생을 포함한 많은 시민들에게는 화학에 대한 이해가 부족하다는 것을 화학 교육자들은 체험하고 있다. 보통 화학 반응이 어떻게 일어나고 화학 구조가 어떻게 변화하고 물성이 화학 구조와 어떤 관련이 있는가 하는 것을 화학에서 학습한다. 그러나 많은 대상자가 화학을 전공하지 않으므로 흥미를 유발하기가 쉽지 않다. 이것 대신에 화학이 우리 생활 및 다른 과학 그리고 기술과의 관계를 이해하고 화학이 이들 분야에 어떤 영향을 미쳤는가를 알려주는 방법도 화학에 대한 호기심과 흥미를 이끌어내는 좋은 방법이 될 것이다. 대한화학회에서 발행한 "화학의 대중화 방안과 활용 자료"는 이런 관점에서 좋은 활용 자료가 된다. 이 내용은 에너지와 교통, 정보와 통신, 건강과 의료, 식품과 농업의 4 분야로 나누어서 각 주제와 관련된 중요한 기록 사진과 연대기 그리고 설명을 간략히 하고 있다. 화학보다는 각 주제에 관심을 가진 독자는 이 내용을 통해서

화학과의 연관성을 이해하고 화학에 대한 흥미를 가지게 된다. 이 내용은 다음 웹 사이트에서도 내려받아서 활용할 수 있다:

<http://www.chemistryculture.org/chemtechmilestones/chemtechmilestones-index.htm>



일시: 2012년 4월 25~27일(수~금) 3일간

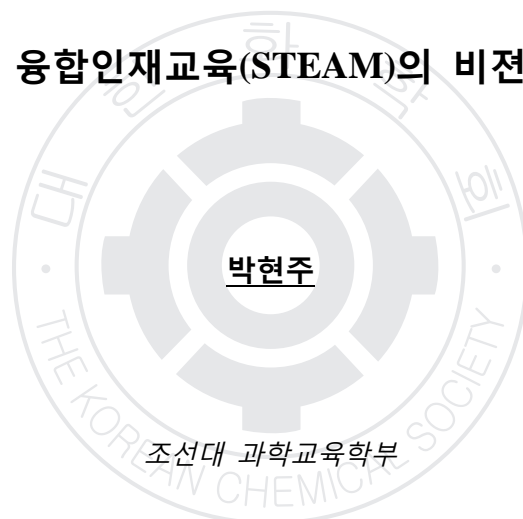
장소: 일산KINTEX

발표코드: EDEC.O-4

발표분야: STEAM Based on Chemistry

발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 유미현

## 융합인재교육(STEAM)의 비전



우리나라 STE(A)M 정책은 도입 초기단계로서, 중앙정부(교과부)의 주도하에 관련 진행되고 있다. 현재 STEM 은 전세계 모든 분야에서 가장 핵심적인 주제이고, 과학교육개혁의 중심이다. 우수한 융합적 사고를 할 수 있는 STE(A)M 인재 양성이라는 목표를 설정하고 이를 달성하기 위해서 중앙정부와 지방정부, 그리고 학교 현장에서 많은 과제를 수행하고 있다. 현재까지의 STE(A)M 연구 및 논의는 미국, 영국 등과 같은 선진국의 배경과 환경에 맞춰져 있는 경향이 있다. 그러나 국가별로 교육환경, 정책적 목표 등 사회적, 문화적 배경이 다른 상황에서 STE(A)M 의 접근 등이 동일하게 적용될 수 있을 지는 충분히 검토해야 한다. 예를 들면, 우리나라와 미국 모두 수학·과학에 대한 낮은 흥미도로 인한 미래 우수 STE(A)M 인재 확보가 어려움이 예상되는 유사한 상황 속에서 우수인재를 과학기술분야로 어떻게 유인할 것인가가 정책의 핵심 키워드로 자리잡게 되었다. 향후 다양한 기술과 지식간의 융복합이 과학기술의 패러다임을 주도할 것으로 예측됨에 따라

이에 적합한 융합형 과학기술인재 또는 연구인력을 양성하기 위해서는 초중고 단계에서부터 과학기술분야에 대한 소양교육 및 인식 제고가 이루어 질 수 있도록 교육정책의 방향이 설정되어야 할 것이다. 또한 우리나라는 대학입시 등 창의적 사고에 걸림돌로 지적되는 제도적 장애물이 존재하고 있다. 현실적인 한계를 고려하여 **STEAM**의 단계별 접근 전략이 요구된다.



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장소: 일산KINTEX

발표코드: POLY.P-1

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Improved Performance of Organic Field Effect Transistors by Doping poly(3-hexylthiophene) with an Organosulfonic Acid

남성호 김화정 김영규

경북대 화학공학과

For the last two decades organic field effect transistors (OFETs) have been widely studied for the application of light-weight electronic devices because of their low-cost advantages utilizing roll-to-roll processes at room temperature. To date, the highest hole mobility of OFETs with semiconducting polymers reached  $\sim 3.3 \text{ cm}^2/\text{V}^2\text{s}$ , which is comparable to that of amorphous silicon FETs ( $\sim 1 \text{ cm}^2/\text{V}^2\text{s}$ ). This improvement can be attributed to the self-organizing tendency leading to enhanced crystallinity in the polymer films. An alternative approach, such as doping of ammonium salt and/or an electron acceptor molecule into organic semiconductors, has been reported to improve the hole mobility of organic semiconductors. In this work, we attempted to dope organic semiconductors with an organosulfonic acid and investigated the optical and electrical characteristics and nanostructures therein. The results showed that the hole mobility of the OFETs with the doped organic semiconductors was improved by ca. 10-fold.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-2

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Polynorbornenes with Methanofullerene Side Group as an Electron Acceptor for OPVs

어맹선 이민형<sup>1</sup> 도영규<sup>2</sup>

KAIST 화학<sup>1</sup> 울산대 화학과<sup>2</sup> KAIST 화학과

Soluble polynorbornenes with side-chain methanofullerene groups (PCBM) were synthesized by the vinyl addition homo- and co-polymerization of norbornene monomer bearing pendant PCBM moiety using Pd(II) catalyst. The homopolymer is insoluble in organic solvents, but the copolymers (62 mol-% and 50 mol-% of PCBM moiety) are soluble in chlorinated solvents such as ODCB. The copolymers exhibited high thermal stability and almost invariant electronic properties when compared to monomer. The BHJ organic solar cells were fabricated based on a blend of P3HT and the copolymer, showing that the polynorbornenes can adequately function as an electron acceptor. Details of synthesis, characterization, and device performances of polymer will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-3

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Fluoride Sensing Behavior of Triarylborane-Functionalized Polynorbornenes

성우영 김태원 이민형

울산대 화학과

Vinyl addition homo- and copolymerization of norbornene monomer bearing an electron-deficient triarylborane moiety using Pd(II) catalyst has been investigated to produce polynorbornene functionalized with triarylborane groups. The catalytic system efficiently led to the soluble polynorbornene with high molecular weight and high thermal stability. While the homopolymer showed enhanced fluorescence quenching efficiency in the sensing of fluoride anions in comparison with monomer, the copolymers with low monomer contents did not exhibit an apparent signal amplification effect. The details of synthesis, characterization, and fluoride sensing behavior will be discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-4

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Layer-by-Layer Assembly of Amino-Functionalized Graphene Nanosheets and Poly(acrylic acid)-Grafted MWNTs

이종희 임정혁 김경민

충주대 나노고분자공학과

Carbon-based materials, graphene and multiwalled carbon nanotubes, have attracted attention owing to their unique properties such as high electrical conductivity, mechanical strength, transparency, and good thermal stability. In this study, the surface of graphene was modified with poly(acryl amide) or ethylenediamine by covalent bonding. Poly(acrylic acid) (PAA) was chemically attached to the surfaces of MWNTs to make PAA-grafted MWNTs. The positively charge amino-functionalized graphene nanosheets and negatively charge PAA-grafted MWNTs assembled together to form a multilayer structure through the electrostatic interaction. The difference between polymer-modified graphene and amine-modified graphene in graphene/MWNTs multilayer was also discussed. The characteristics of the graphene/MWNT multilayer were characterized by various analytical tools. The research was supported by a grant from the academic research program of Chungju National University in 2012.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-5

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Photo-cleavable Block Copolymers Having Multiple *o*-Nitrobenzyl (ONB) Groups

이정원 문봉진

서강대 화학과

As an extension of our previously reported work on ONB-containing block copolymer synthesis,<sup>1</sup> several block copolymers bearing multiple ONB groups were designed and synthesized via living radical polymerization processes such as ATRP and RAFT. In contrast to the case of making polymer bearing a single ONB group, introducing multiple ONB groups was more challenging due to the inhibitory effect of ONB groups under the radical polymerization conditions. In order to circumvent this problem, we have investigated the electronic and structural effect of the ONB group along with the reaction conditions such as catalyst stoichiometry and solvent. We could achieve successful polymerization of newly designed ONB-bearing monomers with reasonable polydispersity and high monomer conversion based on the information from the investigation. The optimum ratio of initiator to copper to ligand and sufficiently high concentration of monomer in the reaction system must be considered which lead to fast polymerization.

1. Kang, M.; Moon, B. *Macromolecules* 2009, 42, 455.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-6

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 이산화탄소를 이용한 지방족 폴리카보네이트의 합성 및 생분해

특성

이명옥 황용택 이문호<sup>1</sup>

호남석유화학(주) 대덕연구소 <sup>1</sup>포항공과대 화학과

지구온난화의 주범인 CO<sub>2</sub>를 원료로 사용하고 프로필렌 옥사이드(PO) 및 생분해 특성이 있는 사이클릭 에스터로 락타이드(LA)를 사용하여 생분해성 지방족 폴리카보네이트를 합성하였다. 합성된 친환경 고분자는 반응 몰비에 따라 수율과 분자량에 차이는 있지만, 수백만의 고분자량을 가졌으며 효소와 미생물에 의한 생분해특성을 나타내었다. 유기용매를 사용하지 않는 청정중합법을 통하여 합성된 친환경 생분해성 고분자는 의료용 및 각종 친환경 소재로의 응용이 가능하다.

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장소: 일산KINTEX

발표코드: POLY.P-7

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 생분해성 polyurethane 합성 및 diol 변화의 특성 조사

오소연 공명선

단국대 나노바이오의과학과

폴리우레탄은 소수성과 친수성을 함께 가지고 있는 대표적인 상분리 공중합체로서 diisocyanate 화합물과 diol 화합물을 반응하여 합성한다. 생체 친화성 재료로서 혈액 적합성이 우수하여 매우 유용하게 이용되고 있으며 혈장 단백질의 점착에 따른 혈전 형성을 조절할 수 있으므로 주로 순환기계의 생체 재료로 널리 이용되고 있다. 본 연구에서는 생체적합성이 우수하고 경직된 구조와 유연성이 큰 구조를 조절할 수 있게 생분해성 키랄 디올인 1,4:3,6-dianhydro-D-sorbitol(isosorbide) 과 1,4:3,6-dianhydro-D-manniol (isomannide)를 사용하고 poly( $\epsilon$ -caprolactone) 디올의 비를 조절하여 hexamethylene diisocyanate (HDI)와의 polyurethane 을 bulk 중합으로 합성하였다. 각 성분의 조성 변화에 따른 물성 변화를 GPC, DSC, TGA, 용해도, 인장강도 등의 기계적 특성 및 열적 특성을 측정하여 디올의 조성 변화에 따른 특성 변화를 조사하였다.

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장소: 일산KINTEX

발표코드: POLY.P-8

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Isosorbide를 이용한 생분해성을 polyester의 합성 및 특성 조사

김정진 공명선

단국대 나노바이오의과학과

생체 적합성 고분자의 중요성과 이용분야가 점차 넓어지면서 약물 전달체, 인공 장기 및 스캐폴드 등과 같이 의료용 분야에 널리 적용되고 있다. 특히 polyester (PEs)는 생분해 능력이 탁월하고 분해 생성물이 인체에 독성을 띄지 않는 것으로 널리 알려져 drug delivery system (DDS)과 조직공학의 재료로서 많은 관심을 받고 있으며 널리 이용되고 있다. 본 연구에서는 succinic acid (SA)와 isosorbide (IS)의 중합체가 경직한 구조를 가지고 있기 때문에 IS와 ethylene glycol (EG)의 비율을 조절하여 여러 가지 조성을 가지는 PEs를 합성하여 여러 가지 물성을 조사하였다. GPC를 이용한 분자량 측정과 DSC, TGA를 이용한 열적 성질 그리고 기계적 성질을 보기위하여 인장강도를 측정하였다. 또한 생체 적합성을 확인하기 위하여 PBS 및 NaOH 수용액을 이용한 생분해성 분해를 조사하였다.

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장소: 일산KINTEX

발표코드: POLY.P-9

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Controlled organic thin film growth via solution-based molecular-layer-deposition

이은혜 박지웅<sup>1</sup>

광주과학기술원 신소재공학부 <sup>1</sup>광주과학기술원 신소재공학과

The 3-dimension cross-linked organic molecular network films were successfully prepared via solution-based molecular-layer-deposition on amine functionalized surface with alternating depositions of tetrakis(4-aminophenyl)methane and phenylene diisocyanate. The films grow linearly by increasing deposition cycles and the thickness of films could be controlled on the molecular level by varying the number of deposition cycles. Morphology and nanometer-scale thickness of the film was studied using scanning electron microscopy (SEM) and atomic force microscopy (AFM). The UV absorption of the film was proportional to the number of deposition cycles. The MLD process was conducted on a nanoporous alumina support to fabricate ultrathin membrane. Performance of the membrane was studied by filtration test using aqueous solution. This work was supported by a Korea Science and Engineering Foundation (KOSEF) grant [2010-0026421] funded by the Korean government (MEST).

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-10

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New Aromatic Coupling Reactions Using a Polymer Reagent

전보람 변인준 신승훈 한양규

한양대 화학과

We synthesized porous crosslinked polymer particles (PDOPAM) from new acrylamide based monomer in the presence of divinyl benzene by a suspension polymerization. The porous polymer was used as a polymer reagent for conventional aromatic coupling 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 polymer reagent enables the highly selective coupling reaction of aryl halides to biphenyl compounds due to its fixation and orientation effects. Keywords: crosslinked porous polymer, polymer reagent, aromatic coupling reaction, suzuki reaction, ullmann reaction.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-11

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization and Properties of a New Conjugated Polymer Containing Thiophene Derivative for Polymer Solar Cells

황선우 장원 김홍선 이상우 김인태 이영남

광운대 화학과

A new conjugated polymer containing thiophene derivative is successfully synthesized by Stille's coupling reaction. The new polymer has good solubility in organic solvents such as  $\text{CHCl}_3$ , and Chlorobenzene. The new polymer was characterized by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, GPC and TGA. Electrochemical and optical properties of the polymer are measured by UV-vis spectroscopy, PL spectroscopy and cyclovoltammetry. The new polymer will be used for polymer solar cell device.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-12

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and properties of a new conducting polymer for all solid state sensor

박은랑 김중일 허민 신재호 김인태

광운대 화학과

New conducting polymer containing heterocyclic ring with carbazole, ethylene dioxythiophene (EDOT) and benzobisthiazole is synthesized and characterized by organic spectroscopic methods. Potentiometric ion-selective membrane electrodes (ISMES) have been extensively used for ion analysis in clinical, environmental, and industrial fields, owing to its wide response range (4 to 7 orders of magnitude), no effect of sample turbidity, fast response time, and ease of miniaturization. Considerable attention has been given to alternative use of room-temperature vulcanizing (RTV)-type silicone rubber (SR) owing to its strong adhesion and high thermal durability. We demonstrate a new method to reduce membrane resistance via addition of a new conducting polymer into the SR-based ISMs.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-13

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dimer acid 함량에 따른 PS계 아이오노머의 기계적 성질 연구

고광환 박혜련<sup>1</sup> 김준섭<sup>2</sup>

조선대 첨단부품소재공학과 <sup>1</sup>조선대 화학과 <sup>2</sup>조선대 응용화학소재공학과

본 연구에서는 술폰화된 폴리스타이렌(PS) 아이오노머인 P(S-co-SA)Na 아이오노머에 다이머산을 넣었을 때 기계적 성질이 어떻게 변하는지에 대해서 알아보았다. 다이머산의 양이 증가함에 따라 비이온성 고분자 사슬로 이루어진 매트릭스의 유리전이온도(matrix Tg)가 113 °C에서 65 °C로 점점 낮아짐을 알 수 있었다. 또한, matrix Tg와 cluster Tg 사이의 모듈러스인 이온 모듈러스 값이 약 150 °C에서 관찰되며 첨가한 다이머 산의 양이 증가함에 따라 점점 감소하는 것을 알 수 있었다. 한편, 고분자의 loss tangent( $\tan \delta$ ) 피크를 보면 matrix와 cluster  $\tan \delta$  피크를 보여 주는데 다이머산의 양이 증가함에 따라 이 두 피크는 낮은 온도 쪽으로 이동하는데 matrix 피크의 크기는 감소하는 반면 cluster 피크의 크기는 약간 증가하는 것을 알 수 있었다.

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장소: 일산KINTEX

발표코드: POLY.P-14

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 다이머/트라이머 산과 블렌드된 스타이렌 아이오노머의 기계적 성

### 질 및 구조

고광환 박혜련<sup>1</sup> 김준섭<sup>2</sup>

조선대 첨단부품소재공학과 <sup>1</sup>조선대 화학과 <sup>2</sup>조선대 응용화학소재공학과

최근 친환경 소재에 대한 연구가 활발하게 진행되고 있어 본 연구에서는 다이머/트라이머 산과 우지 지방산, 대두 지방산, 미강 지방산을 스타이렌 아이오노머에 함량을 다르게 하여 넣었을 때 변화하는 스타이렌 아이오노머의 기계적 물성을 DMA 를 이용하여 연구하였다. 실험에 사용된 아이오노머는 6.9 mol %의 이온기를 가지고 있는 P(S-co-MA)Na 아이오노머이며, 이 고분자는 60 °C 물중탕에서 자유 라디칼 벌크 중합을 시켜 만들었다. 아이오노머와 다이머/트라이머 산-Na 염은 용액 상태로 블렌딩한 후 동결 건조하여 고체형태의 고분자 시료를 얻었다. DMA 측정결과 다이머/트라이머 산의 함량은 matrix 와 cluster T<sub>g</sub> 를 변화시켰고 동시에 이온 모듈러스를 변화시켰다. 이로부터 우리는 다이머/트라이머 산-Na 염이 아이오노머에서 가소제 및 충전제로 작용함을 알 수 있었다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-15

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Morphology-Dependent Electrical Memory Characteristics of a Well-Defined Brush Polymer Bearing Oxadiazole-Based Mesogens

권원상 안병철 고용기 함석규 김영규<sup>1</sup> 김화정<sup>1</sup> 정정운 노예철 김경태 김미희 정성민

권경호 김영용<sup>2</sup> 이진석 이문호

포항공과대 화학과 <sup>1</sup>경북대 화학공학과 <sup>2</sup>포항공과대 첨단재료과학

A new oxadiazole-containing brush polymer, poly-(5-phenyl-1,3,4-oxadiazol-2-yl-[1,10-biphenyl]carboxyloxynnonyl acrylate) (PPOXBPA), was synthesized. The polymer was thermally stable up to 350 °C. Below the degradation temperature, it showed a glass transition, crystal melting transition, and a liquid crystal to isotropic melt transition. Its optical and electrochemical properties were also investigated. This brush polymer was found to always self-assemble into a multilayer structure, with partial interdigitation between bristles from different layers occurring via the  $\pi$ - $\pi$  stacking of the oxadiazole mesogen units. Interestingly, when the polymer film was applied in devices with a bottom and top electrode, it showed either volatile or nonvolatile memory behavior, depending on the ordering and orientation of the multilayer structure (particularly, the  $\pi$ - $\pi$  stacked oxadiazole mesogen units), which

could be controlled via thermal annealing. The switching mechanisms of these electrical memory behaviors were investigated. Collectively, these results demonstrate that this chemically well-defined brush polymer is suitable for use as an active material for the low-cost, mass production of high-performance, programmable volatile and nonvolatile memory devices via control of the morphological structure.



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장소: 일산KINTEX

발표코드: POLY.P-16

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of New Well-defined DNA-Mimicking Brush Polyoxyethylenes Bearing Adenine Moieties

권경호 권원상 정성민 안병철 송성진 김미희 노예철 정정운 김경태 이진석 김용완

김종현 김영용<sup>1</sup> 위동우<sup>1</sup> 이문호<sup>2</sup>

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학부 <sup>2</sup>포항공과대 화학과, 첨단재료과학부

In this study, we describe new well-defined DNA-mimicking brush polyoxyethylenes bearing adenine moieties at the bristle ends : poly[oxy(11-(3-(9-adeninyl)propionato)-undecanyl-1-thiomethyl)ethylene] (PECH-AP) and poly[oxy(11-(5-(9-adenylethoxy)-4-oxopentanoato)undecanyl-1-thiomethyl)ethylene] (PECH-AS). these polymers were found to be thermally stable up to 220 °C and could be applied easily by conventional coating processes to produce good quality films. In thin films, these polymers present selfassembled nanostructures and nucleobase-rich surfaces. Interestingly, both brush polymers formed molecular multi-bilayer structures to provide an adenine-rich surface. Despite the structural similarities, PECH-AS surprisingly exhibited higher hydrophilicity and better water sorption properties than PECH-AP. These differences were attributed to the chemical structures in the bristles of the polymers. The

adenine-rich surfaces of the polymer films demonstrated facilitated HEp-2 cell adhesion, suppressed bacterial adherence, selective protein adsorption, and exhibited good biocompatibility in mice. However, the high hydrophilicity and good water sorption characteristics of the PECH-AS film suggest that this brush polymer is better suited to applications requiring good biocompatibility and reduced chance of bacterial infection compared with the PECH-AP film.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-17

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synchrotron Grazing Incidence X-ray Scattering Study of Hierarchical Nanostructures in Organic-Inorganic Hybrid Diblock Copolymer

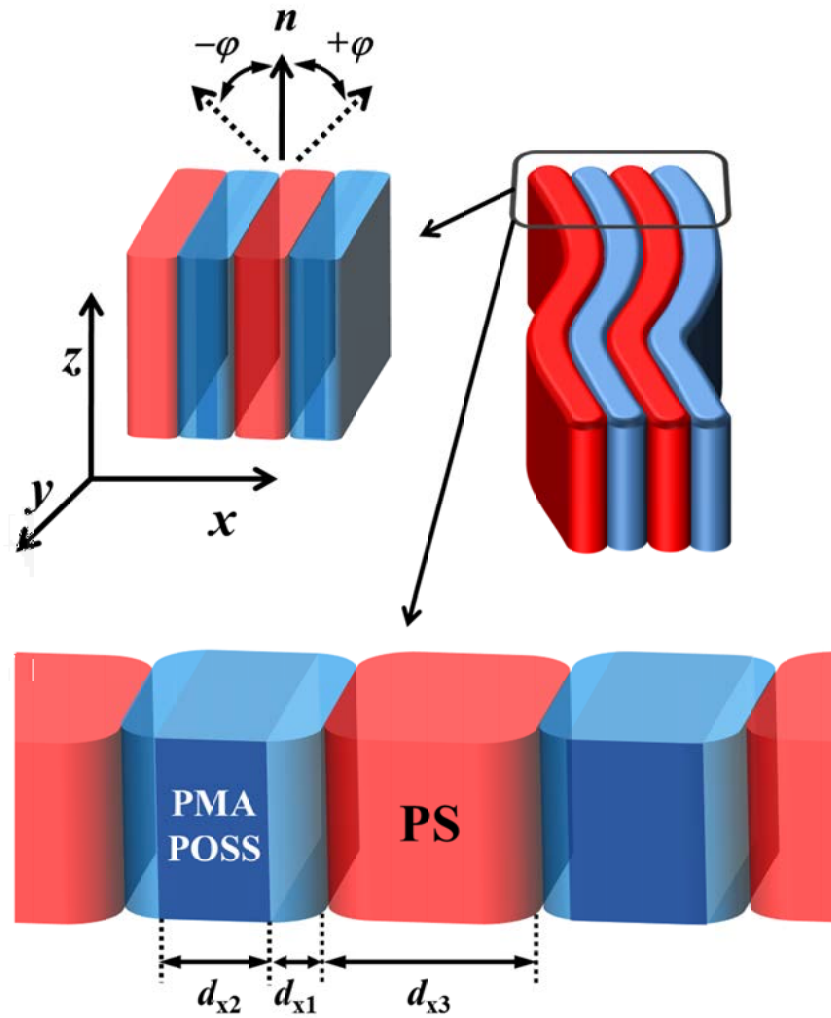
안병철 Sangwoo Jin<sup>1</sup> Tomoyasu Hirai<sup>2</sup> 이문호 노예철 김경태 정성민 김영용<sup>3</sup> 김미희

위동우<sup>3</sup> 김종현 정정운 고용기 김용완 권원상 Teruaki Hayakawa<sup>2</sup>

포항공과대 화학과 <sup>1</sup>Toray Research Center <sup>2</sup>Tokyo Institute of Technology <sup>3</sup>포항공과대 첨단재료과학부

An interesting organic-inorganic hybrid diblock copolymer, poly(styrene-*b*-methacrylate grafted with polyhedral oligomeric silsesquioxane) (PS-*b*-PMAPOSS). The morphological structures in nanoscale thin films of PS-*b*-PMAPOSS were investigated in detail by performing grazing incidence X-ray scattering (GIXS) with a synchrotron radiation source. GIXS formulas based on structural models were derived for the quantitative analysis of the two-dimensional (2D) scattering data. The quantitative 2D GIXS analysis found that the diblock copolymer molecules in the thin films undergo phase separation into PS and PMAPOSS domains, which generates a lamellar structure. Surprisingly, this lamellar structure is completely oriented in the out-of-plane of the film and is stable up to the degradation temperature. The

PMAPOSS layers in the lamellar structure were found to consist of two sub-layers, namely a densely ordered layer composed of vertically oriented orthorhombic crystals and a less ordered layer that consists of molecularly stacked layers that are oriented vertically. In both the sub-layers, the PMAPOSS block chains have helical conformations and thus are present as molecular cylinders.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-18

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Structures of Polymethacrylate block Copolymer Bearing POSS Moieties using Synchrotron X-ray Scattering

김영용 안병철<sup>1</sup> 노예철<sup>1</sup> 권원상<sup>1</sup> 정정운<sup>1</sup> 김경태<sup>1</sup> 김미희<sup>1</sup> 정성민<sup>1</sup> 권경호<sup>1</sup> Tomoyasu

Hirai<sup>2</sup> Masa-aki Kakimoto<sup>2</sup> Teruaki Hayakawa<sup>2</sup> 이문호<sup>1</sup>

포항공과대 첨단재료과학부 <sup>1</sup>포항공과대 화학과 <sup>2</sup>Tokyo Institute of Technology

The morphological behavior of diblock copolymer of methyl methacrylate and polyhedral oligomeric silsesquioxane (POSS) functionalized methacrylate (PMMA-b-PMAPOSS) with volume ratio of 13/87 thin films were studied by using synchrotron grazing incidence small and wide-angle X-ray scattering (GISAXS and GIWAXS), and differential scanning calorimetry(DSC). The quantitative GISAXS and GIWAXS analysis showed that both the PMMA cylinders and the PMAPOSS matrix (i.e., amorphous) are induced from solvent-annealing copolymer films. However, the post thermal annealing process induces aggregation of the POSS moieties, which results in the formation of crystals with an orthorhombic lattice unit cell. Furthermore, the molecular PMAPOSS cylinders in helical conformations are aligned in the film plane. The crystals were found to melt above 190 °C during heating and

subsequent cooling. In contrast, the hexagonally packed structure of the PMMA was found to be retained during the heating and the subsequent cooling. These in-situ experiments were combined with DSC.



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장소: 일산KINTEX

발표코드: POLY.P-19

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization of Structures of Star-shaped Polystyrenes with Varying Numbers of Arms by Small Angle X-ray Scattering

정성민 윤진환<sup>1</sup> 정정운 노예철 안병철 권원상 김미희 Tomoya Higashihara<sup>2</sup> 김경태

권경호 김영용<sup>3</sup> 고용기 Akira Hirao<sup>2</sup> 이문호

포항공과대 화학과 <sup>1</sup> 동아대 화학과 <sup>2</sup> Tokyo Institute of Technology, JAPAN <sup>3</sup> 포항공과대 첨단재료과학

We investigated the structures and shapes of well-defined star-PS polymers with 6, 9, 17, 33, and 57 arms in good and  $\Theta$  solvents using SAXS with a synchrotron radiation source. The SAXS data revealed details of the molecular sizes and shapes of the star-PS polymer series, including blob contributions, the radius of gyration, the pair distributions, radial electron density distributions, and the Zimm-Stockmayer and Roovers g-factors. The molecular size and shape of the star-PS polymers varied with the number of arms. The radius of gyration of star-PS polymers ranged from 30.2 to 49.5 nm, depending on the number of arms, the solvent, and the molecular weights. The shapes of the star-PS polymers containing 6, 9, or 17 arms could be described as fuzzy ellipsoids, consisting of a core and a shell. The aspect ratio decreased with

the increasing number of arms. The fuzziness ranged from 35.6 to 51.9%, depending on the number of arms and the solvent. The ellipsoidal molecular shapes were favored at lower arm numbers by the extended anisotropic architecture of the connection part of arms. The effect of the extended anisotropic branches decreased as the number of arms increased, because the space-filling effects of the arms became more significant. In contrast, the star-PS polymers with 33 or 57 arms could be described as fuzzy spheres. The fuzziness ranged from 25.0 to 31.0%, depending on the number of arms and the solvent. The spherical shapes indicated that with sufficient ( $>33$ ) arms, the effects of the extended anisotropically branched connections in the molecular architecture were compensated by the space filling effects of the large number of arms.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-20

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrical Memory Performance of Nitrogen-Linked Poly(2,7-carbazole)s Polymer Devices and Analysis of Devices Structure Using X-Ray Reflectivity

고용기 함석규 Tsuyoshi michinobu<sup>1</sup> 권원상 김경태 권경호 이진석 송성진 김용완 김

중현 위동우<sup>2</sup> 이문호

포항공과대 화학과 <sup>1</sup>Tokyo Institute of Technology <sup>2</sup>포항공과대 첨단재료과학부

Electrically programmable polymer memory devices based on thermally and dimensionally stable carbazole polymers, nitrogen-linked poly(2,7-carbazole)s thin films were fabricated. As an active layer we adopt three kinds of nitrogen-linked poly(2,7-carbazole)s; Poly(9-Hexadecyl-9H-carbazole-4-hexadecyloxy aniline) (P1), Poly(9-Hexadecyl-N,N'-diphenyl-9H-carbazole-1,3-phenylene) (P2), and Poly(9-Hexadecyl-N,N'-diphenyl-9H-carbazole-1,4-biphenylene) (P3). The memory device has metal-polymer-metal (MPM) structure where metal electrode is aluminum (Al). We investigated I?V curves and stress tests of these devices. These nitrogen-linked poly(2,7-carbazole)s devices show excellent dynamic random access memory (DRAM) characteristic at 8~60 nm thickness. The ON/OFF current ratios are

108-109 for P1, 105-106 for P2, and 107-108 for P3. Besides, P1 has the longest retention time among three nitrogen-linked poly(2,7-carbazole)s. Therefore, P1 devices show excellent memory performance among them. By analysis of I-V curves, DRAM behavior of nitrogen-linked poly(2,7-carbazole) polymers is turned out to be governed by trap-limited SCLC and local filament formation. We also investigated MPM structure devices using atomic force microscopy (AFM) and X-ray reflectivity. By analysis of surface roughness of each layer and interface layers between polymer and Al electrode layer, we verified that the memory characteristics of nitrogen-linked poly(2,7-carbazole)s devices is caused from polymer layer not from defects of MPM devices such as, unknown interface layer and high roughness of layers. And the switching mechanism is ascribed from the conducting filament formation within polymer layer not by the influence of the oxide layer between polymer and metal electrode.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-21

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Guest-initiated Supramolecular Polymerization of Aromatic Amphiphiles

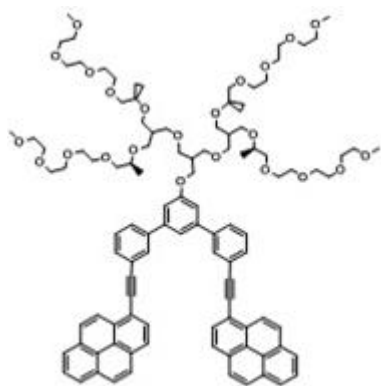
구효진 황철강 이명수

서울대 화학과

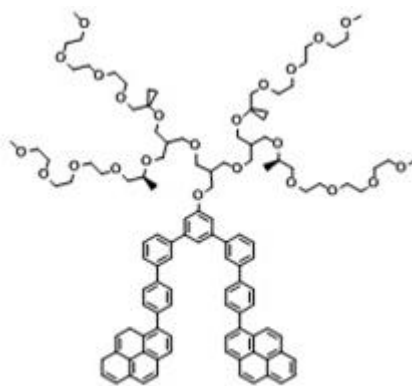
We have synthesized an n-shaped pyrene derivatives which are able to be formed dimeric macrocycles by the charge transfer interaction between pyrene and 2,4,5,7-trinitrofluorenone (TNF). Upon addition of TNF into aqueous solution, the macrocycles can stack to each other to produce a supramolecular polymer. Notably, the average size of the supramolecular polymer (DP) showed to be controlled by electron-deficient guest molecule (TNF). Interestingly, the polymer 1 based on acetyl pyrene showed chiral aggregate in contrast to the polymer 2 based on phenyl pyrene which observed non-chiral caused by steric hindrance by bulky aromatic rod. Graphene exfoliation experiments showed that the black graphene powder was only dispersed in amphiphile 1 solution, indicating that the flat conformation of the aromatic segment of 1 provides efficient interaction with 2-D graphene. On the other hand, the polymerized fibers were observed poor exfoliation ability under the same conditions, suggesting that the charge-transfer interaction of pyrene-TNF is larger than the  $\pi$ - $\pi$  interaction of pyrene-graphene. References[1] H.-J. Kim,

S.-K. Kang, Y.-K. Lee, C. Seok, J.-K. Lee, W.-C. Zin, M. Lee, *Angew. Chem. Int. Ed.* 2010, 139, 8471.[2]

H.-J. Kim, T. Kim, M. Lee, *Acc. Chem. Res.* 2011, 44, 72.



1



2



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-22

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

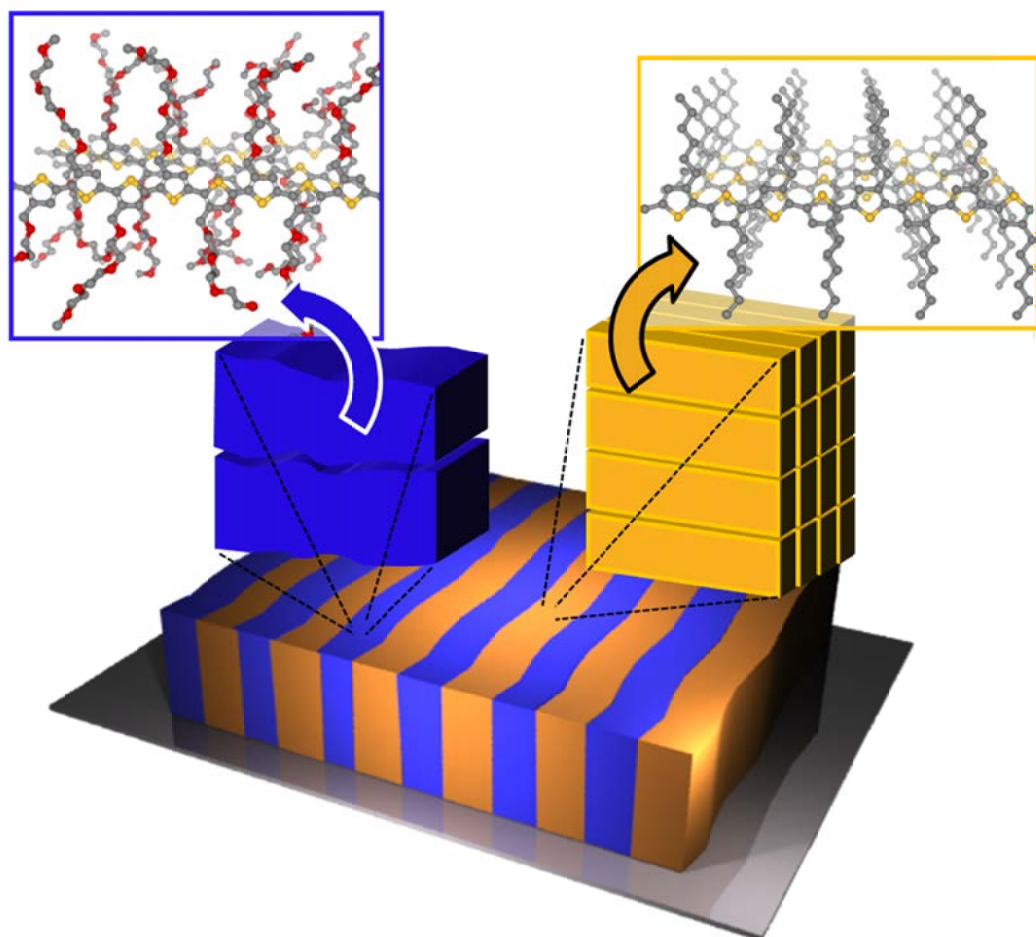
## Well-ordered Lamellar Formation of Amphiphilic Diblock Copolythiophene in Thin Film

노예철 Tomoya Higashihara<sup>1</sup> Kaoru Ohshimizu<sup>1</sup> 안병철 김경태 정성민 권원상 김미희

고용기 김영용<sup>2</sup> 권경호 Shuichi Nojima<sup>1</sup> Mitsuru Ueda<sup>1</sup> 이문호

포항공과대 화학과 <sup>1</sup>Tokyo Institute of Technology <sup>2</sup>포항공과대 첨단재료과학

$\pi$ -conjugated polymer based on diblock copolythiophene was studied using synchrotron X-ray scattering, Differential scanning calorimetry (DSC), ultraviolet-visible (UV-vis) spectroscopy, atomic force microscopy (AFM) and transmission electron microscopy (TEM) for the quantitative analysis. From these analyses, the block copolythiophene thin films formed well-ordered lamellar structure from micro-phase separation and both block domains show self-assembled multi-layered stacking along a direction normal to substrate. The crystalline domains were originated from the  $\pi$ ? $\pi$  stacked thiophene backbones along in-plane direction and the amorphous domains displayed no specific intermolecular packing as can be seen by thermal analysis. From these results, we successfully obtained the well-defined self-assembled structure of the amphiphilic diblock copolymer in thin films for the various applications.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-23

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Bipolar and Unipolar Switching Characteristics of Nonvolatile Memory Device Fabricated with a Novel Polymer Bearing Carbazole and Fullerene Moieties**

김경태 함석규 권원상 고용기 장태현 이재석<sup>1</sup> 권경호 이진석 송성진 김용완 김종현  
위동우<sup>2</sup>

포항공과대 화학과 <sup>1</sup>광주과학기술원 신소재공학과, PIMS <sup>2</sup>포항공과대 첨단재료과학부

We report devices made of a nanoscale thin film of poly(2-(N-carbazolyl)ethyl methacrylate) end-capped with fullerene (PCzMA-C60) sandwiched between aluminum and indium-tin-oxide electrodes and their electrically bistable memory characteristics. The devices were easily fabricated via a simple conventional coating process of the polymer in solution, and found to exhibit programmable, rewritable nonvolatile memory characteristics with a high ON/OFF current ratio of up to  $10^4$ , a long retention time in both ON and OFF states, and low power consumption. Furthermore, the devices revealed unipolar switching behavior as well as bipolar switching behavior, depending on the control of current compliance. The

advantageous properties and ease of fabrication of the PCzMA-C60 based devices open up the possibility of the mass production of high performance digital nonvolatile polymer memory devices at low cost.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-24

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of chemically, dimensionally and thermally stable four different polyimides bearing carbazole and its nonvolatile memory characteristics

김용완 김경태 권원상 정정운 노예철 안병철 김미희 고용기 정성민 권경호 김영용<sup>1</sup>

이진석 송성진 김종현 위동우<sup>2</sup> 이문호

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학 <sup>2</sup>포항공과대 첨단재료과학부

A series of soluble poly(amic acid) precursors were prepared from a new carbazole-containing monomer, 3,30-bis[9-carbazole(ethyloxy)biphenyl]-4,40-diamine (HAB-CBZ) by polycondensation with four different aromatic dianhydrides: pyromellitic dianhydride (PMDA), 3,30,4,40-biphenyltetracarboxylic dianhydride (BPDA), 3,30,4,40-diphenylsulfonfyltetracarboxylic dianhydride (DSDA) , and 3,30,4,40-diphenylethertetracarboxylic dianhydride (ODPA). From the precursors, nanoscale thin films of polyimides (PIs) were prepared by spin-coating and subsequent thermal imidization. All the PIs showed excellent thermal and dimensional stability. In specialty, the PIs based on the PMDA and BPDA units revealed excellent chemical resistance to organic solvents, in addition to the high thermal and

dimensional stability, which are required for the fabrication of high performance memory devices in three-dimensionally multi-stack structure. Devices fabricated with nanoscale thin PI films showed excellent unipolar write-once-readmany-times (WORM) memory behavior with a high ON/OFF current ratio of up to 10<sup>10</sup>. This study found that the imide rings as local charge trap sites are necessary to enhance the memory performance in addition to carbazole moiety. All the results collectively indicate that the chemically, dimensionally and thermally stable PIs of this study are a promising material for the mass production at low cost of high performance, programmable nonvolatile WORM memory devices that can be operated with low power consumption in unipolar switching mode.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-25

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fabrication and Patterning of Polymer-Halloysite Nanotube Multilayer Films

천세연 황선민 강훈구 손대원 노재근

한양대 화학과

Halloysite nanotubes (HNTs), a type of natural occurring clay with nanotubular structures, are promising candidates for various applications such as controlled release, nanotemplating and catalyst carrier. HNTs can be used as a polyanionic material in fabricating Layer-by-Layer (LbL) assembled film due to its negatively charged surface under neutral condition. As a positively charged polyelectrolyte, we employed poly allylamine hydrochloride (PAH). In this study, we fabricated LbL multilayered films on stripe patterned PDMS using two different methods of LbL assembly, dipping and spin coating, and transferred them to silicon wafer. We confirmed the patterning and surface morphology of HNT/PAH multilayered films and measured the patterned film thickness by atomic force microscopy (AFM) measurement. The film thickness was regularly increased as the number of bilayers increased in both assembly methods. We also compared HNT/PAH multilayered film to IMO/PSS multilayered film, which is one of our previous study.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-26

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies of Synthesis and morphological structure of Polythiophenes Containing Aromatic Groups at the 3-Position

김종현 안병철 정정운 권원상 김경태 김미희 고용기 정성민 권경호 김영용<sup>1</sup> 이문호

Kaoru Ohshimizu<sup>2</sup> Tomoya Higashihara<sup>2</sup> Mitsuru Ueda<sup>2</sup>

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학 <sup>2</sup>Tokyo Institute of Technology

Regioregular poly(3-(4'-(3'',7''-dimethyloctoxy)phenyl)thiophene) (P3PhT) and poly(3-(4'-(3'',7''-dimethyloctoxy)-3'-pyridinyl)thiophene) (P3PyT) were successfully synthesized by the Grignard metathesis (GRIM) polymerization. Both Materials had high molecular weights and low polydispersity indices. These polymers were found to be thermally stable up to 360-390 °C, because of the phenyl or pyridinyl linker in the bristle. Both polymer films had a molecularly multilayer structure whose layers stacked normal to the film plane; each lamella consists of two sublayers, namely ordered and amorphous layers. The amorphous sublayer was composed of a bilayer formed from the bristles. The ordered sublayer in P3PhT consisted of laterally stacked 3-phenylthiophene backbone chains, but that of P3PyT consisted of thiophene backbone chains without the pyridinyl linker. These ordered sublayer formations led a longer  $\pi$ -conjugation length. The enhanced  $\pi$ -conjugation lengths were reflected in their optical and

electronic properties, showing that both P3PhT and P3PyT exhibited a lower highest occupied molecular orbital (HOMO) level and lower energy band gap compared to those of poly(3-hexylthiophene) (P3HT). Overall, the structure and properties of P3PhT and P3PyT make them promising materials for advanced polymer solar cells having an excellent performance.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-27

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study of Self-Assembled Films of Brush Polymers Bearing Zwitterionic Sulfobetaine Moieties

위동우 노예철<sup>1</sup> 안병철<sup>1</sup> 정정운<sup>1</sup> 권원상<sup>1</sup> 김경태<sup>1</sup> 김미희<sup>1</sup> 고용기<sup>1</sup> 정성민<sup>1</sup> 권경호<sup>1</sup>

김영용 송성진<sup>1</sup> 이진석<sup>1</sup> 김용완<sup>1</sup> 김종현<sup>1</sup> 이문호<sup>1</sup>

포항공과대 첨단재료과학 <sup>1</sup>포항공과대 화학과

The well-defined brush polymers containing zwitterionic sulfobetaine, poly(oxy(11-(3-sulfonylpropyltrimethylglyciny)undecylesterthiomethyl)ethylene-co-oxy(n-dodecylthiomethyl)-ethylene)s (PECH-DMAPSm, where m is the mol% of DMAPS (sulfobetaine) end group) were synthesized. The thermal properties and phase transitions of these polymers were investigated. The polymers were thermally stable up to 185 °C. The polymers were found to form favorably into multibilayer structure, always providing hydrophilic, zwitterionic sulfobetaine end groups at the film surface. For the films, water sorption behaviors were examined. In addition, surface energy components were determined for the polymer films and the bacterial cells deposited on cellulose acetate membranes. The brush polymer films were found to suppress bacterial adherence significantly. An understanding of

the suppression of bacterial adherence was attempted in terms of surface energies and thermodynamics. The results collectively indicate that the sulfobetaine-containing brush polymers are suitable for use in biomedical applications that require the reduced possibility of post-operative infection.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-28

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-polishing properties of MMA-Zinc methacrylate copolymers

김윤태 황도훈 박현<sup>1</sup>

부산대 화학과 <sup>1</sup>부산대 첨단조선공학연구센터

Zinc containing Acrylic or methacrylic copolymers are easily hydrolyzed in seawater. Fouling organisms, which attach on the surface of a paint film, are eliminated together with the copolymer film which is decomposed by the hydrolysis of the copolymers. In this study, we synthesized several Zn-based methacrylic copolymers by controlling the molar ratio of co monomers and investigated its effect on the polishing rate. Synthesis and properties of copolymer were investigated by <sup>1</sup>H-NMR, gel permeation chromatography (GPC), inductively coupled plasma (ICP) mass and infrared (IR) spectroscopy. The polishing rate was determined by measuring the film thickness after a dynamic immersion test.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-29

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

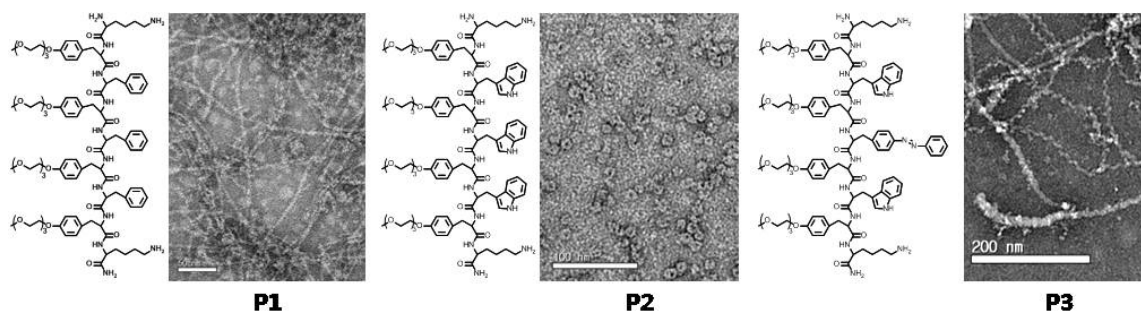
## Structural Evolution of Peptide Nanofibers into Twisted Ribbons and Toroids through Regulation of Intermolecular Interactions

김찬우 유자형<sup>1</sup> 이명수<sup>1</sup>

서울대 화학부 <sup>1</sup>서울대 화학과

Synthetic peptides have been regarded as important biomaterials because of their unique structures like natural peptides. The control of self-assembled nanostructure via molecular design, thus, is crucial to extend our understanding of natural science and living things. In this respect, we synthesized three peptides that have sequential differences of amino acid and investigated their morphologies by using transmission electron microscopy (TEM), circular dichroism (CD), and light scattering experiments. The peptides consist of hydrophilic amino acid, triethylene glycol modified tyrosine, and hydrophobic amino acid, which have amphiphilic characteristics. We varied the hydrophobic part from phenylalanine, tryptophan, to azobenzene modified tyrosine. The sequential differences of amino acid result in various peptide nanostructures. Peptide 1 (P1) that had 3 phenylalanines showed long fibers and P2 which changes 3 phenylalanines to 3 tryptophans, showed toroids nanostructure. P3 that was varied with one central tryptophan to azobenzene modified tyrosine showed twisted ribbons. These results demonstrate

that some sequential alternations make structural differences caused by their intermolecular interaction changes. Eventually, we can regulate synthetic peptide nanostructure by molecular design.



**Figure.** Molecular structure of **P1**, **P2** and **P3** and their nanostructures.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-30

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

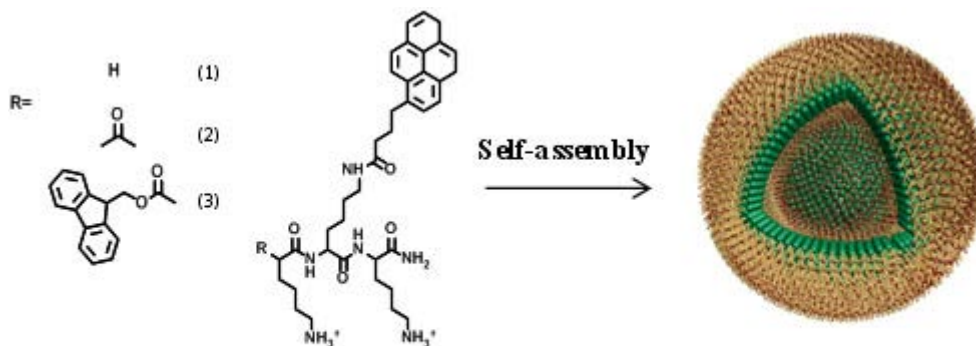
## Controlled Self-Assembly of Peptide Amphiphiles with Nanofibers and Hollow Capsules

최인호 유자형<sup>1</sup> 이명수<sup>1</sup>

서울대 화학부 <sup>1</sup>서울대 화학과

The programmed self-assembly of peptide units into highly ordered nanostructures has a great potential for novel biomaterials displaying a wide range of physical properties often exceeding those of synthetic polymers. For this, we synthesized new self-assembling amphiphiles and investigated their self-assembling behavior in aqueous solution. Peptide amphiphiles are composed of three lysine units with different N-terminal, H, Acetyl, and Fmoc, in pursuance of controlling amphiphilicity. At the second lysine,  $\epsilon$ -position of amine is modified with 1-pyrenebutyric acid. These oligo-peptide units show different structures by modifying N-terminal. The molecule 1 based on H-terminal shows to form hollow capsules. But acetyl-terminated tripeptide unit 2 and Fmoc terminated homologue 3 assemble into well-defined nanofibers. The vesicle structure of 1 arises from increased hydrophilicity of N-terminal, at the same time, hydrophobic pyrene minimize interaction with water. Bulky lysine parts position at outside by electrostatic repulsion and hydrophobic pyrene hide into inside. So these units seem to play an important

role for the formation of hollow capsules. Unlike 1, Fmoc and pyrene part dominate in assembling of 3, then these groups pack into linear nanofiber structures. Such aggregates which can be easily controlled by small modification of molecular architecture may provide a new strategy for creating versatile nanomaterials.



(Fig. 1) Hollow capsule from self-assembly of peptide amphiphiles



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-31

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cells sense the microenvironmental handedness during 3D culture

연보라 최정윤<sup>1</sup> 정병문<sup>2</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 PBL <sup>2</sup>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 chondrocytes and human adipose derived stem cell. Polymers were synthesized by ring-opening polymerization, and were characterized by <sup>1</sup>H-NMR, GPC. Thermal properties were investigated by test tube inverting method and Rheometer to show sol-gel phase transition. In our system, mPEG-L-PA hydrogel system showed selective differentiation of chondrocytes and human adipose derived stem cell.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-32

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cardo Based New Poly(arylene ether)s for Flexible Plastic Substrates



이원중 한양규

한양대 화학과

Transparent and heat resistant polymer materials have gained much attention in the field of next-generation flexible electronic devices such as display, solar cell, e-paper and etc. New poly(arylene ether)s (PAEs) with both transparency and heat-resistance were prepared by a polycondensation of ordered-sequence aromatic dihalide FBPODS with cardo typed aromatic diols. The resulting polymers were found to be amorphous by X-ray diffractometry and T<sub>g</sub> ranged from 200 to 250 °C. Based on TGA and TMA data, they exhibited excellent thermal stabilities. They also had excellent mechanical properties as well as good optical transparency at 450-700 nm. Keywords: poly(arylene ether); flexible display; heat resistant polymer; transparency; CTE

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-33

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Sol-gel transition of PEG-PAF aqueous solution and its application for hGH sustained release

SHINDE USHA PRAMOD 주민경 계은정 정병문

이화여대 화학나노과학과

We report a poly(ethylene glycol)-poly(L-alanine-co-L-phenylalanine) (PEG-PAF) aqueous solution as a polypeptide-based thermogelling system, and its application as an injectable sustained release system for human growth hormone (hGH). The PEG-PAF aqueous solution underwent sol-to-gel transition at 16 - 34 °C in a polymer concentration range of 6.0 wt.% - 14.0 wt.% as the temperature increased. Circular dichroism, FTIR, and <sup>13</sup>C-NMR spectra indicated that the secondary structure of PAF was preserved, however, the molecular motion of the PEG significantly decreased in the sol-to-gel transition temperature range. The polymer was quite stable in water, and therefore, the molecular weight of the polymer did not significantly change and pH of the aqueous polymer solution maintained at 7.2 - 7.8 during the 1 month storage of the polymer as an aqueous solution at room temperature. This point is clearly distinguished from previous thermogelling polymers based on polyesters, polyorthoesters, polyphosphazenes, poly( $\beta$ -amino ester urethane)s, and polyanhydrides, which

generate acid degradation products or can be degraded during storage as an aqueous polymer solution. Therefore, the current system can be used as a ready-to-use injectable implant for biomedical applications. When the polymer aqueous solution (0.5 mL) was injected into the subcutaneous layer of rats, the gel was formed by temperature-sensitive sol-to-gel transition, and the gel was completely eliminated from the implanted site in < 15 days. A haematoxylin and eosin (H&E) staining study suggests the good histocompatibility of the gel in the subcutaneous layer of rats. As a sustained release formulation for hGH, the PEG-PAF showed a 4 day release profile with a pharmacological effective concentration range of > 1 - 5 ng/mL in vivo, suggesting that the system is promising as a once-per-week delivery system for the hGH.



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장소: 일산KINTEX

발표코드: POLY.P-34

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Thermally Activable Bifunctional Reactive Block Copolymers

이진영 Patrick Theato<sup>1</sup> 문봉진

서강대 화학과 <sup>1</sup>University of Hamburg, Germany

In the previous study, ketene-functionalized polymer was synthesized via the ring opening metathesis polymerization (ROMP) using Meldrum's acid derived norbornene as a monomer.<sup>1</sup> In this work, we have synthesized dual functional block copolymers based on 5-norbornene-2-carboxylic acid pentafluorophenyl ester and Meldrum's acid containing norbornene. While many well-known active ester polymers such as poly(N-hydroxysuccinimide acrylate) and poly(N-hydroxysuccinimide methacrylate) suffer from poor solubility in various organic solvents, polymer synthesized from 5-norbornene-2-carboxylic acid pentafluorophenyl ester exhibit much better solubility.<sup>2</sup> TGA study was conducted to confirm that the pentafluorophenyl ester groups were intact at the evaluated temperature for thermolysis of the Meldrum's acid groups. Also, through cyclic voltammetry study, we knew that the polymer was successfully attached to the ITO coated glass via dimerization of ketenes and the active ester group reacted with ferrocenylethylamine efficiently. This dual function polymer is expected to be used in

various material science fields.

- (1) Leibfarth, F. A.; Kang, M.; Ham, M.; Kim, J.; Campos, L. M.; Gupta, N.; Moon, B.; Hawker, C. J. *Nat. Chem.* **2010**, 2, 207-212.
- (2) Theato, P. *J. Pol. Sci. Part A* **2008**, 46, 6677-6687.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-35

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

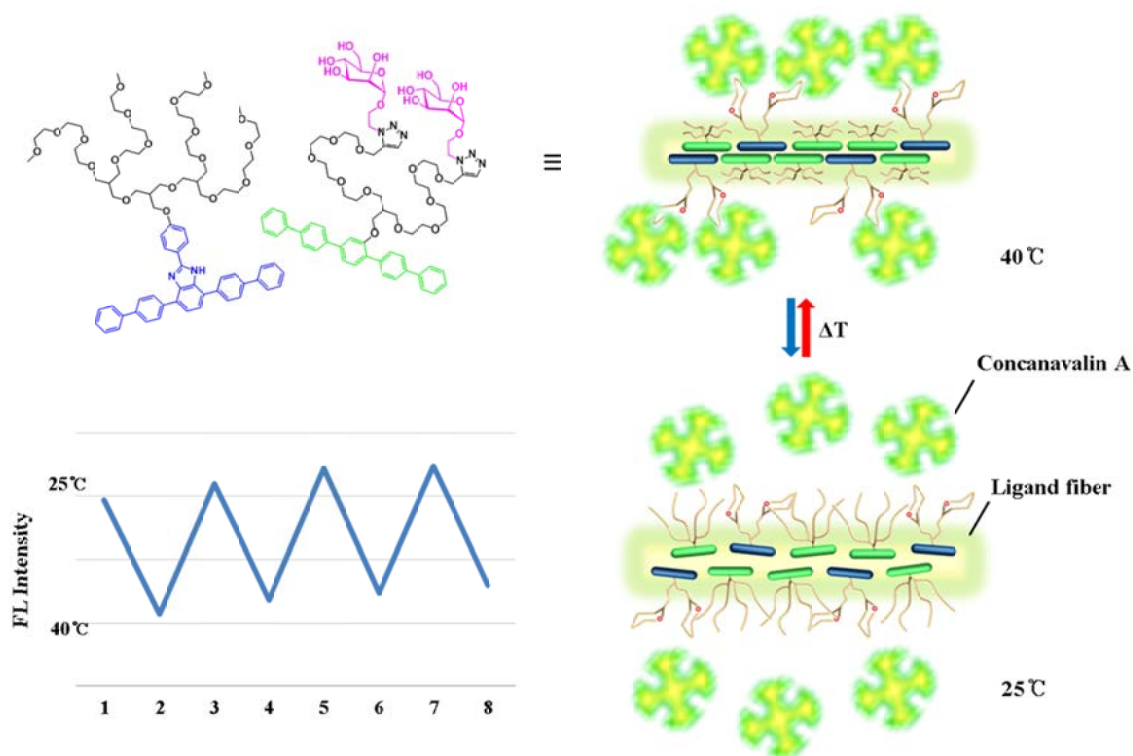
## Stimuli-Responsive Carbohydrate-coated Nanofibers for Multivalent Interactions

김태훈 이명수

서울대 화학부

Cell-surface receptors play an essential role in cell adhesion and signaling. They transmit information of extracellular signals to the internal machinery of the cell. For this purpose, the receptors require higher order macromolecular assemblies rather than isolated entities. Thus, understanding the mechanisms underlying the function of these assemblies is critical. Controlling multivalent ligands interactions can address the role of receptor assembly in signal transduction. In this regard, we synthesized linear aromatic amphiphiles containing oligoether dendrons which are functionalized with bioactive monosaccharides to endow bioactive functions. The density of supramolecular multivalent ligands is regulated by co-assembly with bioactive amphiphiles and inactive one. Investigation on the interactions of the carbohydrate-coated nanostructures with lectin proteins showed that nano-fibers could modulate the amount of multivalent ligands, and the carbohydrate supramolecular structures could bind to lectin

protein by thermo reversible feature through LCST. These results demonstrated that responsive supramolecular nanostructures can provide novel opportunities to control many biological activities.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-36

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Brush Polymers Bearing Alkyl and Sulfobetaine End Group: Synthesis, Multilayer Structure, and Biocompatibility

송성진 정정운 김미희 노예철 권원상 안병철 김경태 고용기 정성민 권경호 김영용<sup>1</sup>

김용완 김종현 이진석 위동우<sup>1</sup> 이문호

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학부

A series of well-defined brush polymers, poly(oxy(11-(3-sulfonylpropyltrimethyl-glyciny)undecylester-thiomethyl)ethylene-co-oxy(n-dodecylthio-methyl)ethylene)s (PECH-DMAS<sub>m</sub>, where m is the mol% of the DMAPS[sulfobetaine] end group) were synthesized. The thermal properties and phase transitions of these polymers were investigated. The polymers were thermally stable up to 185°C and were found to form favorably into multi-bilayer structures, always providing hydrophilic, zwitterionic sulfobetaine end group at the film surface. Because revealed biocompatibility in mice but significantly suppressed protein adsorption. These results collectively indicate that the sulfobetaine-containing brush polymers are suitable for use in biomedical applications, including medical devices and biosensors that require biocompatibility.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-37

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Regulated-Proliferation of Bacterial Cells with Multivalent Carbohydrate Nanofibers

이동우 이명수<sup>1</sup>

서울대 화학부 <sup>1</sup>서울대 화학과

The bio-responsive synthetic aggregates can be used to manipulate biological activities such as cell signalling, micro-environment and cross-linker for cell aggregation. The introduction of carbohydrate functional group on self-assembled nanostructure gives a unique opportunity to promote many biological process. We have explored a system of regulating bacterial cell proliferation by using well-defined self-assembled carbohydrate-coated nanofiber. In this research, we have shown that carbohydrate-functionalized rod-coil amphiphiles are self-assembled into the rigid nanofiber in aqueous solution. This carbohydrate-coated nanofiber efficiently induced e-coli agglutination and can be used as cross-linkers for bacteria. This unique system by using of rod-coil amphiphile can regulate bacterial cell proliferation by controlling biological function of carbohydrate epitope and structural change of self-assembled nanostructure.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-38

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of novel copolymer for selective biomolecule immobilization on gold surface

김동균 이철현

한국기초과학지원연구원 자기공명연구부

Various types of nanoparticles such as quantum dots, magnetic nanoparticles, and liposomes have been studied for numerous biomedical applications. Among these nanoparticles, gold nanoparticles have been extensively exploited for various applications including drug delivery, imaging agents, biosensors, and computed tomography (CT) contrast agents because they have many advantages such as low cytotoxicity, easy size control, high x-ray absorption, unique optical and electrical properties. Stability of gold nanoparticles under physiological conditions is key step for biomedical application. Another key is the immobilization or conjugation of bioactive molecules on gold nanoparticles for targeted drug delivery, molecular imaging, and in vitro diagnosis. To satisfy these key requirements, we developed a novel random copolymer composed of a “surface anchor part” (thiol group), “antibiofouling part” (PEG), and “bioreactivity part” (carboxyl group) for gold surface modification in particular. This polymer could easily be coated on a gold surface by forming polymeric SAM. Biomolecules could be efficiently immobilized

onto the polymer-coated gold surface with high specificity, as well as little non-specific adsorption. Taken together, these results indicate that the polymer described here may be suitable for a variety of gold nanoparticle applications in the fields of biosensing, targeted drug delivery, and molecular imaging.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-39

발표분야: 고분자화학

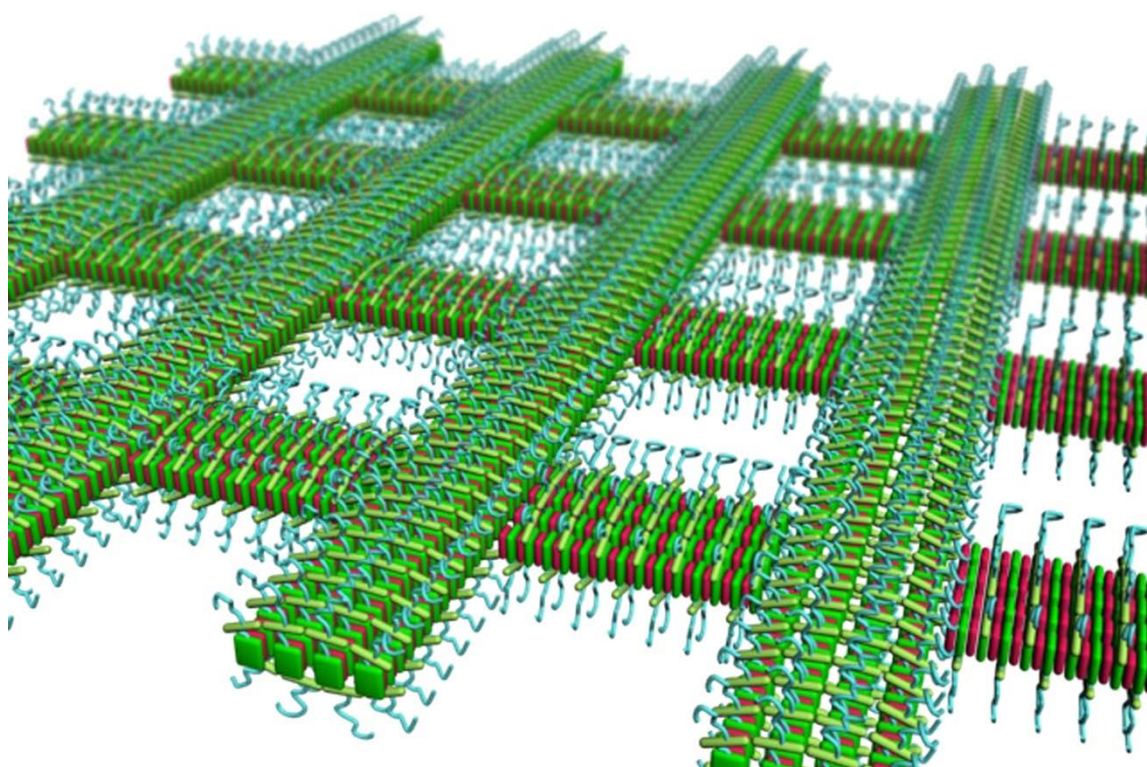
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Formation of Square Grids from Self-Assembly of Peptide Oligomers

박일수 이명수

서울대 화학과

The peptide can make several nanostructures such as fiber, ribbon, sheet, and so on. But, there are limits to make a novel, unique morphology. Addition of guest molecules is one of the good strategies to make unusual nanostructures. 2,4,5,7-Tetranitrofluorenone(TNF) as the guest molecule is hydrophobic and electron-deficient. So, it can interact with hydrophobic and electron-rich segment such as pyrene unit. We have synthesized amphipathic small peptides based a pyrene unit which is hydrophobic and electron-rich. These peptides can make nano-ribbon structures in aqueous solution. When TNF was mixed with peptides, we can show novel and unique square-pore networks in aqueous solution. We confirmed nanostructures by AFM, TEM, and cryo-TEM. The pore-size of networks is nano-scale within 10nm. The square-pore networks were made by addition of TNF 1 equivalent. The mechanisms of forming the networks are suggested from TEM images





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-40

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Radiolytic preparation of poly(ether ether ketone)-grafted-poly(vinyl benzyl chloride) films**

**황미림 손준용 신준화**

한국원자력연구원 첨단방사선연구소 공업환경연구부

Since poly(ether ether ketone) [PEEK] has many advantages such as thermal and chemical stabilities, solvent resistance, high strength, and low cost, it has been widely used for the industrial application. In this study, poly(ether ether ketone)-grafted-poly(vinyl benzyl chloride) (PEEK-g-PVBC) membranes were prepared by a gamma-ray radiation grafting method. The prepared membranes and original PEEK film were investigated by using IR, SEM-EDS, TGA, DSC and DMA.

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장소: 일산KINTEX

발표코드: POLY.P-41

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of new iridium-containing polymers for PLEDs

FEIXU 김희운<sup>1</sup> 미동보<sup>1</sup> 황도훈

부산대 화학과 <sup>1</sup>부산대

PLEDs directly using electrophosphorescent polymers are currently attracting a lot of attention because their internal quantum efficiency is theoretically 100% and the phase separation or dopant aggregation could be restrained. The phosphorescent PLEDs with high luminous efficiency and brightness are expected. In this paper, three series of new iridium electrophosphorescent polymers with fluorene and carbazole as host units have been synthesized via Yamamoto polymerization, respectively. The molecular structures of the polymers were characterized with <sup>1</sup>H NMR spectroscopy and their photophysical, electrochemical and electroluminescence properties were investigated. Note that as increasing the ratio of iridium complex in the polymers, efficient energy transfer from host to dopant unit was observed obviously. Compared with the other host units, the polyfluorene backbone with carbazole as the pendant attached to the 9-carbon position of fluorene by long alkyl chain showed the best performance. External

quantum efficiency of 0.73, a maximum luminous efficiency of 1.21 cd/A, a maximal luminance of 615.2 cd/m<sup>2</sup> and the maximum EL peak at 506 nm were observed.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: POLY.P-42

발표분야: 고분자화학

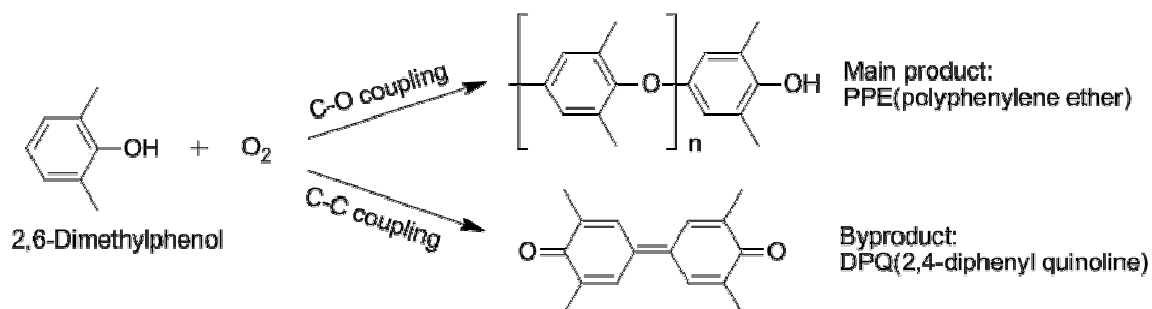
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies of solvent effect on the polymerization of 2,6-dimethylphenol to polyphenylene ether catalyzed by diamine-copper chlorides

김민구 풍신혜 김용태<sup>1</sup> 문성일<sup>1</sup> 윤재숙

성균관대 화학과 <sup>1</sup>제일모직(주) 중앙연구소

The oxidative coupling of 2,6-dimethylphenol to PPE(polyphenylene ether) can be affected by various reaction conditions. We found that an alcohol additive is essential for the fast activation of catalyst, especially for copper(II) chloride. Furthermore, alcohol additives can significantly affect the distribution of molecular weight and PDI of the resulting polymer. More details will be presented.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-43

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The effect of various EB-irradiation doses on the properties of crosslinked SPEEK membranes

송주명 손준용 신준화<sup>1</sup>

한국원자력연구원 첨단방사선연구소/공업환경연구부 <sup>1</sup>한국원자력연구원 정읍방사선과학연구소

Crosslinked sulfonated poly(ether ether ketone) (SPEEK) membranes were prepared by the EB-irradiation crosslinking method with various irradiation doses. The crosslinked membranes are aimed to a study of proton exchange membranes (PEM) for fuel cell application. The pure SPEEK and Crosslinked SPEEK membrane were characterized by using <sup>1</sup>H NMR and <sup>13</sup>C NMR spectroscopy, gel fraction and dynamic mechanical analysis (DMA). The degree of sulfonation of the SPEEK was calculated to be 0.69 from NMR results. The EB-irradiation doses were shown to affect the degree of crosslinking from gel fraction. The DMA results were shown that the CSPEEK membranes have well-developed ionic aggregation in the cluster region. These results indicate that the ionic aggregations are not affected by EB irradiation.

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발표코드: POLY.P-44

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization of crosslinked organic/inorganic composite membrane prepared by radiation

이지홍

한국원자력연구소 첨단방사선연구소/공업환경연구부

In this study, ETFE(ethylene-alt-tetrafluoroethylene)-g-PSSA/PTMSPM (sulfonated poly(styrene-co-(trimethoxysilyl)propyl methacrylate)) membranes were prepared by a simultaneous irradiation grafting of various compositions of binary monomers (styrene and TMSPM) onto ETFE film and followed by sol-gel processing and sulfonation to provide crosslinking structure and proton conducting ability, respectively. The FT-IR and TGA confirmed the crosslinking structure of the prepared films. After sulfonation, the similar IEC value of crosslinked membrane with various degrees of grafting and crosslinking were investigated by stress strain, proton conductivity, dimension stability, and single cell performance.

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장소: 일산KINTEX

발표코드: POLY.P-45

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of Conformational Transition of Silk Fibroin Nanofiber MAt on Biodegradability

김종욱 이미성 김미진 김해경 김도연 진종성

한국기초과학지원연구원 부산센터

Biodegradability is one of the most important parameters for the biomaterial applications. In this study, electrospun silk fibroin (SF) nanofiber nonwoven mat was treated with different alcohol mixtures for controlling the biodegradability. The various properties that morphological structure, conformational transition and etc. of SF mat, treated with various conditions was observed by SEM, FT-IR and DTA. And the observation of feasibility of biodegradability control was evaluated by enzymatic degradation method in vitro.



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장소: 일산KINTEX

발표코드: POLY.P-46

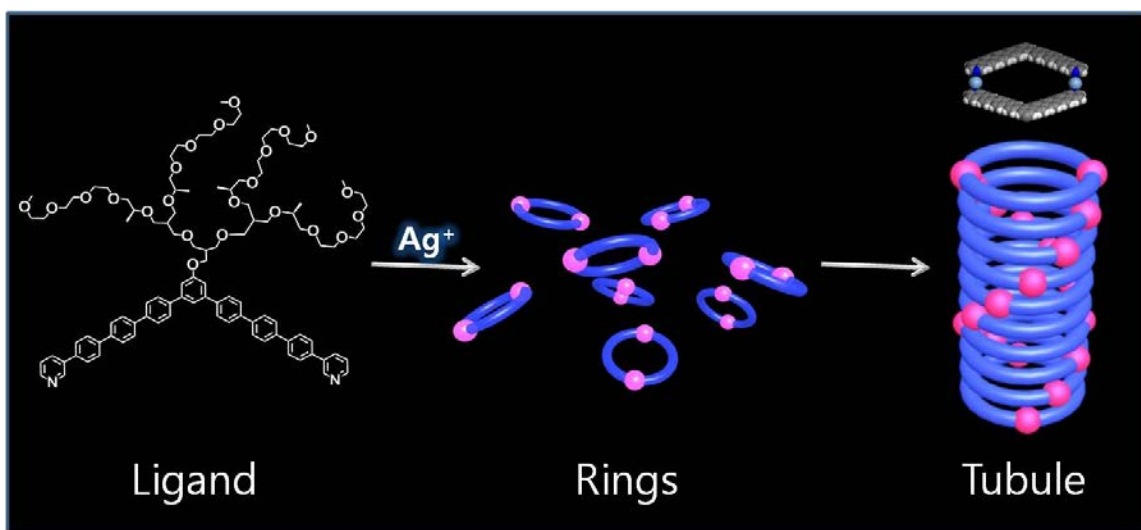
발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dynamic Tubules from Silver-Coordinated Dimeric Cycles



Rigid rod block containing a flexible dendron has already been known to self-assemble into well-defined nanoscopic structure. As an extension of this concept, a bent-shaped amphiphilic molecule containing bipyridine ligand has been synthesized and complexed with silver ion to investigate its secondary structure. The bipyridine ligand showed to be assembled into cylindrical micelles in aqueous solution, as confirmed by TEM. In great contrast, complexation of the ligand with  $\text{Ag}^+$  induces the formation of hollow tubules with hydrophobic cavity. At initial stage, TEM showed the formation of dimeric cycles through complexation. Eventually, the resulting dimeric cycles formed toroidal structure and then toroids stacked on top of each other in the same direction to form helical tubules in aqueous solution. In this meeting, we will present these results on smart tubules together with practical implications.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-47

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Optimization of Active Self-healing Microencapsulation in varying process

고은주 정근우<sup>1</sup> 박수열<sup>2</sup> 김남균<sup>3</sup>

한국화학연구원 그린화학연구단 <sup>1</sup>한국화학연구원 응용화학연구단 <sup>2</sup>한국화학연구원 계면화학  
공정 연구팀 <sup>3</sup>한국화학연구원

**Abstract** In this study investigated optimization of functional microcapsules for self-healing system in the urethane substrate. Diisocyanate group was encapsulated by polyurethane shell wall material, and can be automatically induced self-repairing action by the scratch or crack. We developed microencapsulation process using varying conditions as core-shell materials ratio, agitation rate and different shaped stirring bar. Resultingly, the yield of microcapsules was lessened in an increasing of agitation rate. Mean diameter of microcapsules were decreased with an increasing of core material ratio. Also, the mass of core content has dropped down with an increasing of agitation rate. Characteristics of microcapsules were investigated using by OM and SEM microscopy and analytical technologies.

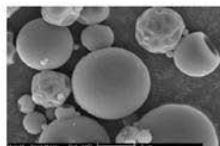
# Influence of the shape of the homogenizer



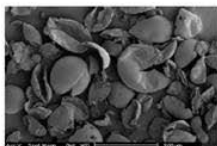
(a) Sawlike shaped stirring bar of the homogenizer



(a) 4-bladed stirring bar of the homogenizer

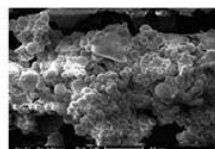


(b) SEM image, at 1000 RPM

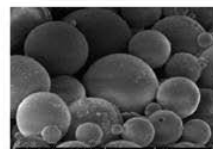


(c) SEM image, at 3000 RPM

Figure 4 Formation of microcapsule using by sawlike shaped stirring bar of the homogenizer



(b) SEM image



(c) SEM image

Figure 5 Formation of microcapsules using by 4-blade shaped stirring bar of the homogenizer



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-48

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Photovoltaic Properties of Organic Semiconducting Polymers

김지훈 김희운 신원석<sup>1</sup> 황도훈<sup>2</sup>

부산대 <sup>1</sup>한국화학연구원 에너지소재연구센터 <sup>2</sup>부산대 화학과

Arylenevinylene based bis(arylhalide) monomers were synthesized as low band gap electron-accepting blocks, and were copolymerized with 9,9-dioctyl-2,7-fluorene or 9-(heptadecan-9'-yl)-2,7-carbazole diboronic esters as electron-donating blocks using Suzuki coupling polymerization. Four alternating copolymers were synthesized through the combination of two different bis(arylhalide)s and diboronic esters, and their optical, thermal and electrochemical properties were characterized. 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. The optical band gap energies of the polymers were measured from their absorption onsets to be 1.97-2.18 eV depending on the polymer structure. Bulk hetero-junction photovoltaic devices were fabricated using the synthesized polymers as the electron donors and [6,6]-phenyl C71-butyric acid methyl ester (PC70BM) as the electron acceptor. One of these devices showed a high power conversion efficiency of 3.22 %, with an open-circuit voltage of 0.74 V, a

short-circuit current of 10.60 mA/cm<sup>2</sup>, and a fill factor of 0.41 under air mass (AM) 1.5 global (1.5 G) illumination conditions (100 mW/cm<sup>2</sup>).



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발표코드: POLY.P-49

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Curing Behaviors and Thermal Conductivities of Silane Treated $\gamma$ -alumina-reinforced Epoxy Composites

권미정 박수진

인하대 화학과

In this work,  $\gamma$ -alumina was used as a filler of epoxy resin to enhance thermal properties of epoxy composites and various thermal properties of the epoxy/alumina composites were investigated. The alumina particles were treated with silane coupling agent to improve the dispersion forces in epoxy resin. Methacryloxy type silane coupling agent was blended with  $\gamma$ -alumina powder. The content of filler was varied between 0 and 20 phr. Effect of  $\gamma$ -alumina particles on thermal stabilities and curing behaviors were studied by thermogravimetric analysis(TGA) and dynamic differential scanning calorimetry(DSC), respectively. Also, the thermal conductivity of epoxy/alumina composites were investigated by laser flash apparatus(LFA). As a result, the thermal conductivity was enhanced by the adding of  $\gamma$ -alumina to epoxy resin.

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발표코드: POLY.P-50

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The effect of silver and gold nanoparticles on dye-sensitized solar cells

윤진선 송홍규 원종욱

세종대 화학과

Metal nanoparticles can contribute to the effective light absorption of dye-sensitized solar cells (DSSCs), both by the localized surface-plasmon resonance and by light scattering efficiency. The plasmonic resonance of silver and gold nanoparticles has been studied because they strongly interact with visible light. We employ polyester hydroxyl acetylene bis (hydroxymethyl) propanoic acid Dendron (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 transmission electron microscopy. Through the analysis of J-V characteristics and Electrochemical Impedance Microscopy, Incident Photon to Current Conversion Efficiency, we observed the effect of silver and gold nanoparticles on DSSCs.



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장소: 일산KINTEX

발표코드: POLY.P-51

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## CO<sub>2</sub>흡착용 Metal Organic Frameworks 합성 및 특성 분석

최지영 박성진 원종욱

세종대 화학과

최근 대기중의 CO<sub>2</sub>의 양의 증가로 인하여 지구 온난화가 문제로 대두 되고 있다. 이러한 문제로 인하여 CO<sub>2</sub>를 선택적으로 흡착하기 위한 연구를 하였다. layering 시스템을 이용하여 MOFs를 합성하는 실험을 하였다. 전이 금속인 Copper(?) (Cu)와 에스테르 계열인 Disodium Succinate(suc)를 리간드로 이용하여 Wall 형태의 two-dimensional(2D)를 얻을 수 있다. 이 2D판의 Cu와 Bis(4-pyridyl)기를 가진 리간드인 4,4'-trimethylenedipyridin(bpp)가 결합하여 입체형식의 frame을 얻었다. 얻어진 입체구조의 frameworks를 dehydrate하여 그 구조를 Single crystal XRD를 이용하여 비교해 보았다. TGA를 이용하여 Dehydrate frameworks의 열에 의한 안정성을 측정하였다. B.E.T 시스템을 사용하여 이 frameworks의 CO<sub>2</sub>흡착정도를 측정하였다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-52

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 염료 감응 태양 전지 전해질에 도입한 polyrotaxan 이온 채널의

효과

송홍균 윤진선 원종욱

세종대 화학과

기존의 액체상 전해질을 이용한 염료 감응 태양 전지의 약점인 전해질의 누수와 증발을 막기 위해 준고체상 전해질을 이용하여 염료 감응 태양 전지를 제작하였다. 이에 따른 Short-circuit photocurrent density ( $J_{sc}$ )와 효율의 감소를 극복하기 위해  $\alpha$ -cyclodextrin 을 이용해 제작한 polyrotaxane 이온 채널을 준고체상 전해질에 포함시켰다.  $\alpha$ -cyclodextrin 과 Polyoxyethylene bis(amine)을 합성하여 pseudopolyrotaxane 을 만든 후, dinitrofluoro benzene 과 혼합하여 polyrotaxane 을 만든다. 이 polyrotaxane 이온 채널은 counter electrode 에서 전자를 받아 conductive electrode 로 빠르게 전달 시켜 주는 역할을 기대한다. 이에 따른 결과를 확인하기 위해 photovoltaic performance 의 측정을 통해 향상된 변환 효율을 측정하고, IPCE (Incident Photon-to-electron Conversion Efficiency)를 통해  $J_{sc}$  가 증가하는 것을 확인하였다.

또한 EIS (Electrochemical Impedance Spectroscopy)를 측정하여 염료 감응 태양 전지에 미치는 영향을 연구하였다.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: POLY.P-53

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 염료감응태양전지에서 organic redox mediator를 기반으로 한 고분자 전해질의 효과

박성진 최지영 원종욱

세종대 화학과

Organic redox couple 은 Dye-sensitized solar cell (DSSC)에서  $I^-/I_3^-$  redox couple 의 단점을 감소시킬 수 있는 물질로서 인정을 받았다. 그러나 acetonitrile(ACN)을 solvent 로서 이용한 액체 전해질의 중요 단점인 누액현상과 longterm stability 는 만족시키지 못하였다. 또한 액체 전해질의 경우 sensitizer 로서 이용되는 organic dye 가 흡착된 nanocrystalline  $TiO_2$ -layer 에서 solvent 인 ACN 으로 해리되는 현상으로 인하여 DSSC 의 전체적인 안정성이 감소한다. Redox couple 을 용해가능하고 고분자 gel 로서 점성을 가지며 증발현상이 적은 poly(ethylene glycol) dimethyl ether(PEG-DME)을 solvent 로써 이용하여 organic redox couple 을 기반으로 한 새로운 고분자 전해질을 제작하였다. 제작된 전해질을 N719 및 D-149 sensitized solar cell 의 적용하고 cyclic voltammetry(CV)를 측정하여 TEMPO 와 TMTU redox couple 의 전기화학적 성질을

확인하고 photocurrent-voltage 및 electrochemical impedance spectroscopy(EIS)를 측정하여 고분자 전해질의 성능 및 효과를 확인하였다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-54

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization of Anion Exchange Membrane Prepared with High Energy Radiation-induced Graft Polymerization and Cross-linking

고범석 손준용 신준화

한국원자력연구원 첨단방사선연구소 공업환경연구부

Anion exchange membranes for solid alkaline fuel cell (SAFC) were prepared with a simultaneous radiation graft polymerization method of vinylbenzyl chloride and divinylbenzene onto poly(ethylene-alt-tetrafluoroethylene) film by gamma-ray (1.25 MeV) and subsequent quaternarization with triethylamine. The prepared anion exchange membranes were characterized by AFM, SEM-EDS, SANS and IEC, etc. The results indicate that the domain of the poly(vinylbenzyl chloride) graft polymer were formed with separated phase in the poly(ethylene-alt-tetrafluoroethylene) and the water uptake, ionic conductivity, dimensional stability, and chemical stability were influenced by the structure of poly(vinylbenzyl chloride) graft polymer.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-55

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mechanical and Morphology Properties of Epoxy Based Composites using $\text{MgAl}_2\text{O}_4$ -spinel Powders as Filler

권미정 박수진

인하대 화학과

In this work, we have prepared  $\text{MgAl}_2\text{O}_4$ -spinel powders as an epoxy filler. For epoxy composites, magnesium-aluminum spinel has been synthesized by citrate-nitrate route using hydrated nitrates of Mg and Al as the precursors with a citrate-nitrate ratio of 1:1. And then, the  $\text{MgAl}_2\text{O}_4$ -spinel powders were heat-treated in an atmosphere control furnace at  $900^\circ\text{C}$  for 1 h with a heating rate of  $10^\circ\text{C}/\text{min}$  and these powders were blended with epoxy resin. The calcined  $\text{MgAl}_2\text{O}_4$ -spinel powders were characterized by X-ray diffraction(XRD), and scanning electron microscopy(SEM) was used to observe the morphology properties of  $\text{MgAl}_2\text{O}_4$ /epoxy composites. Also, the critical stress intensity factor ( $K_{IC}$ ) of epoxy composites was measured by universal testing machine(UTM).

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장소: 일산KINTEX

발표코드: POLY.P-56

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Encapsulation of Light-Emitting Diodes with Silver  
Nanoparticles/Silicone Composite and High Refractive index  
Nanoparticles/Silicone Composite**

**맹일호 김진권 김상호 PIAO LONGHAI**

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 수행하며 봉지재 자체의 굴절률에 의해 휘도를 향상시킨다. 굴절률이 0.1 증가하면 휘도가 10% 증가하는 것으로 알려져 있다. 우리는 고 굴절 투명 나노입자와 봉지재 composite 를 만들어 투과율과 굴절률의 변화를 연구하였다. 또한 AgNPs 와 형광체, 봉지재 composite 를 만들어 LED 칩에서 방출되는 청색 파장이 전환되는 효율을 연구하였다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-57

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of silver nanowires using PVP-b-PEG diblock copolymers

ZHAOHESONG 김상호 PIAO LONGHAI

공주대 화학과

**ABSTRACT:** 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 of silver nanowires mixing little nanoparticles were synthesized through a simple one-step method by reducing  $\text{AgNO}_3$  with ethylene glycol in the presence of PVP-b-PEG diblock copolymer without seed forming procedure. Importantly, these nanowires can be dispersed into not only polar solvent such as ethanol but also non-polar solvent like toluene and THF. This may be attributed the success to the PEGs block tails on the surface of silver nanowires. The diameter of silver nanowires can be controlled by changing the molar ratio of  $\text{AgNO}_3$  and PVP-b-PEG diblock copolymers from 100nm to 400nm with the average length of 17 $\mu\text{m}$ .

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-58

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of Crosslinked Poly (Styrene-Butadiene-Styrene) Block Copolymers by Irradiation Method and Their Characterization

이선영 송주명<sup>1</sup> 손준용<sup>1</sup> 설용건 신준화<sup>1</sup>

연세대 화학공학과 <sup>1</sup>한국원자력연구원 첨단방사선연구소 공업환경연구부

In this study, cross-linked poly(styrene-butadiene-styrene)[SBS] block copolymers were prepared by radiation and the effects of various irradiation factors on the crosslinking were evaluated. The SBS films and SBS solution (10 wt.%) were irradiated at 25, 50, 100, 200, and 300 kGy by electron beam or gamma ray radiation. The gel fraction study indicates that the irradiated SBS solution was quickly crosslinked than the irradiated SBS films. FT-IR data showed that butadiene double bond peak was decreased with increasing irradiation dose. The thermal property and morphology of the cross-linked SBS block-copolymer were characterized by TGA and SEM, respectively.

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장소: 일산KINTEX

발표코드: POLY.P-59

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication and analysis of open digital microfluidic chips based on electrowetting on dielectric technique**

**고효진 권오선 신관우<sup>1</sup>**

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

Open digital microfluidic chips removed a top cover plate, driven by the electrowetting-on-dielectrics (EWOD) force, were fabricated. The patterned nano-multilayers on a glass substrate of the open chips were prepared by applying optical photolithography, ion sputtering and spin coating techniques: Using mask-aligner, an array of micro patterned ITO electrodes on the most bottom layer of 60 nm thickness was coated in a combined method of sputtering and a lift-off method with an aid of photoresist GXR. For second dielectric layer, a 1 $\mu$ m thickness of parylene-C or SU-8 was deposited uniformly with the chemical vapor deposition and the spin coating technique respectively, to cover completely the array of patterned electrodes. For providing a hydrophobic surface, the second layer was, subsequently, coated with an amorphous Teflon solution, AF 1600, in 200 nm thickness. The morphology of parylene and AF 1600 surfaces was studied by using an atomic force microscopy indicating that there are no pin holes with the small roughness enough to resistive water penetration. Furthermore, analyzing the x-ray reflectivity

data showed that the thickness of top Teflon AF 1600 layer was easily controlled by adjusting only the concentrations of solution. We successfully demonstrated the basic motions of a water drop that are necessary to operate the microfluidic chips with the full functionality for any possible applications, such as, the rapid droplet oscillation between two of neighbor arrayed electrodes, the linear translational motion on the rail of array and the merging at Y-junction of the array, except the drop separation. For the drop separation which is not easy operation in the open-type chips due to the high water surface tension, the AF 1600 surface should be converted to be hydrophilic to make a drop be flatten that reduces the total force for drop splitting. For the hydrophilic conversion, the Xe<sup>+</sup> ion beam irradiation was employed with the fluence of  $(1-10) \times 10^{16}$  ions/cm<sup>2</sup> producing the decrease of the contact angle from 120° to 80°. Because it was not so enough to be overcome by the drop splitting force of EWOD, the drop separation has been failed so far. Hence to find the specific condition of irradiation to prepare the more reduction of surface tension will be studied furthermore.



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장소: 일산KINTEX

발표코드: POLY.P-60

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Molecular sieving by ultrathin membrane of organic molecular nets

변민선 박지웅<sup>1</sup>

광주과학기술원 신소재공학부 <sup>1</sup>광주과학기술원 신소재공학과

A new molecular sieve membrane was demonstrated using molecular nets. A solution-based molecular layer deposition (MLD) was conducted on a nanoporous alumina support to fabricate molecular nets as an ultrathin skin layer of thin film composite (TFC) membrane. Alternating deposition of multi-functional, polyhedral molecules gave nanometer thick films of three-dimensionally cross-linked organic molecular networks. Varying the number of deposition cycles enabled to control the pore size of the TFC membrane precisely on the molecular level. The morphology of the membrane was studied using scanning electron microscopy (SEM) and atomic force microscopy (AFM). The flux and rejection of the TFC membrane were investigated by filtration of the aqueous solutions containing organic solutes. This work was supported by a Korea Science and Engineering Foundation (KOSEF) grant [2010-0026421] funded by the Korean government (MEST).

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장소: 일산KINTEX

발표코드: POLY.P-61

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Amphiphilic Polymers Consisting of Alternating Rod and Coil Blocks

김택경 박지웅<sup>1</sup>

광주과학기술원 신소재공학부 <sup>1</sup>광주과학기술원 신소재공학과

In this study, we synthesized the amphiphilic polymers consisting of alternating oligoaniline and oligo(ethylene glycol) (OEG) blocks with various weight fractions. The polymers were produced by polycondensation di-amino aniline heptamers, protected with the *tert*-butoxycarbonyl (*t*-BOC) groups, and Bis-dPEG<sub>n</sub>-NHS ester (*n*=13, 21, 25), respectively. The resultant polymers exhibited good solubility in common solvents, such as CHCl<sub>3</sub>, MC, THF, and NMP. We have also investigated the self-assembly behaviors of the polymers in the different oxidation states obtained by employing distinct deprotection methods. In case of synthetic polymers in a mixture of THF/water, micellar aggregates or vesicles formed in different sizes varying with weight fractions of blocks. The nanostructures of the polymers in other oxidation states will be further studied. This work was supported by the Korea Science and Engineering Foundation (KOSEF) grant [2010-0026421] funded by the Korean Government (MEST) and the Program for Integrated Molecular Systems (PIMS) at GIST in Korea.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-62

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Homo- and mixed polymer brushes prepared by surface-grafting of asymmetric non-sticky/sticky diblock copolymers and their stimuli-responsive behaviors**

**한민구 박지웅**

광주과학기술원 신소재공학부

We synthesize a nonsticky/sticky diblock copolymer, poly[styrene-*b*-3-(trimethoxysilyl)propylmethacrylate] (PS-*b*-PTMSM), to produce polymer brushes by the grafting-to technique. Uniform coatings of PS brushes are efficiently produced thanks to the multiple reactive groups offered by the sticky PTMSM block and the surface coverage and nanoscopic morphology of the brush layer are adjusted by varying the concentrations of immersion polymer solutions and the immersion time of the substrate. The nanoscopic pattern of PS brushes with the trimethoxysilyl group terminated poly(ethyleneoxide)s (PEO-TMS) is utilized further to produce mixed polymer brushes via step-wise coating method. The resultant mixed polymer brushes change their nanoscopic morphology in response to external stimuli by temperature and solvent. This work was supported by the Korea Science and

Engineering Foundation (KOSEF) grant [2010-0000282 and 2010-0026421] funded by the Korean government (MEST) and the Program for Integrated Molecular System (PIMS) at GIST, Korea.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-63

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Deposition control of parylene film with quartz crystal microbalance (QCM)

이가연 고희

연세대 신소재공학과

The parylene is a polymer of p-xylene and it is polymerized by pyrolysis of parylene dimer called di-paraxylylene. Usually, the thickness of parylene film has been controlled by adjusting the amount of parylene dimer and the deposition time which is defined to be the time taken for deposition process. This work presents that the quartz crystal microbalance (QCM) sensor can be used for the control of parylene film thickness with a small deviation from the targeted thickness. For the on-line monitoring of parylene thickness, the QCM sensor was installed at the deposition chamber of a parylene coater and the QCM signal was on-line monitored during the whole deposition process. And for the correlation of the QCM response and the thickness of parylene film, the atomic force microscope (AFM) analysis was carried out with standard samples with measured QCM responses. By comparison with the conventional methods by adjusting the amount of parylene dimer and the deposition time, the on-line QCM monitoring is determined to be feasible for the accurate and reproducible control of parylene thickness.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-64

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

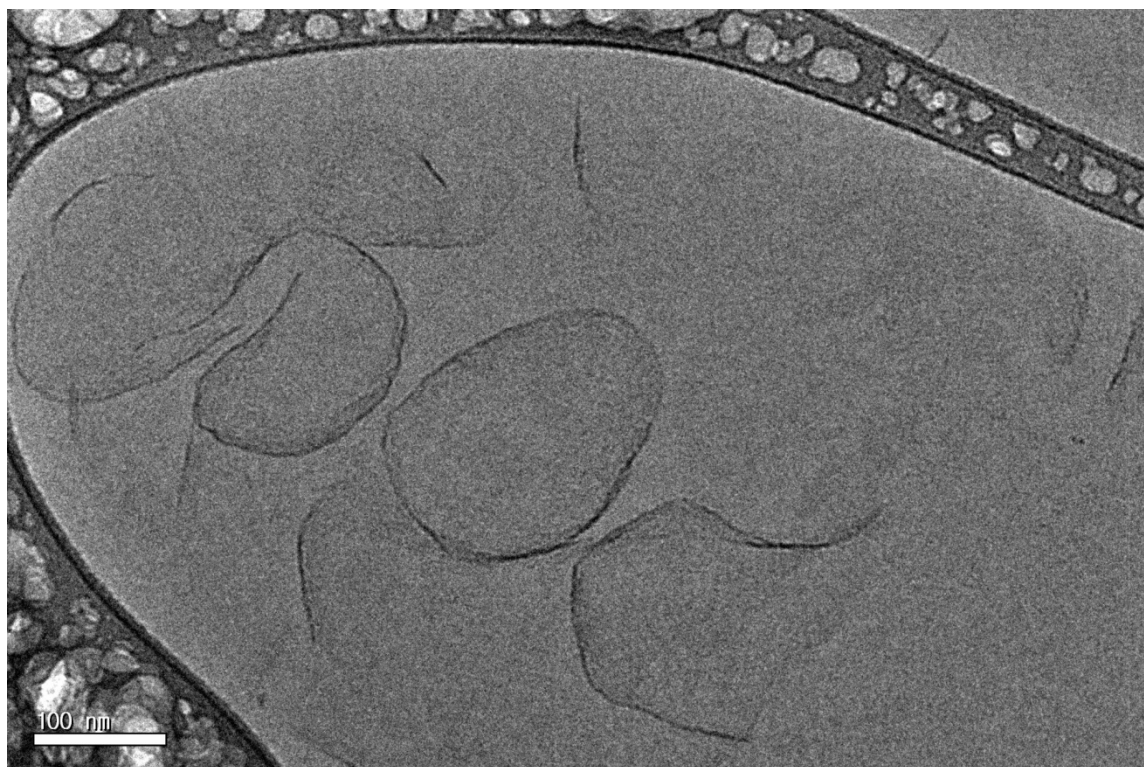
## Self-Assembling Molecular Sheets and Their Aggregation

강선영 이명수

서울대 화학부

Well-defined aqueous nanostructures can be constructed by self-assembly of aromatic amphiphiles. Along this line, we have explored amphiphilic block molecules based on a planar aromatic sheet and a hydrophilic oligoether dendron. Additionally, we have made an effort to prove an influence of a small single alkyl chain which is attached at aromatic sheet. These small block molecules were synthesized through a multistep fashion starting from m-linked terphenyl units. These molecules showed to self-assemble into discrete nanostructures in aqueous solution through strengthened  $\pi$ - $\pi$  stacking interactions of the flat aromatic segments. The aggregation behavior of the molecules has been characterized by cryo-TEM and DLS. We have also demonstrated that the molecules can selectively exfoliate graphite powder into graphene sheets in water. In this presentation, we will discuss the synthesis of the laterally-grafted molecular sheets and their self-assembly behavior in aqueous solution and the functionalization of graphene.[1] J.-K. Kim, E. Lee, M.-C. Kim, E. Shim, M. Lee, J. Am. Chem. Soc. 2009, 131, 17768[2] J.-

K Kim, E. Lee, M. Lee, *Macromol. Rapid Commun.* 2010, 31, 980[3] D.-W. Lee, T. Kim, M. Lee, *Chem. Commun.* 2011, 47, 8259



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-65

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Microporous nanocomposites comprised of the polyimides and the molecular network nanoparticles

전은경 박지웅

광주과학기술원 신소재공학과

Microporous network nanocomposite consisting of microporous organic nanoparticles and polyimide was synthesized that are potentially applicable in mass transport membrane. Nanoparticles were synthesized from tetrakis(4-aminophenyl)methane and hexamethylene diisocyanate by organic sol-gel polymerization to produce the 3D microporous organic molecular network. The nanoparticles dispersions were mixed with poly(amic acid) using various dianhydrides and diamines. Casting onto the glass plate followed by thermal curing gave nanocomposite film. We investigated on the morphological structures subjected to different reaction time and composition of nanoparticles. Continuous interconnected nanostructures in polymer matrix were prepared by controlling spinodal decomposition and reaction between numerous reactive amino and isocyanato functional groups of nanoparticles and polyimide chains. The microporosity of synthesized nanocomposite was characterized under carbon dioxide isotherm at 273K and their permeability of the membranes to small molecules such as helium, carbon dioxide, and nitrogen

was also measured. This work was supported by the Korea Science and Engineering Foundation (KOSEF) grant [2010-0026421] funded by the Korean government (MEST).



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장소: 일산KINTEX

발표코드: POLY.P-66

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Surface structure comparison of blend homopolymers and copolymer films by AFM and TOF-SIMS

강민화 이지혜<sup>1</sup> 이연희<sup>1</sup>

과학기술연합대학원대 나노및바이오표면과학<sup>1</sup>KIST 특성분석센터

Atomic Force Microscopy(AFM) and Time-of-Flight Secondary Ion Mass Spectrometry(TOF-SIMS) are useful instruments to analyze material surfaces. Two kinds of polymer films were analyzed by AFM and TOF-SIMS. One is blend homopolymers consisted of deuterated polystyrene and poly(2-ethyl hexylacrylate). The other polymer sample is poly(styrene(d8)-b-2-ethyl hexylacrylate) copolymer. To compare the difference of surface structure depending on temperature and concentration, various polymer solutions were prepared by dissolving in toluene. Films were annealed at 120℃ for 2 hours in vacuum dry oven and then were compared with samples stored at room temperature to observe microphase separation. Surface morphologies of blend homopolymers and block copolymers were investigated by AFM and their surface compositions were characterized by TOF-SIMS.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-67

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Inkjet Printing of CNT inks for flexible patterned electrodes

김한수 이병노 권오선 신관우<sup>1</sup>

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

Compare to another conductivity polymers, Multi-walled Carbon nanotube(MWCNT) is a comparative material for fabricating a flexible electrical circuit. Even if CNT is not dispersed well in the water because of its hydrophobic property, we make highly concentrated CNT-ink, which could be one of the highest conductivity water based CNT-inks. The printable CNT-ink is obtained by ball-milling process with surfactants in water. After ball-milling, the solution is centrifuged at 3000 rpm for 10 minutes. The supernatant solution is collected and centrifuged again. It is also patterned on the several substrates such as common paper, glossy paper, photo paper and OHP films by using piezoelectric head of inkjet printer, which is also environment-friendly and low cost process since the ink-jet printing is drop-on-demand (DOD) process, no waste of ink and substrates. The pattern can be free from curing process dissimilar to nano-silver conductive ink. Sheet resistance of the CNT patterns printed on the photo paper is measured up to the 168Ω/sq by applying 20 times prints, respectively. The conductivity of CNT solution could be

improved by the addition of doping reagents, which are currently under investigation. Several effective binders are also investigated.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-68

발표분야: 고분자화학

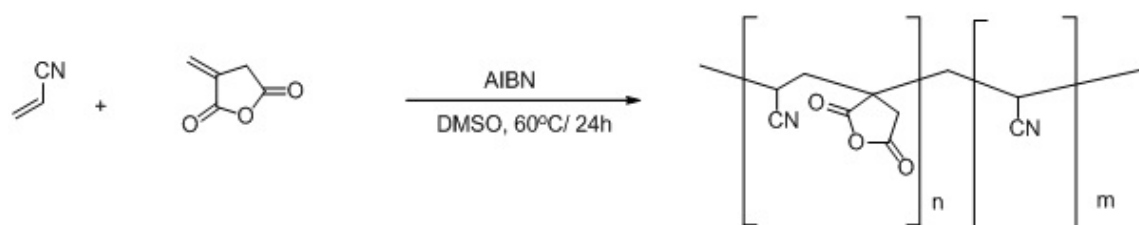
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermal Behavior of Carbon Fiber Precursor from Acrylonitrile and Itaconic anhydride as a Comonomer

신동근 한진욱 김기영<sup>1</sup>

한양대 화학과 <sup>1</sup>한국생산기술연구원 섬유융합연구그룹

The P(AN-ITAh) copolymers with different ITAh(Itaconic anhydride) contents (0.125 ~ 1.5 mol% in the feed) were polymerized using solution polymerization with 2,2'-azobis(isobutyronitrile) (AIBN) as an initiator. The chemical structure and composition of P(AN- ITAh) copolymers were determined by proton nuclear magnetic resonance (<sup>1</sup>H-NMR) and elemental analysis, and the copolymer composition was similar to the feeding ratio of the monomers. The effects of ITAh comonomer on the thermal properties of its copolymers were characterized differential scanning calorimetry (DSC) in nitrogen and air atmospheres.



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장소: 일산KINTEX

발표코드: POLY.P-69

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Graphene Sheet Exfoliation with the Aid of Polymer Nanoparticles

**J. S. Siddique N. F. Attia<sup>1</sup> K. E. Geckeler<sup>2</sup>**

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Nanomaterials have attract a lot interest especially carbon nanomaterials. Graphene is unique 2-dimensional carbon allotropes which has promising electronic and mechanical properties demanded in various applications. There are a number of methods for generating graphene sheets from graphite and derivatives of graphite. Here in this study the exfoliation of graphene sheets have been prepared from commercial graphite using effortless green synthesis method by using spherical polymer nanoparticles. The spherical polymer nanoparticles having ~20 nm in diameter have been prepared by two different methods i.e. wet milling and magneting stirring process. These nanoparticles penetrate the graphite with help of ultrasonification producing graphene sheets. Showing the crucial role of polymer nanoparticles in the synthesis of graphene which couldn't achieved by the normal polymer chain. This prepared graphene sheets have characterized by using UV-VIS, Raman, FTIR spectroscopy, and Transmission electron microscopy TEM.

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## Effect of cardiolipin on the size and shape of small unilamellar vesicle interacting with cytochrome C

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The effect of cardiolipin lipid on the size and shape of dioleoyl-phosphocholine (DOPC)/cardiolipin small unilamellar vesicle interacting with cytochrome C was studied by small angle neutron scattering (SANS) and dynamic light scattering (DLS) measurements. Small unilamellar vesicles containing various mol-ratio of cardiolipin were prepared in PBS buffer by the extrusion method. When the small unilamellar vesicles were prepared from mixed lipid solution with higher mol % of cardiolipin, the membrane thickness of vesicle was thinner. And the polydispersity of the vesicles containing cardiolipin is also lower than the polydispersity of pure DOPC vesicles. We found that cytochrome c binds strongly to cardiolipin-rich vesicle by DLS measurements. Furthermore, we will investigate the binding structure of cytochrome c on the DOPC/cardiolipin lipid bilayer by AFM study.

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## Sulfonated poly(biphenylsulfone ketone) block copolymers containing biphenylsulfone and perfluorobiphenylene units

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본 연구에서 우리는 4,4'-bis[(4-chlorophenyl)sulfonyl]-1,1'-biphenyl 단량체에 sulfuric acid 를 가하여 일련의 과정을 거쳐 대량스케일로 4 개가 술폰화된 단량체를 제조하였다. 이 합성된 단량체와 4,4'-(hexa-fluoroisopropylidene) diphenol 을 사용하여 우선 친수성을 갖는 고분자를 합성하였고, 또한 bis (4-chlorophenyl) methanone 과 4,4'-(hexafluoroisopropylidene) diphenol 을 사용하여 소수성을 갖는 고분자를 합성하였다. 합성된 두 고분자를 연결자 역할로 decafluorobiphenyl 을 사용하여 친핵성 방향족치환반응을 통하여 공중합 반응을 시켰다. 선 술폰화(pre-sulfonation)방법으로 친수성 부분의 비율이 각각 10%, 30%, 50%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 고분자로서 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), 물흡수도 및 양이온 전도도를 확인하였다. Block copolymer 30%에서 가장 높은 값인 75 mS/cm (90 °C, RH 100%)의 양이온 전도도 성능을 얻을 수 있었다. 이들을 결과를 예측하기 위해 AFM phase image 을 통해 확인해 본 결과, block copolymer 30 이 소수성 부분과 친수성 부분이 잘 나누어져서 이온 통로가 가장 효과적으로 형성되어 block copolymer 30 에서 가장 좋은 전도도 값을 보인 것으로 예측된다.



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## Sulfonated poly(biphenylsulfone ketone) multi-block copolymers for PEMFC: structural, thermal, electrochemical and morphological characteristics

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본 연구는 새로운 술폰화된 poly(biphenylsulfone ketone) 블록공중합체를 제조하여 이들의 특성들을 분석하여 고찰하였다. 신규 블록공중합체는 다음과 같이 합성하였다. 먼저, 친수성 올리고머와 소수성 올리고머를 합성하고, 이 합성한 친수성 올리고머를 chlorosulfuric acid 를 가하여 술폰화를 진행하였다. 그리고 나서 앞에서 제조한 친수성 올리고머와 수소성 올리고머를 직접 공중합반응을 시킴으로써 새로운 블록코폴리머를 합성하였다. 블록코폴리머의 술폰화도 (degree of sulfonation)는 친수성 올리고머(10%, 30%, 50%)의 비율의 조절함으로써 결정하였다. 합성한 블록코폴리머들은 <sup>1</sup>H NMR, FT-IR 및 GPC 를 통하여 폴리머의 구조분석을 확인하였으며, DMSO 용매를 사용하여 각각 제막하였다. 상용의 Nafion 을 비교물질로 하여 열적 안정성을 확인하였는데, TGA 와 DSC 측정한 결과, 우수한 열적 안정성을 보여주었다. 또한 막의 술폰화도가 증가함에 따라 이온교환능력 (IEC)과

water uptake (물흡수도)가 증가하는 경향을 보여주었다. 블록코폴리머 50 의 이온전도도는 60 °C 100 %RH 에서 184 mS cm<sup>-1</sup> 나왔으며, 같은 조건에서 Nafion 115 는 160 mS cm<sup>-1</sup> 로 측정되었다. 이는 AFM image 를 관찰한 결과, 친수성 부분과 소수성 부분이 매우 효과적으로 분리 되어 있음으로써 양이온 통로가 잘 형성되어 만족할 만한 성능이 나온 것으로 판단되어진다. 따라서 이 고분자는 고분자 전해질 연료전지의 고체 전해질막으로 적용하기에 좋은 대체 물질로서 판단된다.





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## Synthesis of Thienylenevinylene based Copolymers with High Mobility Ambipolar Charge Transport in Organic Thin-Film Transistors

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Thienylenevinylene (TV) based materials can show a high charge-carrier mobility as a result of a high planarity by introduction of vinylene with double bond character between thiophene units and a large intermolecular attractive force by the thiophene. The presence of vinylene linkages as a conjugated spacer in a backbone of aromatic polymers can increase the degree of coplanarity by the limitation of the rotational disorder inherent between consecutive bulky aromatic units. Therefore, the introduction of a vinylene moiety between the thiophene units resulting in a TV is an attractive building block for the active layer of OTFTs or organic photovoltaics (OPVs). We synthesized alkyl-substituted TV based donor-acceptor type copolymers using Grignard, Kumada, and Stille coupling reactions. These polymers showed crystallinity and ambipolar charge transport property. This ambipolar polymers showed good hole and electron mobilities ( $\mu_h = 0.75 \text{ cm}^2/\text{Vs}$  and  $\mu_e = 0.06 \text{ cm}^2/\text{Vs}$ ). In addition, these polymers showed excellent solubility in common organic solvents such as chloroform and chlorobenzene (30~50 mg/mL at

25 °C) because of sufficient solubilizing groups. To understand the nature of polymer structure, charge transport and electronic properties, these polymers were investigated using X-ray diffraction, Raman spectroscopy, quantum calculation and morphological study. Finally, CMOS-like organic integrated circuits (ICs) were demonstrated by solution process and optimized ICs exhibit ideal behavior characterized by very high voltage gains ( $>50$ ) and high noise margin ( $\sim 75\%$  of  $1/2V_{DD}$ ).



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## Solution-processable New HOST Materials based on Triphenylene and Diphenylbenzothiophene Derivatives for PHOLEDs

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OLEDs(Organic Light-Emitting Diodes)은 형광성 또는 인광성 유기 화합물 박막에 전류를 흘려주면, 전자와 정공이 유기막에서 결합하면서 빛이 발생하는 현상을 이용한 자체발광형 표시 소자로서, 경량, 부품이 간소하고 제작공정이 간단하고 고화질에 넓은 시야각이 특징으로 최근 1월 미국 2012 CES 에서 삼성전자와 LGD 에서 55 인치 TV 급 AMOLED 를 발표할 만큼 급속도로 발전하고 있는 분야이다. 발광층 형성 재료는 발광 메커니즘에 따라 일중항 상태의 엑시톤을 이용하는 형광 재료와, 삼중항 상태의 엑시톤을 이용하는 인광 재료로 나뉘지만, 형광재료를 이용하는 OLED 소자는 생성되는 엑시톤 중 75%는 전혀 이용할 수 없었지만 인광재료를 사용하여 이론적으로 100% 발광효율을 높이려는 연구가 활발히 진행되어 왔다. 그러나 그 효율을 극대화시키기 위해서는 에너지는 전달하는 HOST 와 그것을 받아 발광하는 Dopant 와의 삼중항 에너지레벨의 효율적인 맞춤이 필요하고 대부분의 경우 그 필수조건으로 높은 삼중항 에너지준위를 가진 HOST 재료가

필요하게 된다.

본 연구는 기본적으로 높은 삼중항 에너지준위를 갖는 Carbazole 을 사용한 mCP 에 성능 개선을 위해 Triphenylene 과 Diphenylbenzothiophene 을 도입하여 분자를 디자인하였다. Triphenylene 은 평평한 구조로 charge transporting 향상이 기대되고, Diphenylbenzothiophene 구조에는 sulfur 분자가 존재하여 인광 효율 향상을 기대할 수 있다. 이들 새로운 HOST 재료를 합성하고, 용액공정으로 OLED 소자를 제작하여 그 특성에 대해 조사하였다.



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## **Solution-processable New Asymmetric Hole-Transporting Materials Based on Phenylanthracene Core for OLEDs**

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OLEDs 의 발광효율과 lifetimes 은 electrons 과 holes 의 charge balance 에 영향을 받는다. HTL, ETL 등과 같은 다층 구조(multilayer system)를 이용하지 않으면 고효율 및 고휘도의 발광특성을 기대하기는 불가능하다. 그리고 증착공정이 아닌 대면적화에 유리한 용액공정으로 device 를 제작하기 위해서는 재료의 용해성 및 균일한 박막 형성 능력이 매우 중요하다. 따라서 열적 안정성이 낮으면 구동시 발생하는 열에 의하여 분자의 재결정 현상이 나타나 발광효율이 떨어지고 소자의 수명이 크게 단축되는 등의 문제가 발생한다. 본 연구에서는 phenylanthracene core 를 분자에 도입하여 열적 안정성이 우수하고, 분자구조적으로 비대칭이며 뛰어난 용해성과 amorphous 한 박막 형성 특성을 갖는 새로운 HTL 재료를 분자디자인하여 합성하였고, 치환기의 종류와 치환위치에 따른 열적, 전기화학적 특성의 차이와 또한 증착공정과 용액공정을 이용해 제작한 devices 의

전계발광적 특성의 변화를 상용화된 HTL 재료인 NPB 를 비교물질로 사용하여 체계적으로 조사하였다.



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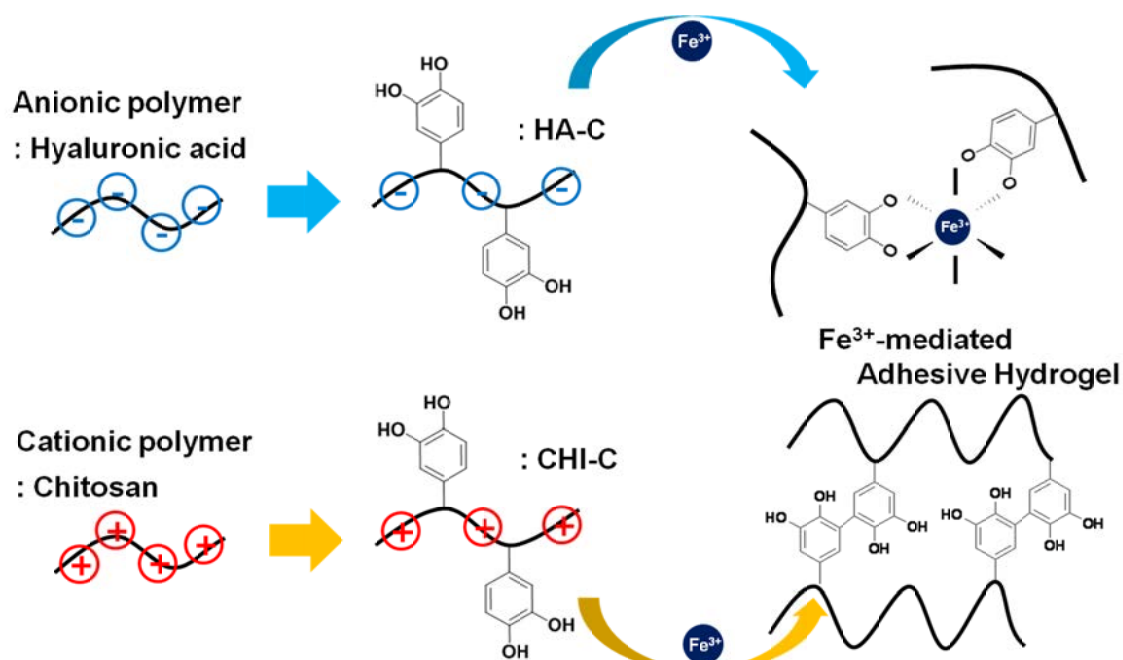
## Mussel-Inspired Instant Medical Adhesives Using $\text{Fe}^{3+}$ Ion-Mediated Rapid Crosslinking for Immobilizing Drug-Loaded Polymeric Patch

유지현

KAIST 나노과학기술대학원

Metal-ion based polymer hydrogel is an emerging tissue engineering material adhesives because of its reversibility and self-healing properties upon crosslinking by coordination bonds. Bio-inspired by mussel cuticle cohesion, rapid curing catechol-functionalized hyaluronic acid and chitosan based medical adhesives were synthesized to immobilize a polymeric patch via iron-mediated crosslinking. Catechol groups were first introduced on hyaluronic acid and chitosan, and both were cross-linked with  $\text{Fe}^{3+}$  ions respectively. The instantaneous  $\text{Fe}^{3+}$ -mediated cross-linking which are strong binding affinity with catechol groups and redox activity of  $\text{Fe}^{3+}$  ions in longer times, and anchorage effects could contribute the high elastic modulus values and adhesion forces of hydrogels. In addition, amine and carboxylic acid groups in polymer backbone could affect the mechanical properties such as stability of hydrogels. Furthermore, these hydrogels could immobilize the polycaprolactone film on mouse peritoneal region.

Thus, these  $\text{Fe}^{3+}$ -mediated medical adhesives have enormous potential to apply medical applications as drug delivery, tissue engineering and tissue adhesives.





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## **An electrochemical immunosensor with self assembled monolayer for GP73 determination**

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GP73 is a cancer biomarker, which is strongly up-regulated expressed in HCC. A label-free immunosensor for sensitive determination of GP73 is prepared by immobilizing antibody on MPA SAM decorated Au electrode. EIS was used for determination of different concentrations of target molecules, the result showed that the electron transfer resistance increased linearly with GP73 concentration in the range of 0.005 - 0.1 ng/ml with high sensitivity, specificity and good reproducibility.

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## Copolymers of 2-Pyrrolidone and Various Beta-lactams

김선미 조창기

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Copolymers of nylon-4 and  $\beta$ -lactam was prepared via anionic ring-opening polymerization in the presence of a strong base and imide initiator. Because the reactivity of  $\beta$ -lactam is higher than 2-pyrrolidone, we used the  $\beta$ -lactams with hydrocarbon substituents to reduce the reactivity. The  $\beta$ -lactam monomers were obtained via N-chlorosulfonylisocyanate cycloaddition reactions with alkenes. And the copolymerization was carried out in organic solvent at 20~50°C. The monomer composition in the copolymers was characterized by nuclear magnetic resonance spectroscopy (NMR) and thermal properties was checked by differential scanning calorimetry (DSC), and thermal gravimetric analyser (TGA).

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## Bernoullian copolymerization of 2-pyrrolidone and $\epsilon$ -caprolactam

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Monomer reactivity ratios were investigated in the copolymerization of 2-pyrrolidone and  $\epsilon$ -caprolactam. Experiment was performed in the temperature range of 60~90°C. 2-Pyrrolidone with  $\epsilon$ -caprolactam copolymer was synthesized by anionic ring-opening polymerization and the mole fraction in the copolymer was obtained by H-NMR. The potassium tert-butoxide was used as an initiator and the N-acetylcaprolactam was used as the activation reagent. According to the obtained reactivity ratio, it is determined that it has the value of the  $r_1 \approx r_2 \approx 1$  in 75~80°C and the copolymer composition is the same as the comonomer feed with random placement of the two monomers along the copolymer chain.

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발표코드: POLY.P-80

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Mercury Sensing Characteristics and Layer-by-Layer Self-Assembly Structures of Novel Brush Polymers Bearing Thymine Moieties

정정운 노예철 김미희 안병철 권원상 김경태 고용기 정성민 김영용<sup>1</sup> 권경호 이문호

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학부

We report herein two polymers which have same functional end group, thymine, which served as sensors for detecting mercury ion but having different structure. Interestingly, thin films of these brush polymers showed different sensitivity for mercury ion in water via different physicochemical properties and reversible character. Various physical properties were measured using DSC, TGA, contact angle meter and ellipsometry. These differences were greatly influenced by structure difference. The structures of these polymers were analyzed using synchrotron radiation source and characterized using surface plasmon resonance spectroscopy (SPRs). The combination of functional studies with structure analysis has shown that importance of structure study for design new sensor materials

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: POLY.P-81

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Magnetic-Cored Dendrimers terminalized with Carboxyl and Amine groups for Cadmium and Chromium adsorption

여인환 박효숙 장준원 박재우<sup>1</sup>

한양대 건설환경공학과 <sup>1</sup>한양대 토목공학과

Two types of magnetic-cored dendrimer terminalized with carboxyl groups and amine groups were synthesized and evaluated for adsorption capacity of both cadmium and chromium. The samples were prepared in four steps: (1) preparation of magnetic-core with ferric chloride and ferrous sulphate using coprecipitation method, (2) amino silanization of magnetic-core with 3-aminopropyltrimethoxysilane (3) growth of dendrimer branches with a repeating injection of ethylene diamine and methyl acrylate using michael addition, and (4) development of functional groups by ethylene diamine and glutaric acid. Transmission electron microscopy and X-ray diffraction measurement showed magnetic-cored dendrimer has magnetite core and 10-15 nm size. Fourier Transform Infrared Spectroscopy measurement showed various bonds in dendrimer such as Si-O, -NH<sub>2</sub>, -OH, C-H, C=O(amide) and Fe-O. ThermoGravimetric Analysis measurement showed growth of repeating units by dendrimer generation. Atomic Absorption Spectrophotometer showed amine terminalized magnetic-cored dendrimer could adsorb 30.3 mg/g of

cadmium and carboxyl terminalized magnetic-cored dendrimer could adsorb 33.8 mg/g of chromium. In addition, dendrimer showed almost comparable adsorption capacity after five times recycle test.



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장소: 일산KINTEX

발표코드: POLY.P-82

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of evaporation rate of solvent on the diameter and morphology of electrospun nanofibers

김태훈 박종래

서울대 재료공학부

Electrospinning is a facile and effective method to process solution into continuous fibers with diameters ranging from a few nanometers to a few micrometers. Because control of diameter and morphology of the fibers are important issue in nanofabrication, many papers have discussed the key factors that determine the diameter and morphology of electrospun fibers. Most of them have concentrated on either solution parameters such as viscosity, conductivity, and surface tension or experimental parameters such as electric field and flow rate. Although the evaporation rate of a solvent must influence the diameter/morphology of the electrospun fibers from a theoretical viewpoint, most of studies on the effect of evaporation rate have been focused on the pore generation on the surface of electrospun fibers. In this report, we investigated the effect of the evaporation rate of solvent during electrospinning on the diameter and morphology of the resultant fibers. Humidity and temperature was controlled to change the evaporation rate of the solution without changing other solution parameters. The result showed that long

evaporation time decreased the average diameter and generated beads on the fibers. It indicates beadless nanofibers can be obtained by optimizing the ambient conditions without change of polymers and solvents.





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장소: 일산KINTEX

발표코드: IND.P-83

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 대화면 의료모니터용 PDP를 위한 속경성 및 저취형 UV경화

### Coating제 개발

이상원 정재원<sup>1</sup> 이창섭

계명대 화학과 <sup>1</sup>한국이엔에쓰(주)

본 연구에서 개발하고자 하는 UV 경화수지의 용도는 PDP의 패널과 FPCB의 터미널을 ACF로 열융착시킨 후 Ag전극의 부식을 방지하기 위해 사용되는 UV 경화형 방습 코팅제이다. 의료용 디스플레이로는 LCD보다 PDP가 자연색을 그대로 표현하고, 가격이 낮기 때문에 화질이나 명암비에서 열세일지라도 더 선호된다. 본 실험에서는 UV 경화수지의 최대 문제점인 경화속도와 냄새 2가지 문제점을 개선하는 것을 목표로 하였다. 기존의 제품은 Metal-Halide lamp로서  $2400\text{mJ}/\text{cm}^2$ 의 노광량에서 99%이상 경화되는 타입인데 이것을  $1500\text{mJ}/\text{cm}^2$ 에서도 99%이상 경화되도록 경화속도를 높여 생산성을 향상시키는 실험을 하였다. Migration test, 열충격 test 및 미량이온농도 분석 결과 Monomer로서 2-HPA, Oligomer는 Aliphatic urethane Acrylate, 표면 경화용 광개시제로는 DC-1173(2%), 심부 경화용

광개시제는 IC-819(0.2%)을 적용하였을 때 최대의 경화속도와 저취형의 UV 경화수지 코팅제가 개발되었다.



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장소: 일산KINTEX

발표코드: IND.P-84

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Significance of irreversible formation of “electromer” in 1-bis[4-[N,N-di(4-tolyl)amino]phenyl]-cyclohexane layer associated with the stability of deep blue phosphorescent organic light emitting diodes**

위경량 이종대<sup>1</sup> 강상욱

고려대 소재화학과 <sup>1</sup>조선대 화학과

We demonstrate that injection of electrons in 1-bis[4-[N,N-di(4-tolyl)amino]phenyl]-cyclohexane (TAPC) layer irreversibly induces defect sites responsible for “electromer” emission. We also show that the defects alter the charge transporting properties of TAPC layer to influence the charge balance of iridium(III)[bis(4,6-difluorophenyl)pyridinato-N,C2']tetrakis(1-pyrazolyl)borate (FIr6) based deep blue phosphorescent organic light emitting diodes (PHOLED). The present investigation implies that deep-blue PHOLEDs should be carefully designed for the emission zone to be located far enough from the TAPC layer so as to avoid or minimize the emission from TAPC layer.

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장소: 일산KINTEX

발표코드: IND.P-85

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The relationship between the device performance and hole mobility of host materials in mixed host system for deep blue phosphorescent organic light emitting devices**

**위경량 이종대<sup>1</sup> 강상욱**

고려대 소재화학과 <sup>1</sup>조선대 화학과

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 ( $1.1 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ), 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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장소: 일산KINTEX

발표코드: IND.P-86

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Asymmetric anthracene-based blue host materials: synthesis and electroluminescence properties of 9-(2-naphthyl)-10-arylanthracenes

위경량 이종대<sup>1</sup> 강상욱

고려대 소재화학과 <sup>1</sup>조선대 화학과

A series of bulky aryl-substituted asymmetric anthracene blue host materials, 9-(2-naphthyl)-10-(3-(1-naphthyl)phenyl)anthracene, where phenyl was varied from H (5a), Me (5b), Ph (5e), and 1-Naph (5f) at the 6-position and Me (5c) at the 2-position, was synthesized by Suzuki coupling reaction between 10-(2-naphthyl)anthracene-9-boronic acid and 1-(3-iodophenyl)naphthalene derivatives. A less bulky aryl-substituted anthracene, 9-(2-naphthyl)-10-(2,5-diphenyl)phenyl)anthracene (5d), was also synthesized for comparison. All asymmetric anthracenes showed high glass transition temperatures in the range of 84~153 °C. The photophysical and electrochemical properties in solution showed that the substituent at the 10-positions of the anthracene unit did not influence the blue emission of 420 nm and HOMO~LUMO energy level (5.5~2.5 eV). However, a gradual decrease of bathochromic shift in solid state PL was observed from the increase of the substituent bulkiness, exhibiting 5e (18 nm) ≤ 5f (19 nm) < 5c (25 nm) ≤ 5b (26 nm) < 5a (30 nm) < 5d (41 nm), respectively. When 5a was used as a blue host material in the

multilayered device structure of ITO/DNTPD/NPD/host:dopant (9%)/PyPySPyPy/LiF/Al, enhanced OLED device performance was observed, showing a luminous current efficiency of  $9.9 \text{ cd A}^{-1}$ , power efficiency of  $6.3 \text{ lm W}^{-1}$  at  $20 \text{ mA cm}^{-2}$ , deep blue color coordinates of (0.14, 0.18), and a 932 h device lifetime at  $L0 = 3000 \text{ cd m}^{-2}$ .



일시: 2012년 4월 25~27일(수~금) 3일간

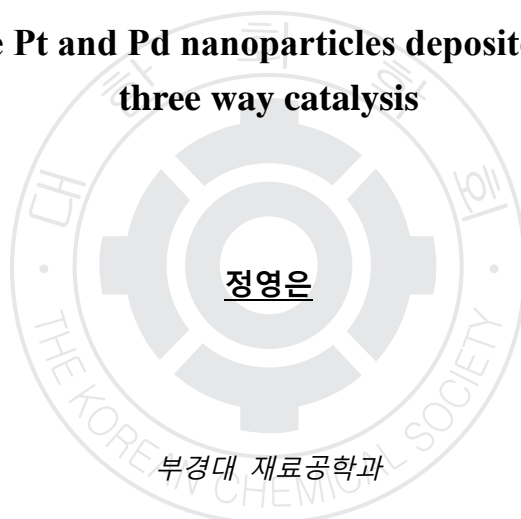
장소: 일산KINTEX

발표코드: IND.P-87

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermally stable Pt and Pd nanoparticles deposited on $\gamma$ -Al<sub>2</sub>O<sub>3</sub> for three way catalysis



Noble-metal nanoparticles have been the subject of a considerable amount of study because of their unique behavior and their applicability in catalytic and many other fields. Precious metals like Pt and Pd play efficient role to remove the emission components in auto exhaust system such as nitrogen oxide (NO<sub>x</sub>), hydrocarbon (HC), and carbon monoxide (CO). Throughout the world the usage of precious metals has dramatically increased which tends the catalysts more expensive. Thus to minimize the amount of these metals is highly promising approach. In the present investigation we adopted a novel approach to reduce the noble metal content as well as desperation of these active components by Arc plasma deposition (APD). In this method one can synthesize the homogeneously dispersed Pt and Pd on powders like  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> [1,2]. Both deposited Pt and Pd particles on alumina improved the overall TWC performance at lower temperature. APD samples also suppress the usual sintering of active metal at higher temperatures, which expanding the lifespan of TWC catalysts. In addition, we compare APD

materials with conventional impregnation samples. As synthesized Pt/Al<sub>2</sub>O<sub>3</sub> and Pd/Al<sub>2</sub>O<sub>3</sub> material were characterized by BET surface area, X-ray diffraction, TEM, ICP analysis and evaluated for TWC reactions. References: [1] Hinokuma S., Murakami K., Uemura K., Matsuda M., Ikeue K., Tsukahara N., Machida M. Top Catal 52, 2108, (2009) [2] Hinokuma S., Okamoto M., Ando E., Ikeue K., and Machida M. Catal Today, In press, (2011)





일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: IND.P-88

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Purification of MFB from industrial waste to available high-value green resources and synthesis of AMCA and AMBA from MFB**

**김기림 함미정 정효진 Dagvajantsan Oyuner**

국민대 화학과

MFB(4-methylformylbenzoate) 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 CO<sub>2</sub> and cost and it leads to environmental pollution. Accordingly, We synthesize high-value green resource from industrial waste of PET process. High-purity MFB can be a precursor of pharmaceuticals, cosmetics, and polymer additives, and so on. Most of all, we think that AMCA and AMBA are especially high-value green resources. These compounds be used to base material of pharmaceutical and cosmetics. Synthesizing of compounds is using autoclave, react with MFB or HBA adds to Hydrogen gas and various metal source catalysts. As a

result, synthesis of AMCA and AMBA are effective and mild condition. Identification of reaction is using by FT-NMR, HPLC, GC.



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발표코드: IND.P-89

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Tetraglyme-mediated synthesis of Pd nanoparticles for dehydrogenation of ammonia borane**

**김성관 강상욱 위경량 이종대<sup>1</sup>**

고려대 소재화학과 <sup>1</sup>조선대 화학과

Palladium nanoparticles (PdNPs) were conveniently prepared in tetraglyme (TG) solution using a variety of palladium precursors. At 140 °C, TG promoted  $\text{Pd}_3(\text{OAc})_6$  to produce irregular shaped PdNPs with an average size of 4 nm. When these PdNPs were re-dispersed in TG and used for the dehydrogenation of ammonia borane (AB) at 85 °C, remarkably enhanced catalytic performance was achieved to release 2.3 equiv. of  $\text{H}_2$  in 1 h.

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발표코드: IND.P-90

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Silane-based hydrogen storage materials for fuel cell application:  
Hydrogen release via methanolysis and regeneration by hydride  
reduction from organosilanes**

김성관 강상욱 위경량 이종대<sup>1</sup>

고려대 소재화학과 <sup>1</sup>조선대 화학과

A series of cyclic- and linear organosilanes was prepared and examined as potential hydrogen storage materials. When a stoichiometric amount of methanol was added to a mixture of cyclic organosilane,  $(\text{CH}_2\text{SiH}_2)_3$  (1) or  $(\text{CH}_2\text{SiH}_2\text{CHSiH}_3)_2$  (2), and 5 mol% NaOMe, rapid hydrogen release was observed at room temperature within 10-15 s. The hydrogen storage capacities of compounds 1 and 2 were estimated to be 3.70 and 4.04 wt.-%  $\text{H}_2$ , respectively. However, to ensure the complete methanolysis from organosilanes including methanol evaporation at exothermic dehydrogenation condition, two equivalents of methanol were used. The resulting methoxysilanes,  $(\text{CH}_2\text{Si}(\text{OMe})_2)_3$  (6) and  $(\text{CH}_2\text{Si}(\text{OMe})_2\text{CHSi}(\text{OMe})_3)_2$  (7), were regenerated to the starting organosilanes in high yields by  $\text{LiAlH}_4$  reduction. Linear organosilanes,  $\text{SiH}_3\text{CH}_2\text{SiH}_2\text{CH}_2\text{SiH}_3$  (3),  $\text{SiH}_3\text{CH}_2\text{CH}(\text{SiH}_3)_2$  (4), and  $\text{SiH}_3\text{CH}_2\text{CH}(\text{SiH}_3)\text{CH}_2\text{SiH}_3$  (5) also showed fast hydrogen release kinetics at room temperature with

hydrogen storage capacities of 4.26, 4.55, and 4.27 wt.%  $H_2$ , respectively; the corresponding methoxysilanes were successfully regenerated by  $LiAlH_4$ . Compound 1 was further tested as a hydrogen source for fuel cell operation.



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장소: 일산KINTEX

발표코드: IND.P-91

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of some thiadiazole and thiocarbamate derivatives for friction reduction additives

이신호 김영준

충남대 화학과

Some thiocarbamate and thiadiazole fatty acid ester derivatives fatty acid ester were synthesized and compared friction reducing properties. All organic derivatives (1wt%) were added to the different lubricant oil systems, such as diester oil, 100N base oil, and vegetable oil to investigate the effect of their friction reducing properties using a 4-ball WSD tester. The monothiocarbamate derivative with nonanoyl functional group gives higher performance in all kinds of base oil than that of dithiocarbamate derivatives whereas dithiocarbamate derivative with oleolyl function group gives higher friction reducing properties in all kinds of base oil except soybean. Also friction reducing properties was compared in the thiadiazole derivatives.

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장소: 일산KINTEX

발표코드: IND.P-92

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 인산 알칼리토금속계 촉매를 이용하여 젯산으로부터 아크릴산 합

성

박정우 조한아 김형록 장종산 한요한<sup>1</sup>

한국화학연구원 바이오리파이너지연구센터 <sup>1</sup>한국화학연구원 바이오리파이너지연구센터

바이오매스로부터 발효에 의해 젯산이 대량생산이 가능하게 되어 합성된 젯산을 일단계 탈수반응하여 공업적으로 유용한 아크릴산을 제조하는 촉매와 공정을 조사하였다. 알코올의 탈수에 의한 올레핀 합성 촉매로 고체산촉매와 고체염기촉매가 사용가능하지만, 반응물인 젯산의 특성상 탈수반응보다 탈탄산반응 및 수소화분해 반응 등의 부반응이 일어나기 쉽고, 생성물인 아크릴산의 고온에서의 높은 중합성으로 촉매의 비활성화가 문제가 되므로 고선택성 및 고안정성을 가진 촉매와 공정이 요구된다. 본 실험에서는 인산 알칼리토금속계 촉매를 사용하여 젯산에스테르로부터 탈수반응에 의해 아크릴산을 제조하였다. 인산칼슘 촉매의 경우, 350℃, 상압 조건에서 젯산에스테르 전환율 90%, 아크릴산 선택도 65%를

나타내었다. 위 촉매는 산성과 염기성을 복합적으로 가지고, 수열반응조건에서 비교적 열안정이 높은 것으로 확인되었다.





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장소: 일산KINTEX

발표코드: IND.P-93

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Method for preparing p-aminobenzoic acid from useless MFB

김경덕 유영 김아나 김석찬

국민대 화학과

4-Aminobenzoic acid (also known as para-aminobenzoic acid or PABA because the number 4 carbon in the benzene ring is also known as the para position) is an organic compound with the formula  $\text{H}_2\text{NC}_6\text{H}_4\text{CO}_2\text{H}$ . PABA is a white grey crystalline substance that is only slightly soluble in water. It consists of a benzene ring substituted with an amino group and a carboxyl group.

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장소: 일산KINTEX

발표코드: IND.P-94

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A study on the synthesis of o-monoalkylglycerol

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Monoalkylglycerols are known as immunity stimulant, cardiovascular protector and anti-ageing agent. The synthesis of alkylglycerol was reported by the reaction of alkyl glycidyl ether and NaOH in BuOH as solvent in 1995. However, the reaction product is not mono-alkyl glycerol product. New reaction methods, reaction mechanism and characterization by H1-NMR, FT-IR, HR/MS of the named compounds will be presented. The yield of monoalkylglycerol is about 83~95% according to the alkyl chain length.

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## Specifically designed ionic liquids for highly efficient SO<sub>2</sub> absorbents

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경희대 화학과

Specifically designed room temperature ionic liquids (RTILs) such as ether-functionalized imidazolium methanesulfonates exhibit extremely high SO<sub>2</sub> solubility, at least 2 moles of SO<sub>2</sub> per mole of RTIL at 30 °C and at atmospheric pressure. The solubility of SO<sub>2</sub> in these RTILs increases with increasing number of tethered ether oxygen atoms and also with the pressure rise. FT-IR spectroscopic and quantum mechanical calculation results show that such high SO<sub>2</sub> solubility is originated from the combined interactions of SO<sub>2</sub> with methanesulfonate anion and ether oxygen atom or atoms on the imidazolium ring. The absorbed SO<sub>2</sub> gas can be readily and completely desorbed from the RTILs by heating at 100 °C in a N<sub>2</sub> flow, thereby allowing the RTILs to be reused up to 5 cycles without loss of their initial capacity.

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## 1,2-Ethanedithiol 농도에 따른 PbS 콜로이드 상 양자점 태양전지 의 효율 변화

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콜로이드 상으로 합성되는 PbS 양자점을 이용한 태양전지의 효율에 1,2-Ethanedithiol(EDT)의 농도가 미치는 영향을 연구하였다. 일반적으로, oleate 리간드를 가지는 콜로이드 상 양자점의 캐리어 이동도를 증가시키기 위해서 리간드 교환이 필요한 것으로 알려져 있다. 본 연구에서는 1.4 eV의 밴드갭을 가지는 PbS 양자점을 디핑 후 EDT의 농도를 10 mM에서 50 mM로 변화시켜 리간드 교환 과정을 15회 반복함으로써 태양전지의 광흡수층을 형성하였다. 이때, 태양전지를 제작하기 위한 실험조건은 EDT의 농도를 제외하고 모두 동일하게 하였고, 쇼트키 접합 형성을 위해서 하부전극으로 알루미늄을 열증착법을 이용하여 증착하였다. EDT 농도를 10 mM에서 30 mM로 증가함에 따라 태양전지의

단락전류가 약 6 % 증가하였고, 50 mM 로 추가적인 EDT 농도의 증가에서는 약 2 %의 단락전류 감소현상이 나타났다. 또한, 태양전지의 변환효율도 단락전류의 변화 양상과 일치하였으며, 30 mM-EDT 를 이용하여 리간드 교환을 실시한 태양전지의 변환효율이 가장 높게 나타났다. 이러한 결과는 EDT 의 농도가 태양전지의 변환효율에 직접적으로 영향을 미치며, 최적화된 태양전지 제작을 위해서는 적합한 EDT 농도가 존재함을 의미한다. This work was supported by the Global Frontier R&D Program by the Center for Multiscale Energy Systems funded by the National Research Foundation under the Ministry of Education, Science, and Technology, the Industrial Core Technology Development Program funded by the Ministry of Knowledge Economy (No. 10035274).



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## Preparation of porous carbon materials from 2,2'-biphenol under acidic and basic condition

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Porous carbon materials have wide application fields including catalysis, separation, and energy storage for their huge surface area, high thermal and chemical stability, and high electric conduction. The novel phenolic resins have been synthesized using 2,2'-biphenol (BPh) in the presence of surfactants under acidic and basic conditions. Porous carbon materials have been prepared by pyrolysis under inert atmosphere and ambient pressure. The porosity could be controlled by varying the ratios of BPh and surfactants during the polymerization reactions and also by varying the pyrolysis temperature. Interestingly, mesoporous carbons were obtained in acidic condition, while microporous carbons were obtained in basic condition.

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## 광 흡수층 두께에 따른 쇼트키 접합 태양전지의 성능 변화

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본부 <sup>3</sup>충북대 화학과

본 연구에서는 양자점 태양전지의 광흡수층으로 응용하기 위하여 용액 공정으로 제조된 PbS 콜로이드 상 양자점을 이용하여 광흡수층을 형성하였다. 광흡수층 두께에 따른 태양전지의 성능 변화를 고찰하여, 쇼트키 접합 양자점 태양전지의 최적화된 광흡수층의 두께를 제시하고자 한다. 광흡수층은 PbS 양자점을 디핑하여 증착하였으며, 두께는 디핑 회수를 5~50 회로 다양화하여 변화시켰다. 디핑 회수의 증가에 따라서 PbS 양자점 층의 두께가 선형적으로 증가할 것으로 예상하였으나, 주사전자현미경을 이용하여 분석한 결과에서도 알 수 있듯이 40 회 이상의 디핑에서는 불균한 표면을 가지는 층이 형성되기 시작하였다. 이러한 결과는 균일한 PbS 양자점 층을 형성하기 위해서는 광흡수층의 두께 조절이 필요함을 나타낸다. 태양전지의 변환효율은 디핑 회수가 10 회에서 25 회로 증가함에 따라 증가하였고, 그 이상의 디핑 회수 증가에서는 감소하였다. 이러한 결과는 광흡수층이

두꺼우면 직렬저항 성분의 증가로 단락전류가 줄어들게 되고, 얇으면 광자에 의해 생성되는 전자-전공 쌍의 밀도가 줄어들기 때문인 것으로 판단된다. This work was supported by the Global Frontier R&D Program by the Center for Multiscale Energy Systems funded by the National Research Foundation under the Ministry of Education, Science, and Technology, the Industrial Core Technology Development Program funded by the Ministry of Knowledge Economy (No. 10035274).





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## Conversion of CdTe nanoparticles into nanowires via self-assembly

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Highly luminescent water soluble CdTe nanoparticles were prepared with assistance of the mixed ligand system of thiolglycolic acid and CdTe nanowires were successfully synthesized from nanoparticle. The light and dark-controlled self-assembly of CdTe nanoparticles led to nanowires. Slow oxidation of  $\text{Te}^{2-}$  in CdTe nanoparticles resulted in the individual or single nanocrytals. Transmission electron microscopy, scanning electron microscopy, and atomic force microscopy were performed to characterize the synthesized nanostructures. The suggested synthetic procedure provides a viable pathway for the fabrication of nanomaterials.

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## **Influence of Modified Silica with Silane Coupling Agents on properties of Silica Filled SBR/BR Compounds for Green Tire**

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Since 1990s, sulfur-functional silanes with silica filler have been used widely in the green to balance the magic-triangle properties of tire treads. Recently, the various silane coupling agents are used with silica filler for improve performance (magic-triangle properties) such as rolling resistance, wet traction and trade wear of tire treads.1-3 Sulfur-functional organosilanes, such as 3-mercaptopropyltrimethoxysilane (MPTMS) and bis-(triethoxysilylpropyl)tetrasulphide (TESPT), can be more increased mechanical properties than other functional silanes in existing simple mixed method (in situ method).4 However, it is known that SBR-MPTMS system has disadvantage of short vulcanization time and SBR-TESPT system has disadvantage of incompletely hydrolyzed in compounding step. The incomplete hydrolyzed alkoxy-functional groups can cause volatile organic compounds (VOCs) and decreased performance in SBR/BR compounds.5 This study explains influence of completely hydrolyzed TESPT and then treated silica affording hydrophobic and reactive modified silica applicable to SBR/BR compounds of tire tread. In

addition, SBR/BR-modified silica with olefinic-functional silanes compared the properties of SBR/BR-simple mixed silica with olefinic alkoxysilane and SBR/BR-modified silica with sulfur-functional silane.



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## Facile synthesis of silica aerogel using urea aqueous solution

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경희대 화학과

Taking urea aqueous solution as a solvent, silica aerogels were prepared by sol-gel method at an ambient temperature and pressure. Formic acid was added to the mixture of urea solution and tetramethylorthosilicate (TMOS) to provide acidic condition and wet aqueous gels were prepared. Stable porous structure of aerogels can be obtained by varying the molar ratio of urea and TMOS. Silica aerogels were obtained successfully by simple extraction of urea with water without adopting the supercritical drying process. The prepared silica aerogels have surface area ranging from  $700 \text{ m}^2 \text{ g}^{-1}$  to  $970 \text{ m}^2 \text{ g}^{-1}$ .

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## Nobel strategy for the preparation of bio-compatible silica aerogel

Agawal Shalu 정민석 이제승

경희대 화학과

Silica aerogels were prepared by sol-gel method in the presence of glucose. Wet gels were prepared from tetramethylorthosilicate (TMOS) under acidic condition by addition of formic acid. Stable porous structure of silica aerogels were obtained by varying the molar ratio of glucose and TMOS. Silica aerogels were obtained successfully by simple extraction of excess glucose with water instead of using solvent exchange and supercritical drying. Newly prepared silica aerogels have surface areas at a range of 650-750 m<sup>2</sup> g<sup>-1</sup>.

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## Process for the preparation of polyesters controlled molecular by using chain extenders

김하영

호남석유화학(주) 연구4팀

폴리에틸렌 이소프탈레이트 제조하는 과정에서 축합반응 시 기존 축합 촉매와 chain extender 를 혼합한 신규 촉매를 이용하여 분자량 조절이 가능한 폴리에틸렌 이소프탈레이트 연구를 수행하였다. 기존 축합 촉매와 chain extender 를 혼합한 신규 촉매는 축합 반응 시 ester 반응으로 생성된 비스(2-하이드록시에틸)이소프탈레이트들이 결합하면서 고분자를 형성할 때, 비스(2-하이드록시에틸)이소프탈레이트 사이에서 분자량을 증진 시켜주는 역할을 하는 것으로 예측된다. 이렇게 제조된 폴리에틸렌 이소프탈레이트의 물성 및 performance 에 대해 분석하였고, 특정 솔벤트에 녹여 PET flim 위에 코팅을 하여 산소투과도를 평가해 보았다.

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## CO<sub>2</sub> capture using $\beta$ -amino acid-derived ionic liquids

전영은 신승훈 김훈식 정민석

경희대 화학과

As task-specific ionic liquids for CO<sub>2</sub> capture, tetrabutylammonium  $\beta$ -aminocarboxylates (TBACs) were synthesized from the Michael reaction of simple amines with methyl acrylate followed by hydrolysis with tetrabutylammonium hydroxide. The CO<sub>2</sub> absorption capacities of 30 wt.% TBAC solutions in ethylene glycol (EG) or water were evaluated at 0.1 MPa and at 313 K. The absorption capacities of TBAC solutions were found to vary in the range 0.6~0.9 mol of CO<sub>2</sub> per mol of TBAC, depending on the anion and the solvent used. FT-IR and <sup>13</sup>C NMR spectroscopic studies suggest that the type of CO<sub>2</sub>-adduct of TBAC varies with the solvent employed: carbamates in EG and bicarbonate in water.

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## Adsorptive Removal of Pharmaceuticals and Personal Care products (PPCPs) from Water with Metal-organic Frameworks

imteaz ahmed HASAN ZUBAIR<sup>1</sup> 정성화<sup>2</sup>

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Removal of naproxen and clofibric acid, two typical PPCPs (pharmaceuticals and personal care products), has been studied by adsorption using metal-organic frameworks (MOFs) for the first time. The removal efficiency decreases in the order of MIL-101 > MIL-100-Fe > activated carbon both in adsorption rate and adsorption capacity. The adsorption kinetics and capacity of PPCPs generally depend on the average pore size and surface area (or pore volume), respectively, of the adsorbents. The adsorption mechanism may be explained with a simple electrostatic interaction between PPCPs and the adsorbent. Finally, it can be suggested that MOFs having high porosity and large pore size can be potential adsorbents to remove harmful PPCPs in contaminated water. Acknowledgement This work 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] G. Frey, Chem. Soc. Rev., 37 (2008)191.[2] Z. Hasan, J. Jeon, S. H. Jung, J. Hazard. Mater., in press (2012)



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## Desulfurization of benzothiophene and thiophene with oxidation using WO<sub>x</sub>/ZrO<sub>2</sub> catalysts: Effect of calcination temperature of catalysts

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Oxidative desulfurization (ODS) of model fuel containing benzothiophene (BT) or thiophene (Th) has been carried out with WO<sub>x</sub>/ZrO<sub>2</sub> catalyst, which was calcined at various temperatures. Based on the conversion of BT in the model fuel, it can be shown that the optimum calcination temperature of WO<sub>x</sub>/ZrO<sub>2</sub> catalyst is around 700 °C. The most active catalyst is composed of tetragonal zirconia (ZrO<sub>2</sub>) with well dispersed polyoxotungstate species and it is necessary to minimize the contents of the crystalline WO<sub>3</sub> and monoclinic ZrO<sub>2</sub> for a high BT conversion. The oxidation rate was interpreted with the first-order kinetics, and it demonstrated the importance of electron density since the kinetic constant for BT was higher than that for Th even though the BT is larger than Th in size. A WO<sub>x</sub>/ZrO<sub>2</sub> catalyst, treated suitably, can be used as a reusable active catalyst in the oxidative desulfurization. Acknowledgement This work was supported by a grant (B551179-10-03-00) from the cooperative R&D

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References[1] Z. Hasan, J. Jeon, S. H. Jhung, J. Hazard. Mater., 205-206 (2012) 216.



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## Syntheses of SAPO-34 molecular sieves in wide reaction conditions and dehydration of simple alcohols with the molecular sieves

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경북대 화학과

SAPO-34 molecular sieves have been synthesized in wide reaction conditions including temperature, time and type and concentration of templates in order to facilitate the synthesis of the molecular sieve. SAPO-34 molecular sieve can be synthesized rapidly with microwave irradiation from a gel containing tetraethylammonium hydroxide (TEAOH) as a template. Other several templating molecules, however, lead to SAPO-5 molecular sieve under microwave irradiation even though SAPO-34 is obtained by conventional electric synthesis from the same reactant gels. Moreover, SAPO-34 can be obtained more easily by increasing the TEAOH or silica concentration or by increasing the reaction temperature. SAPO-34 can be obtained within 5 min in a selected condition with microwave heating, which may lead to a continuous production of the important material. SAPO-34 synthesized by microwave irradiation is homogeneous and small in size and shows acidity and a stable performance in the dehydration of methanol and butanols to olefins, suggesting potential applications in acid catalysis. Acknowledgement

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발표코드: IND.P-108

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Adsorption of benzothiophene using virgin and CuCl<sub>2</sub>-loaded isotypic metal-organic framework material, Metal-benzenedicarboxylates

Nazmul Abedin Khan 전종원 정성화

경북대 화학과

Benzothiophene (BT) in n-octane has been adsorbed over isotypic metal-organic frameworks (MOFs), Me-BDCs (Me: Al, Cr and V; BDC: benzenedicarboxylates), to understand the effect of central metal ions on the adsorption. Among the isotypic MOFs, MIL-47 (V-BDC) shows the best performance in adsorption kinetics and adsorption capacity probably due to high acidity. Therefore, the favorable adsorption of BT over MIL-47 is due to a specific interaction like the acid-base one. Moreover, CuCl<sub>2</sub>-loaded MIL-47 shows a remarkable adsorption capacity for BT probably because of CuI derived from CuII via  $\pi$ -complexation. The CuI may be obtained at ambient condition by auto-reduction of CuII with VIII in MIL-47. Acknowledgement This work 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] G. Férey, Chem. Soc. Rev., 37 (2008) 191. [2] N.A. Khan, J.W. Jun, J. H.

Jeong and S.H.Jhung, Chem. Commun., 47 (2011) 1306.[3] N.A. Khan and S.H.Jhung, Angew. Chem. Int. Ed. 51 (2012) 1198.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND.P-109

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study on the preparation and optical properties of the core-shell structured ZnS nanoparticles

강민수 한준수<sup>1</sup> 황영애 유복렬<sup>1</sup>

상명대 화학과 <sup>1</sup>KIST 나노재료센터

ZnS nanoparticles (NPs) have been extensively studied during the last decade due to their unique optical and electrical properties. In this study, ZnS NPs on the monodispersed spherical silica NPs (Z@S, ZnS NPs weighed from 1 wt % to 16 wt % of ZnS based on the amount of silica used) were synthesized and covered with silica thin layer on their surface (S@Z@S). In PL analysis, PL intensities of Z@S NPs were increased to 1->8 wt %, but it decreased at more than 8 wt %. These phenomena can be explained by electron coupling (EC) and photoinduced charge transfer (PCT). Their optical, structural properties, surface morphology analysis were investigated by PL instrument, UV-Vis spectrophotometer, XRD, SEM, TEM respectively.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND.P-110

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **N-octyl-N-methylpyrrolidine tetrafluoroborate for Methane Hydrate Inhibitor**

김현택 강완규 김기섭

충주대 화공생물공학과

The performance of ionic liquids (ILs) as a new type gas hydrate inhibitors has been attention. [OMP][BF<sub>4</sub>] (octylmethylpyrrolidine tetrafluoroborate) is one of the ionic liquid has surface active property. In this study we experimented the effect of [OMP][BF<sub>4</sub>], one of the surfactant type ILs, on the formation of the methane hydrate. We measured [OMP][BF<sub>4</sub>]'s induction time. [OMP][BF<sub>4</sub>] have 140 min induction time at 1.0 wt%. It is very long time when it was compare with those of classic kinetic hydrate inhibitors such as PVP(1.8min, 1.0 wt%), PVCap(43min, 1.0 wt%). [OMP][BF<sub>4</sub>] is the expected material as methane hydrate inhibitor.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: IND.P-111

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization and Catalytic activity of Saturated N-heterocyclic carbene Pt Complexes

송진우 한준수<sup>1</sup> 유복렬<sup>1</sup>

KIST 물질제어연구단 <sup>1</sup>KIST 나노재료센터

Hydrosilylation, one of the fundamental methods of Si-C bond forming reaction, is usually catalyzed by platinum complexes. Speier's catalyst ( $\text{H}_2\text{PtCl}_6/\text{IPA}$ ) or Karstedts' catalyst [ $\text{Pt}_2(\text{DVTMS})_3$ ] are the most popular catalysts in industrial process. Recently, a series of platinum (0) complexes, bearing a N-heterocyclic carbene (NHC) and divinyltetramethylsiloxane (DVTMS), was reported. And they argued these new types of catalysts have superior selectivity over the classical catalysts. To verify the catalytic activity by the structure of NHC ligand, we synthesized saturated N-heterocyclic carbene-Pt(0)-(DVTMS) complexes having various substituents (Me, Et, i-Pr, cy-Hex). In this presentation, synthesis and characterization of novel saturated NHC-Pt catalysts will be presented. And their catalytic activity, such as efficiency and selectivity, will be compared with Karstedts' catalyst.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-112

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Colorimetric Turn-On Fluoride Sensing Properties of a Cationic Triarylborane Bearing Benzothiazolium

송기철 이민형<sup>1</sup> 도영규

KAIST 화학과 <sup>1</sup>울산대 화학과

We have synthesized a novel cationic triarylborane bearing benzothiazolium moiety, 2-(4'-dimesitylborylphenyl)-3-methylbenzo[d]thiazol-3-ium. Upon addition of fluoride, the cationic triarylborane undergoes a red-shift of the absorption band which tails over visible region, giving rise to the color change of the solution from colorless to yellow. As a result, color change could be easily observed with naked eye even in the presence of very low level of fluoride ions in THF/H<sub>2</sub>O (9/1, v/v). The fluoride binding constant in THF/H<sub>2</sub>O (9/1, v/v) is calculated to be  $1.3 \times 10^4 \text{ M}^{-1}$  that is much greater than that of a neutral triarylborane ( $K = 4.2 \times 10^2 \text{ M}^{-1}$ ). DFT calculation results suggest that the absorption process in the fluoroborate is involved with  $\text{[(Mes)} \rightarrow \text{[(phenylbenzothiazolium)}$  intramolecular charge transfer and the greater elevation of the  $\text{[(Mes)}$  donor level is responsible for the turn-on colorimetric response of the cationic triarylborane. Details of synthesis, characterization, DFT calculation, and fluoride sensing properties of the cationic triarylborane will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-113

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Reaction of 14-Membered Tetraaza Macrobicycles Containing One Methylene Bridge

강신걸 장보우

대구대 화학과

The macrotricycles 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazatricyclo[9.3.1.1<sup>4,8</sup>]hexadecane ( $L^1$ ) and 2,5,5,7,9,12,12,14-octamethyl-1,4,8,11-tetraazatricyclo[9.3.1.1<sup>4,8</sup>]hexadecane ( $L^2$ ) containing two N-CH<sub>2</sub>-N linkages react with Ni(OAc)<sub>2</sub>·4H<sub>2</sub>O to form the macrobicyclic complexes [NiL<sup>3</sup>(OAc)]<sup>+</sup> ( $L^3$  = 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazabicyclo[9.3.1]pentadecane) and [NiL<sup>4</sup>(OAc)]<sup>+</sup> ( $L^4$  = 2,5,5,7,9,12,12,14-octamethyl-1,4,8,11-tetraazabicyclo[9.3.1]pentadecane), respectively, containing one N-CH<sub>2</sub>-N linkage. The free macrobicycles  $L^3$  and  $L^4$  can be obtained by the demetallization of the complexes. The reactivity of [NiL<sup>4</sup>(OAc)]<sup>+</sup> in methanol is quite different from that of [NiL<sup>3</sup>(OAc)]<sup>+</sup>. Synthesis, characterization, and chemical properties of the compounds are presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-114

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Template Synthesis of Pentaaza Non-macrocyclic and Macrocyclic Nickel(II) Complexes Containing One 1,3-Diazacyclohexane Ring

강신걸 이윤택 정수경<sup>1</sup>

대구대 화학과 <sup>1</sup>김포대학 호텔조리학과

A new pentaaza macrocyclic complex  $[\text{Ni}(\text{A})]^{2+}$  ( $\text{A} = 1-(2\text{-aminoethyl})-3-(\text{N}\{2\text{-aminoethyl}\}\text{aminomethyl})-1,3\text{-diazacyclohexane}$ ) with a 5-6-5 chelate ring sequence has been prepared by reaction of formaldehyde with 1,4,8-triazaoctane and ethylenediamine in the presence of the metal ion. The complex reacts with nitroethane and formaldehyde to yield the macrobicyclic complex  $[\text{Ni}(\text{B})]^{2+}$  ( $\text{B} = 8\text{-methyl-8-nitro-1,3,6,10,13-pentaazabicyclo}[11.3.1]\text{heptadecane}$ ) with a 5-6-5-6 chelate ring sequence. Both complexes have square-planar coordination geometry in the solid state. In coordinating solvents (S), however, they exist as equilibrium mixtures of the octahedral  $[\text{Ni}(\text{L})(\text{S})_2]^{2+}$  ( $\text{L} = \text{A}$  or  $\text{B}$ ) and square-planar species. Synthesis, characterization, and solution behaviors of the complexes are presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-115

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Nickel(II) Complexes of 14-Membered Tetraaza Macrocycles Bearing Tetrazole Pendant Arm(s)

강신걸 방순무 곽지훈<sup>1</sup>

대구대 화학과 <sup>1</sup>순천대 화학과

The reaction of sodium azide with  $[\text{Ni}(\text{C-meso--L}^1)]^{2+}$  or  $[\text{Ni}(\text{C-racemic--L}^1)]^{2+}$  ( $\text{L}^1 = 1,8\text{-bis(cyanoethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane}$ ) bearing two N-cyanoethyl groups produces  $[\text{Ni}(\text{C-meso--H}_2\text{L}^2)]^{2+}$  or  $[\text{Ni}(\text{C-racemic--H}_2\text{L}^2)]^{2+}$  bearing two N-tetrazol methyl pendant arms. They are readily deprotonated in basic aqueous solutions to yield the deprotonated form  $[\text{Ni}(\text{C-meso--L}^2)]$  or  $[\text{Ni}(\text{C-racemic--L}^2)]$ . The crystal structures of  $[\text{Ni}(\text{C-meso--H}_2\text{L}^2)]^{2+}$  and  $[\text{Ni}(\text{C-racemic--H}_2\text{L}^2)]^{2+}$  have been determined. Synthesis, crystal structures, and chemical properties of the macrocyclic compounds are presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-116

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Heteroleptic Ir(III) Complexes Supported by Triarylborylpicolinate Ligand: Turn-On Phosphorescent Sensing of Fluoride Ion

Sanjeev Sharma 김태원 성우영 이민형

울산대 화학과

Owing to detrimental effects on humans and environment, detection of fluoride anion has been recently of great interest. Among the fluoride receptors developed so far, phosphorescent heavy-metal complexes bearing triarylborane Lewis acid moiety has been found to be efficient in sensing of fluoride because of advantageous phosphorescent properties of heavy metal complexes. In this regard, we designed and synthesized novel heteroleptic Ir(III) complexes  $[\text{Ir}(\text{C}^{\text{N}})_2(\text{LX})]$  (where  $\text{C}^{\text{N}}$  is dfppy, ppy, and btp and  $\text{LX}$  is 5-(4-(dimesitylboryl)phenyl)-2-picolinate). It is found that depending on the nature of the cyclometalating ligand ( $\text{C}^{\text{N}}$ ), the complexes showed ratiometric or turn-on phosphorescent sensing behaviors towards fluorides. The details of synthesis, characterization, and photophysical properties of Ir(III) complexes upon fluoride binding will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-117

발표분야: 무기화학

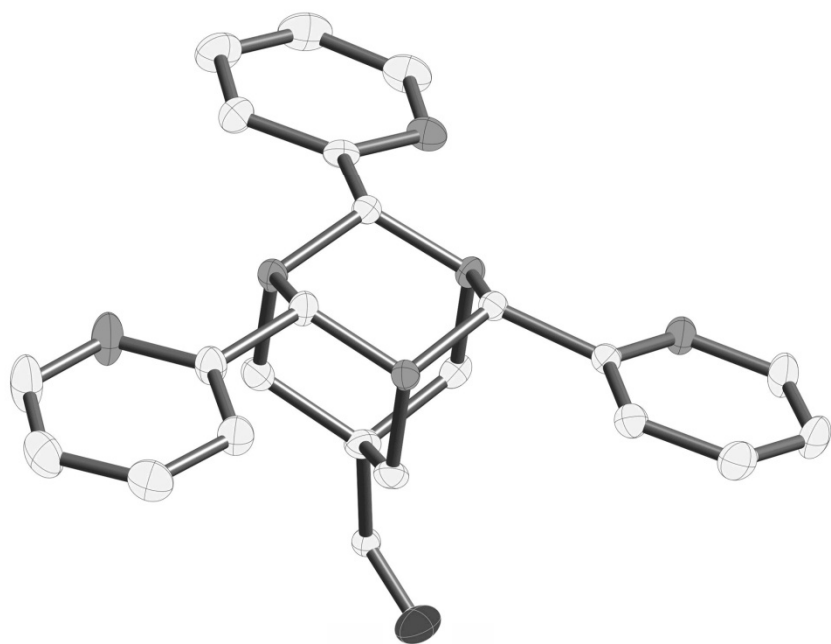
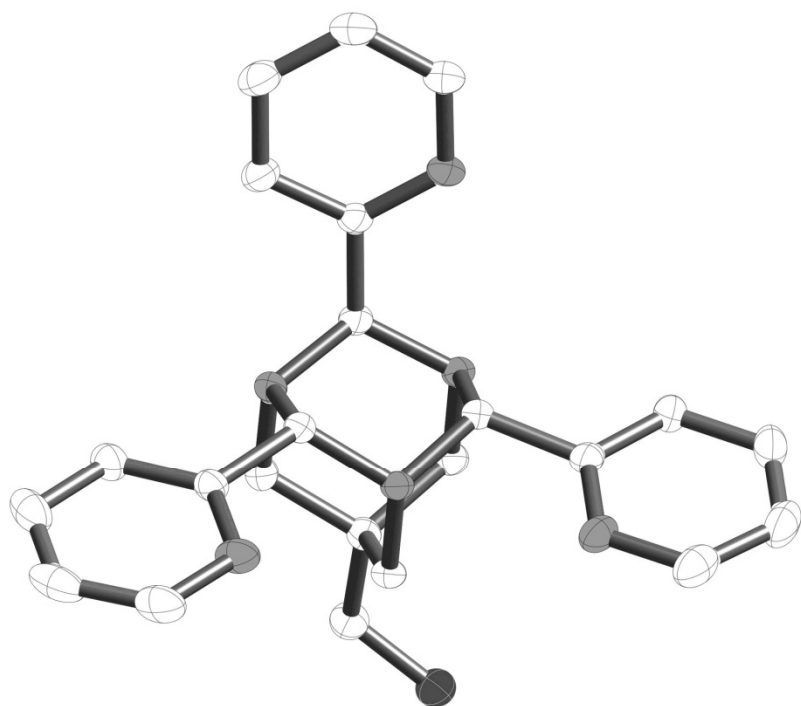
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chelation-Controlled Molecular Morphology

우아림 원미선 김양<sup>1</sup>

고신대 화학신소재학과 <sup>1</sup>고신대 화학 신소재학과

An issue in regard to the metal ion-catalysed rearrangement is whether it is dependent upon the isomeric form of the triaza-adamantane, especially given that the form most obviously closely related to the pendant sexidentate ligand is the unknown triaxial isomer. All these questions were the subject of the present work based upon the reactions of hytame with the isomeric pyridine aldehydes.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-118

발표분야: 무기화학

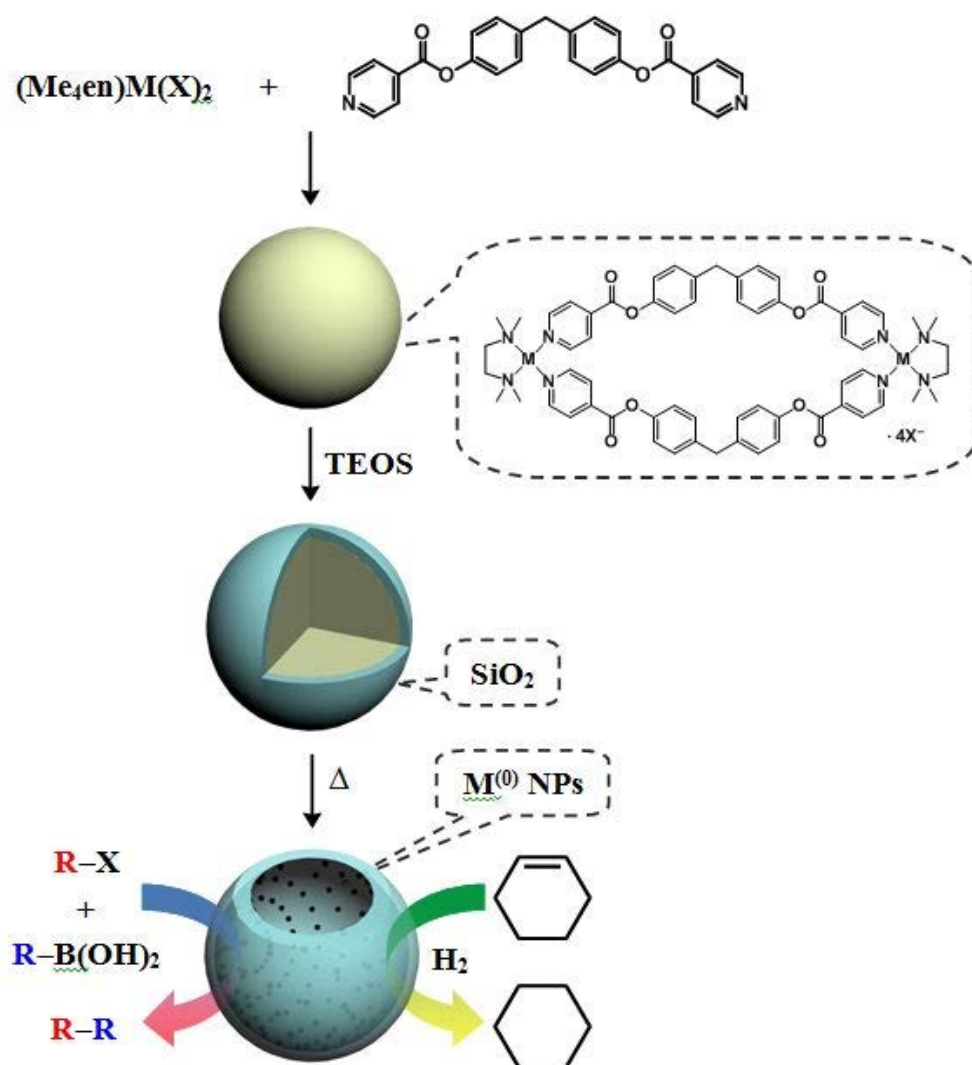
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Advanced Strategy for Silica Submicro-reactor Dotted with Novel Metal Nanoparticles as Catalyst

김성민 정옥상

부산대 화학과

Submicrospheres consisting of ionic palladium(II) and/or platinum(II) complexes were coated with TEOS, and then calcined in air at 550 °C for 1 h, forming an SiO<sub>2</sub> submicro-reactor dotted with palladium(0) and/or platinum(0) nanoparticles. The reactor was proved to be very effective catalyst for Suzuki-Miyaura cross-coupling and hydrogenation reactions. The reactor was characterized by NMR, IR, SEM, TEM, EDS and XPS.



**Scheme 1** Procedure and catalysis for  $\text{SiO}_2$  submicro-reactor dotted with  $\text{M}^{(0)}$  nanoparticles. ( $\text{M} = \text{Pd}$  and/or  $\text{Pt}$ ;  $\text{X}^- = \text{ClO}_4^-$  or  $\text{BF}_4^-$ ; TEOS = tetraethoxysilane)

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-119

발표분야: 무기화학

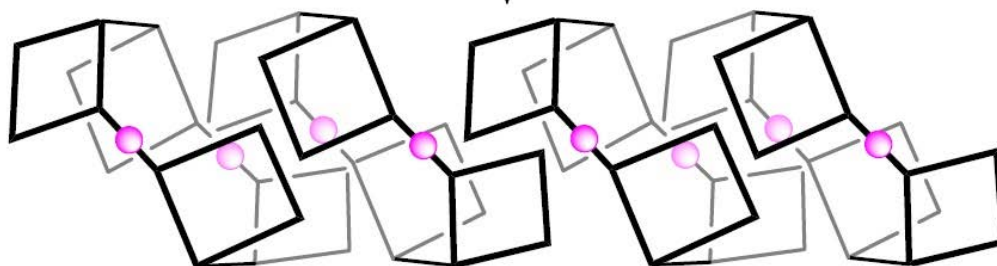
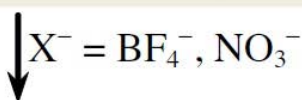
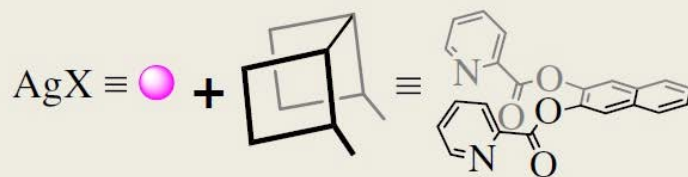
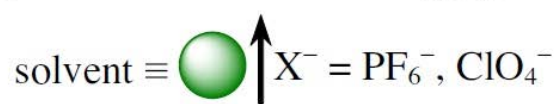
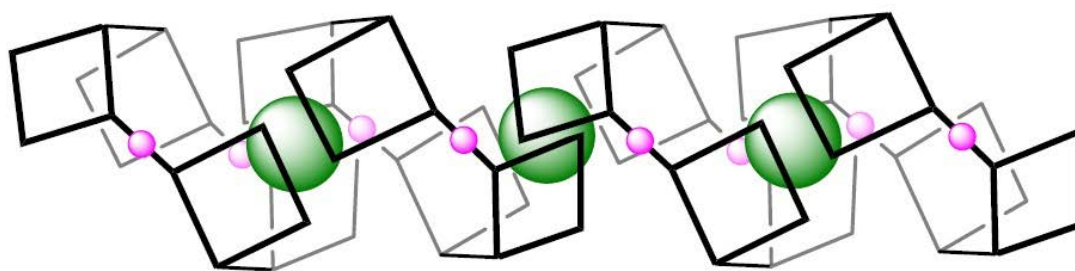
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Anion Effects on Formation of Metallacyclodimeric Silver(I) Complexes as storage of small molecules

이해리 정옥상

부산대 화학과

Ionic macrocyclodimeric silver(I) complexes,  $[Ag(L)]_2(X)_2$  ( $L = 2,3$ -bis(picolinoyloxy)naphthalene;  $X^- = PF_6^-, ClO_4^-, BF_4^-$ , and  $NO_3^-$ ) were synthesized and characterized. Single crystals consisting of cationic 22-membered metallamacrocycles with four pyridyl groups and two naphthyl groups were proven to have inter-cyclodimeric cavity with aromatic walls suitable for storage of small organic molecules. The nature of polyatomic counteranions plays a significant role in storage of small organic molecules. Their physicochemical properties are discussed in terms of solubility.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-120

발표분야: 무기화학

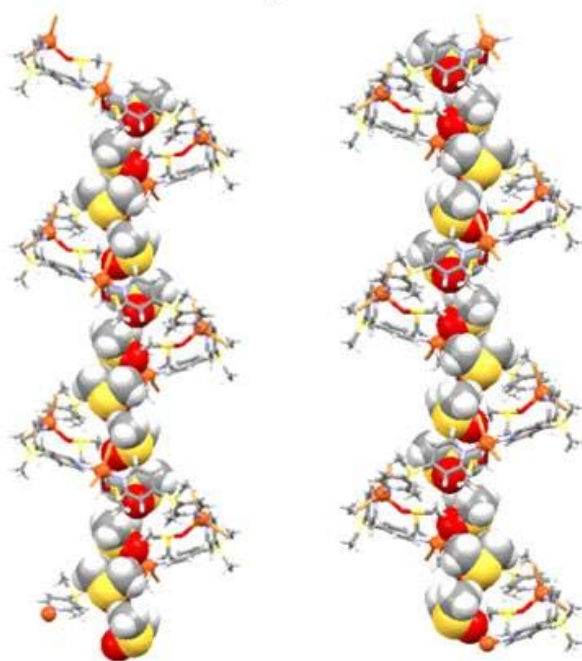
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Time-Dependent Crystallization. Double Strand vs Helix of $\text{CuBr}_2$ with Bis(4-pyridyl)dimethylsilane

문소연 정옥상

부산대 화학과

The reaction of  $\text{CuBr}_2$  with L (bis(4-pyridyl)dimethylsilane) in a mixture of methanol and ethanol produces a greenish yellow precipitate. After vapor diffusion of ethyl acetate into the dimethylsulfoxide solution of the resulting solid yields blue single crystals consisting of loop chain structure,  $[\text{CuBr}(\text{L})_2]_n\text{Br}_n(\text{DMSO})_{2n}$ , and green single crystals consisting of helical skeletal structure,  $[\text{CuBr}_2(\text{L})(\text{DMSO})]_n(\text{DMSO})_n$ . They were characterized by IR, X-ray single crystallography etc.



BY CHEMIST

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-121

발표분야: 무기화학

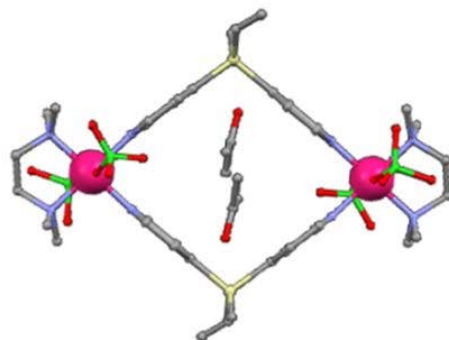
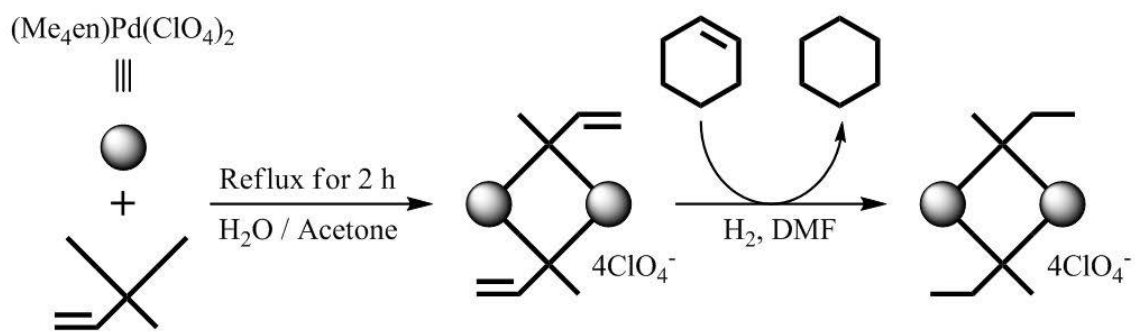
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Ionic Metallacyclodimeric Palladium(II) Complexes of Silicon Containing Pyridyl Ligands and Catalytic Properties

김성민 홍우식 정옥상

부산대 화학과

Metallacyclodimeric complexes of  $[(\text{Me}_4\text{en})\text{Pd}(\text{L})]_2(\text{ClO}_4)_4$  ( $\text{Me}_4\text{en} = \text{N},\text{N},\text{N}',\text{N}'$ -tetramethylethylenediamine;  $\text{L} = \text{bis}(4\text{-pyridyl})\text{dimethylsilane}$  (p-dmps);  $\text{bis}(4\text{-pyridyl})\text{methylvinylsilane}$  (p-mvps);  $\text{bis}(4\text{-pyridyl})\text{allylmethylsilane}$  (p-amps)) have been synthesized. Delicate structural and properties depending on alkyl chains attached to silicon along with catalytic effects were investigated. In order to test the catalytic effects of the metallacyclodimeric palladium(II) complexes, a preliminary hydrogenation was achieved. In the case of the metal complex of p-mvps ligand, the vinyl group was also hydrogenated.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-122

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Olefin Epoxidation of Nonheme Cobalt(III) Catalyst: Partition of Multiple Active Oxidants $\text{Co}^{\text{V}}=\text{O}$ , $\text{Co}^{\text{IV}}=\text{O}$ , and $\text{Co}^{\text{III}}\text{-OO(O)CR}$ Species

현민영 배정미 김현 김경범 김철

서울과학기술대 정밀화학과

A mononuclear nonheme cobalt(III) complex of a tetradentate ligand containing two deprotonated amide moieties,  $[\text{Co}(\text{bpc})\text{Cl}_2][\text{Et}_4\text{N}]$  (1), were prepared and then characterized by IR, elemental analysis, UV-vis and electron paramagnetic resonance spectroscopy. Complex 1 was also characterized by X-ray crystallography. This nonheme  $\text{Co}^{\text{III}}$  complex catalyzes olefin epoxidation upon treatment with *meta*-chloroperbenzoic acid. It is proposed that complex 1 shows partitioning between the heterolytic and homolytic cleavage of an O-O bond to afford  $\text{Co}^{\text{V}}=\text{O}$  and  $\text{Co}^{\text{IV}}=\text{O}$  intermediates, proposed to be 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  $\text{Co-OOC(O)R}$  (2) might be a possible reactive species for epoxidation. Evidence for these multiple active oxidants was derived from product analysis, the use of peroxyphenylacetic acid as peracid and EPR measurements. Our

results suggest that a less accessible  $\text{Co}^{\text{V}}=\text{O}$  moiety can form in a system wherein the supporting chelate ligand comprises a mixture of neutral and anionic nitrogen donors.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-123

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Novel Mn<sup>II</sup> coordination compounds constructed from benzoate and various bipyridyl ligands: magnetic property and catalytic activity

배정미 현민영 김경범 김현 김철<sup>1</sup> 김영미<sup>2</sup> 김성진<sup>3</sup>

서울과학기술대 정밀화학과 <sup>1</sup>서울과학기술대 정밀화학과 친환경소재제품센터 <sup>2</sup>이화여대 화학-나노과학과 <sup>3</sup>이화여대 화학과

Three new Mn<sup>II</sup>-benzoates coordination polymers containing various bipyridyl ligands (3,3'-dpicam, 3-methylisoquinoline, and 4,4'-dtp) and a [Mn<sub>6</sub>(O<sub>2</sub>CPh)<sub>10</sub>(μ<sub>4</sub>-OH)<sub>2</sub>(CH<sub>3</sub>OH)<sub>3</sub>(H<sub>2</sub>O)]·1.5(C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>) cluster have prepared and their structures were determined. The bipyridyl ligands can act as bridging ligands to produce 1-D or 2-D polymeric compounds. The pyz produced a Mn<sub>6</sub> cluster molecule, and 3-methylisoquinoline did a benzoate-bridged 1-D Mn<sup>II</sup> compound. The Mn<sub>6</sub> cluster (1) and 1-D Mn<sup>II</sup> compound containing 3,3'-dpicam (3) show antiferromagnetic property. The compounds 1, 3, and 4 have catalyzed efficiently the transesterification of a variety of esters, while 5 has displayed a very slow conversion. The thermal stabilities of these complexes were also examined.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-124

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Advanced fabrication of metal-organic frameworks

이희정 오문현

연세대 화학과

Zeolite imidazolate frameworks (ZIFs), considered being a new sub-family of MOFs, have been receiving many attention because of their exceptional chemical and thermal stabilities. In particular, ZIF-8, which has a sodalite topology, is one of the most studied typical ZIFs. ZIF-8 was prepared as a type of nano-scaled crystal or thin film as well as a classic macro-scaled crystalline material for its practical applications in gas storage, catalysis and gas separation. Herein, we report important advancement in the conjunction of porous MOFs with other compositional particles for the preparation of core-shell structure from ZIF-8 and polystyrene spheres. In addition, we report a simple approach for the fabrication of hollow structure from ZIF-8.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mixed-linker effects on the formation of coordination polymer particles (CPPs)

정동욱 이희정 오문현

연세대 화학과

In recent, many efforts have focused on tuning the structure and property of coordination polymers. Several methods to alter or enhance the properties of coordination polymers have been studied. Such techniques include modification of their composition via post-synthesis, controlling interpenetration and the co-introduction of different kinds of linkers within a coordination polymer structure. However, the mixed-linker effects on the formation of coordination polymer particles (CPPs) and the gas sorption properties of the resulting CPPs have not yet been studied. Here we report the solvothermal reactions for the preparation of five types of CPPs with distinct morphologies based on  $\text{In}^{3+}$  and three well-known organic linkers,  $\text{H}_2\text{NDC}$ ,  $\text{H}_2\text{BPDC}$  and  $\text{H}_2\text{BDC}$ .

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발표코드: INOR.P-126

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Structure and Spectroscopy of Dinitrato[3,14-diethyl-2,6,13,17-tetraazatricyclo(16.4.0.0<sup>7,12</sup>)docosane]copper(II)

최종하 유건상<sup>1</sup>

안동대 화학과 <sup>1</sup>안동대 응용화학과

The newly prepared complex crystallizes in the space group P-1 of the triclinic system with one mononuclear formula unit in a cell of dimensions  $a=7.9468$  (4),  $b=9.1175$  (4),  $c=9.8268$  (5) Å and  $\alpha=72.826(4)^\circ$ ,  $\beta=100.665(1)^\circ$  and  $\gamma=69.839(4)^\circ$ . The copper(II) ion with 3,14-diethyl-2,6,13,17-tetraazatricyclo(16.4.0.0<sup>7,12</sup>)docosane (L) has a tetragonally distorted octahedral environment with the four N atoms of the macrocyclic ligand in equatorial positions and the O atoms of two nitrate groups in axial positions. The macrocyclic ligand adopts the most stable trans-III conformation. The Cu-N distance of 2.0304(16) Å is normal, but the elongation of Cu-ONO<sub>2</sub> bond, 2.5061(14) Å may be due to the pseudo Jahn-Teller effect and the strong in-plane ligand field. The crystal is stabilized by a three-dimensional network of hydrogen bonds among secondary N hydrogens and O atoms of nitrate anions.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-127

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Crystal structure and IR spectroscopy of 3,14-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0<sup>7,12</sup>]docosane (1-naphthyl)methanol

최종하 유건상<sup>1</sup>

안동대 화학과 <sup>1</sup>안동대 응용화학과

In the centrosymmetric co-crystal, C<sub>20</sub>H<sub>40</sub>N<sub>4</sub>·2(C<sub>11</sub>H<sub>10</sub>O), the nitrogen atoms show pyramidal coordination, and the cyclohexane ring that is fused to the 14-membered C<sub>10</sub>N<sub>4</sub> ring exists in a chair conformations whereas the methyl substituent occupies an axial site. The 14-membered macrocyclic molecule adopts the pseudo trans-III configuration. The (1-naphthyl)methanol molecule forms a hydrogen bond to an N atom. The mean-square-plane passing through the 14-membered ring is approximately coplanar with the naphthalene fused-ring (dihedral angle 6.6(1)<sup>o</sup>). The crystal may be stabilized by the intermolecular O-H...N, and very weak intramolecular NH...N hydrogen bonds. The IR spectral properties and assignments of main absorptions are also discussed.

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장소: 일산KINTEX

발표코드: INOR.P-128

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, structure, and properties of NHC(N-heterocyclic carbene)- Pd(II) complexes containing $\sigma$ -allenyl or propargyl group

김용주 김현경 이선계 ZHENG ZHENNU<sup>1</sup> 이순원<sup>1</sup>

강릉원주대 화학과 <sup>1</sup>성균관대 화학과

Various s-allenyl and -propargyl Pd(II) Complexes were prepared from the oxidative addition of propargyl halides to the Pd(0) compound Pd(CH<sub>2</sub>=CHPh)(PR<sub>3</sub>)<sub>2</sub>. New s-allenyl or propargyl complexes were characterized by spectroscopic analyses and some of X-ray diffraction study. Treatments of the s-allenyl complex, trans-[ClPd(CH=C=CH<sub>2</sub>)(PMe<sub>3</sub>)<sub>2</sub>] with NHC (N-heterocyclic carbene) ligand also caused the ligand substitution to give new s-allenyl Pd(II) complex containing a NHC group. Other reactivities toward the s-allenyl Pd(II) complex with organic thiols and trimethylsilyl pseudohalides were examined.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-129

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of ( $\pi$ -allyl) Pd azides having NHC(N-heterocyclic carbene) ligand and their reactivity toward organic isothiocyanates

김용주 김현경 최근영 ZHENG ZHENNU<sup>1</sup> 이순원<sup>1</sup>

강릉원주대 화학과 <sup>1</sup>성균관대 화학과

Various ( $\pi$ -allyl) Pd azides having a NHC ligand were obtained from the reactions of bis( $\pi$ -allyl) dinuclear Pd azides with 2 equiv. of NHC group. The isolated complexes were characterized by spectroscopic analyses and some of X-ray diffraction study. Treatments with organic isothiocyanates(R-NCS) to the ( $\pi$ -allyl) Pd-NHC azides caused the formation of tetrazol-thiolato ( $\pi$ -allyl) Pd-NHC complexes. Also, the catalytic C-C coupling reactions using the some of complexes underwent. Experimental details will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-130

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization, Photoluminescence, and Catalytic Activities of Cd(II) Complexes with a Bipyridyl Ligand

강주혜 조영단 노진영 황인홍 송은주 김철<sup>1</sup> 김성진<sup>2</sup> 김영미<sup>3</sup>

서울과학기술대 정밀화학과 <sup>1</sup>서울과학기술대 정밀화학과 친환경소재제품센터 <sup>2</sup>이화여대 화학과 <sup>3</sup>이화여대 화학-나노과학과

Six new structures of Cd(II) complexes with chelating ligands (Hdpa) have been synthesized and characterized. With chloride and bromide, Cd(II) ions produce halide-bridged dinuclear units 1 and 2 while CdI<sub>2</sub> produces mononuclear unit 3 without halide-bridging. Cd(II) produces different types of structures: with chelating benzoate, Cd(II) produces mono-Hdpa complex 4; with coordinating anions, Cd(II) does di-Hdpa complex 5; with non-coordinating anions, Cd(II) does tri-Hdpa complexes 6 and 7. These results indicate that an anion effect is very important for construction of Cd(II) complexes containing chelating Hdpa ligands, and intermolecular hydrogen bonds are also very important roles for construction of polymeric crystal structures. We have also shown that the homogeneous catalyst 4, 5, and 6 catalyzed efficiently the transesterification of a variety of esters with different alcohols, while 1, 2, 3 and 7 has displayed a very slow conversion. Importantly, the transesterification reaction catalyzed by the

catalyst 6 is the best among the catalytic systems reported previously in Cd-containing coordination and polymeric compounds, to our best knowledge.



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장소: 일산KINTEX

발표코드: INOR.P-131

발표분야: 무기화학

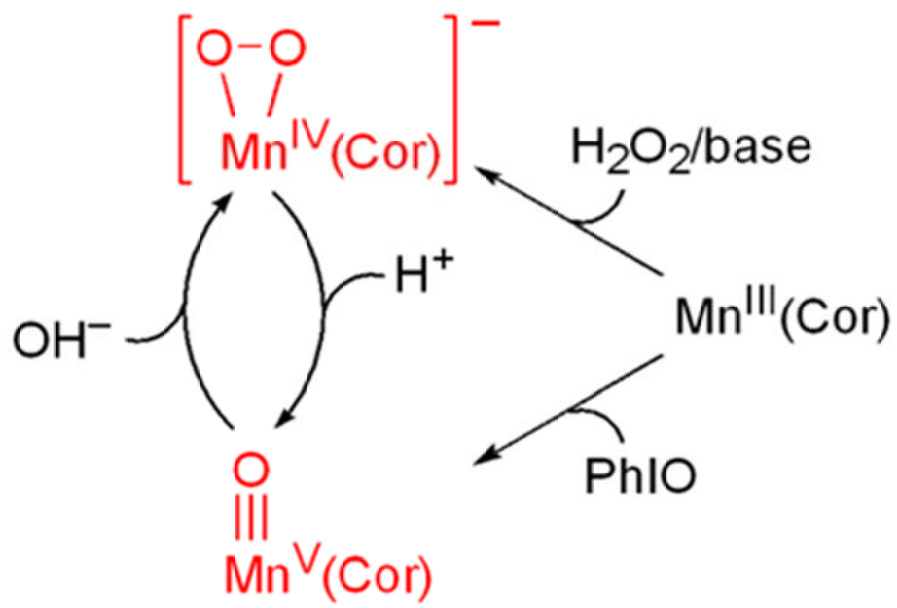
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Generation and Characterization of Mn(V)-Oxo and Mn(IV)-Peroxo Corroles, and Their Inter-conversion

박혜진 이용민<sup>1</sup> 남원우<sup>2</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 기초과학연구소 <sup>2</sup>이화여대 화학과

Manganese-catalyzed oxidations of organic substrates involving manganese-oxo and manganese-peroxo complexes have been extensively studied. Although O-O bond activation of Mn-O<sub>2</sub> adducts has been investigated, the functional model for oxygen-oxygen bond formation is still elusive. Herein we report the first example of reversible O-O bond cleavage and formation by manganese corroles. Mn(V)-oxo and Mn(IV)-peroxo corroles, were independently synthesized and characterized with various spectroscopic techniques. Reversible inter-conversion between Mn(V)-oxo and Mn(IV)-peroxo corroles was also found by acid-base titration.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: INOR.P-132

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

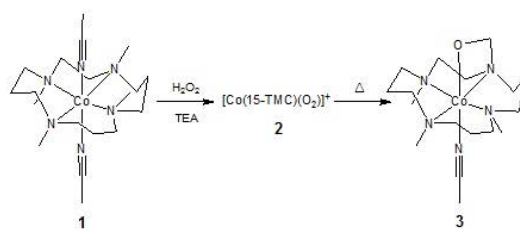
## Synthesis, Characterization, and Reactivity Studies of Cobalt(III)-Oxygen Complexes Bearing a Macrocyclic TMC Ligand

김도연 조재흥<sup>1</sup> 남원우<sup>2</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 나노과학부 <sup>2</sup>이화여대 화학과

Mononuclear metal-dioxygen adducts such as metal-superoxo and peroxo species are generated as key intermediates in the catalytic cycles of dioxygen activation by metalloenzymes and their model complexes have been characterized and investigated in electrophilic and nucleophilic reactions. Recently, we reported that the synthesis and structural and spectroscopic characterization of side-on cobalt(III)-peroxo complexes with 12- and 13-membered macrocyclic ligands which show the O<sub>2</sub>-transfer reactivity. Herein, we have shown the synthesis, spectroscopic characterization, and reactivity of cobalt(III)-peroxo complex, [Co<sup>III</sup>(15-TMC)(O<sub>2</sub>)]<sup>+</sup> (2) (15-TMC = 1,4,8,12-tetramethyl-1,4,8,12-tetraazacyclopentadecane), obtained by the reaction of [Co<sup>II</sup>(15-TMC)(CH<sub>3</sub>CN)<sub>2</sub>]<sup>2+</sup> (1) with ten equiv. of H<sub>2</sub>O<sub>2</sub> in the presence of five equiv. of triethylamine (Et<sub>3</sub>N) in CH<sub>3</sub>CN at 0 °C. In addition, 2 gradually decomposes, leading to aliphatic hydroxylation of the ligand side arm at its methyl position to give [Co<sup>III</sup>(15-TMC-O)(CH<sub>3</sub>CN)]<sup>2+</sup>

(3) (15-TMC-O = (4,8,12-trimethyl-1,4,8,12-tetraazacyclopentadecan-1-yl)methanolate), which was confirmed by UV-vis, ESI-MS and X-ray analysis.



Scheme



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-133

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Metal-directed assembly of metal(II) benzoates (M = Mn, Ni, Co, Cu, Zn, and Cd) with 1,2-bis(4-pyridyl)ethene: light- and photo-induced [2 + 2] cycloaddition**

**황인홍 조영단 강주혜 노진영 송은주 김철<sup>1</sup> 김성진<sup>2</sup> 김영미<sup>3</sup>**

서울과학기술대 정밀화학과 <sup>1</sup>서울과학기술대 정밀화학과 친환경소재제품센터 <sup>2</sup>이화여대 화학과 <sup>3</sup>이화여대 화학-나노과학과

We showed a systematic investigation on the coordination polymers assembled from metal(II) benzoates and bpe ligands. Their structures show various coordination modes depending on metal ions: a tetragonal pyramidal (five-coordinate) Cu<sup>II</sup> ion, a trigonal-bipyramidal (five-coordinate) Zn<sup>II</sup> ion, octahedral (six-coordinate) Mn<sup>II</sup>, Co<sup>II</sup>, and Ni<sup>II</sup> ions, and a pentagonal-bipyramidal (seven-coordinate) Cd<sup>II</sup> 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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발표코드: INOR.P-134

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Naparticle-based 3 Colour Indicator for Target Detection

김필용 남좌민

서울대 화학부

콜로이드상태에서 금 나노입자(sphere)는 빨간색, 금 나노입자(rod)는 파란색, 그리고 은 나노입자(sphere)는 노란색을 가진다. 그리고 이러한 나노입자들을 적절한 비율로 서로 혼합하면 마치 물감을 섞는 것처럼 다양한 색깔을 만들 수 있다는 사실을 발견하였다. 이를 바탕으로 하여 나노입자를 이용한 기존의 colorimetric assay 를 보완하는 방법을 구현해보았다. 이전의 colorimetric assay 방식에서는 1 가지 DNA 목표물을 검지하기 위해서는 두 종류의 나노입자가 필요했다. 그런데 빨강, 노랑, 파랑 등의 색깔을 가지는 3 가지 종류의 나노입자들을 혼합하여 특정한 target 에 반응하는 바이오센서를 만들면, 복잡한 장비의 도움 없이도 색깔 변화로서 3 가지 DNA 를 각각 구분할 수 있다. 이와 더불어 UV-vis spectrophotometer 를 사용하면 UV-vis spectra 의 peak 변화를 이용해서 서로 다른 2 가지 DNA 도 동시에 검지가 가능하다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-135

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ion-Selective Electrodes with Tin(IV) Porphyrins for Detection of Alkylammonium Cations

이민정 김희준 오진호<sup>1</sup>

금오공과대 응용화학과 <sup>1</sup>한국과학영재학교 화학생물학부

Tin(IV) porphyrins have made a resurgence of interest in the recent years due to the successful utilization of the particular properties conferred by the highly charged main group metal center. The ditopic porphyrins such as dihydroxotin(IV) pyridylporphyrins, possessing the cooperative binding sites in their axial and peripheral positions, have great potential in molecular recognition leading to the construction of functional multiporphyrin supramolecular arrays and nanostructures. Aiming at this goal, we have recently investigated molecular recognition by [(2-pyridyl)porphyrinato]tin(IV) complexes using cooperative interactions of axial ligands and peripheral functional groups. We here present the development of ion-selective electrodes with tin(IV) porphyrins to detect alkylammonium cations in aqueous solutions.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-136

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of Reaction Temperature on Li (I) Adsorption Performance of Hydrogen Manganese Oxide Complex

이슬이 박수진

인하대 화학과

In this study, we prepared hydrogen manganese oxide complex (HMOC) using a mixture of  $\text{Li}_2\text{CO}_3$  and  $\text{MnCO}_3$  by a solid-state reaction with reaction temperatures, in order to investigate the Li (I) adsorption behaviors. X-ray diffraction analysis was used to observe the crystalline of HMOC's structure. The feature and particle size of samples were investigated by scanning electron microscopy and zeta-potential analysis, respectively. Textural properties were determined by  $\text{N}_2/77\text{ K}$  adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Barrett-Joyner-Halenda method. The Li (I) adsorption capacity was determined by an atomic absorption spectrometer. From the results, it was found that the reaction temperature played a key role in the Li (I) adsorption capacity, resulting from the structural and textural characteristics of HMOC samples.

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장소: 일산KINTEX

발표코드: INOR.P-137

발표분야: 무기화학

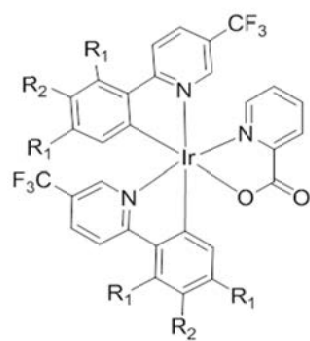
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Phosphorescent Heteroleptic Ir(III) Complexes with Two Substituted - phenylpyridine and One Picolinic acid

윤성재 김대영<sup>1</sup> 황인혜<sup>2</sup> 진성호<sup>2</sup> 김영인<sup>2</sup>

부산대 첨단정보및디스플레이소재협동<sup>1</sup> 부산대 첨단정보 및 디스플레이소재협동과정<sup>2</sup> 부산  
대 화학교육과

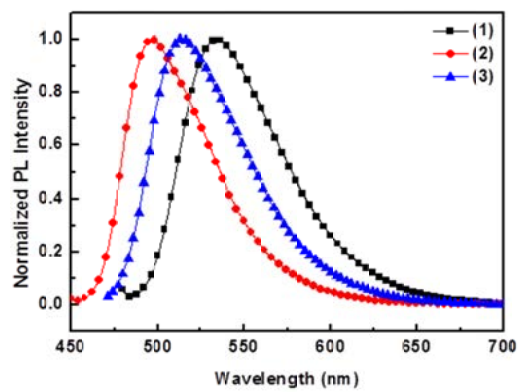
Novel green phosphorescent heteroleptic Ir(III) complexes for the fabrication of PhOLEDs were prepared and characterized; (pCF<sub>3</sub>py)<sub>2</sub>Ir(pic) (1), (dfpCF<sub>3</sub>py)<sub>2</sub>Ir(pic) (2) and (tfpCF<sub>3</sub>py)<sub>2</sub>Ir(pic) (3), where pCF<sub>3</sub>py = 2-phenyl-5-(trifluoromethyl)pyridine, dfpCF<sub>3</sub>py = 2-(2',4'-difluorophenyl)-5-(trifluoromethyl)pyridine, tfpCF<sub>3</sub>py = 2-(2',3',4'-trifluorophenyl)-5-(trifluoromethyl)pyridine and pic = picolinic acid. The absorption, luminescence and cyclic voltammetry of Ir(III) complexes were investigated, and OLED performances were significantly affected by the introduction of electron donating and electron withdrawing substituents into the phenylpyridine backbone. The developed Ir(III) complexes exhibited the photoluminescence at 497 ~ 534 nm in solution and 499 ~ 537 nm in film. The fabricated PhOLEDs of 1 and 2 showed green and greenish-blue emission, luminance efficiency of 24.71, 16.40cd/A, external quantum efficiencies of 6.87, 5.63 % and the CIE of (0.39, 0.58), (0.21,0.57), respectively.



1 :  $R_1=H$ ,  $R_2=H$

2 :  $R_1=F$ ,  $R_2=H$

3 :  $R_1=F$ ,  $R_2=F$



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: INOR.P-138

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescent Chemosensors for Aromatic Residues Based on Supramolecular Assemblies with Porphyrin, Viologens and Cucurbit[8]uril

조수민 김희준

금오공과대 응용화학과

The design of chemosensors capable of recognizing biologically important molecules in aqueous solution is a challenging field in the chemical and biomedical sciences. The unique phenomenon of the charge transfer complex formation inside cucurbit[8]uril (CB[8]) can be utilized for the detection of biologically important molecules containing aromatic side chains. On the other hand, porphyrins and metalloporphyrins are attractive molecular components for the design of chemosensor systems and applications in molecular photoelectronic materials and devices because of their unique structures and rich photoelectronic properties as well as a variety of coordination geometries. Thus we have been interested in supramolecular assemblies with porphyrin, viologen and cucurbituril homologues to develop efficient fluorescent chemosensors for aromatic residues. Here we present the syntheses of porphyrin-

viologen complexes, their inclusion behaviors in CB[8], and their spectroscopic properties as a fluorescent chemosensor in detail.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

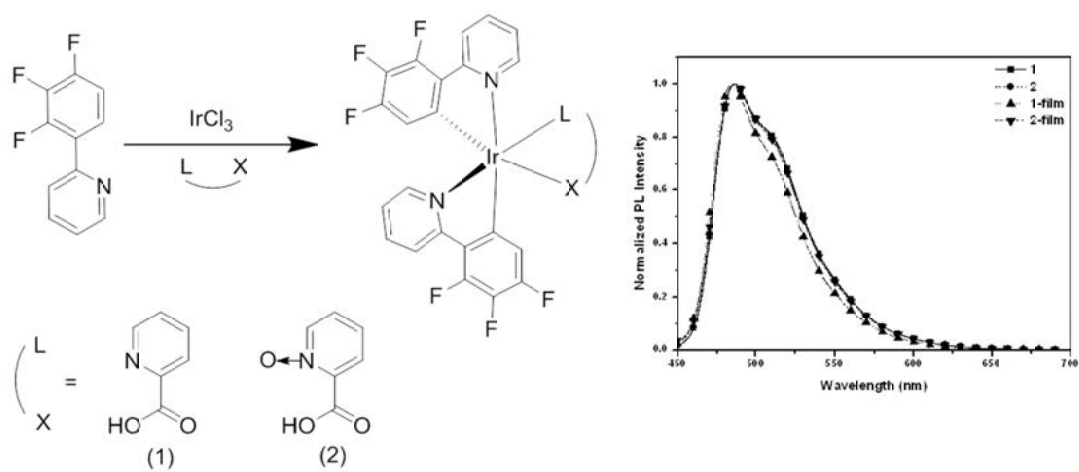
## Phosphorescent Iridium(III) Complexes Based on 2-(2,3,4-Trifluorophenyl)pyridine: The Effect of 3-Substituted Fluorine in Phenyl Ring on Color Tuning

김대영 윤성재<sup>1</sup> 황인혜<sup>2</sup> 진성호<sup>2</sup> 김영인<sup>2</sup>

부산대 첨단정보 및 디스플레이소재협동과정 <sup>1</sup>부산대 첨단정보및디스플레이소재협동 <sup>2</sup>부산  
대 화학교육과

We have designed and synthesized heteroleptic cyclometalated Ir(III) complexes,  $(C^N)_2Ir(L^X)$ , where  $C^N$  = 2-(2,3,4-trifluorophenyl)pyridine(tfppy) and  $L^X$  = picolinic acid(pic), picolinic acid N-oxide(pic-N-O);  $(tfppy)_2Ir(pic)$  (1),  $(tfppy)_2Ir(pic-N-O)$  (2). The complexes exhibited the photoluminescence peak at 485 and 486 nm, and quantum yields of 16 and 19% in solution, respectively. The complex (1) exhibited a red-shift emission compared to  $Irpic$ , indicating that the conjugation effect of 3-substituted fluorine increased the electron density of the phenyl ring resulting in an increase of the HOMO energy level. The electroluminescent properties of complex (1) showed CIE coordinates of (0.18, 0.47), maximum external quantum efficiency of 8.48% and luminance efficiency of 21.18 cd/A.





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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of New Pd (II) Complex with Ligand Bispyrazole Derivative

김성훈 이하진<sup>1</sup> 이효선<sup>2</sup>

경북대 화학과 <sup>1</sup>한국기초과학지원연구원 전주센터 <sup>2</sup>경북대 자연과학대학 화학과

The development of well-defined palladium-based complexes capable of catalyzing  $\alpha$ -olefin Polymerization, has been particularly focused due to their increased tolerance to functional group in the substrate. In this regard, the chemistry of N-donor palladium complexes have been extensively reported applying for various catalyst precursors. Here, we report new palladium complexes,  $\text{PdLnCl}_2$  ligated to Ln (L1~L3), where (L1 = (Z)-N ((pyridinyl)methylene)cyclohexanamine), L2 = N-((pyridin-2-yl)methyl)benzenamine), L3 = N-methyl-N-((pyridin-2-yl)methyl)benzenamine) from substitution reaction of starting material  $\text{Pd}(\text{CNCH}_3)_2\text{Cl}_2$ . The synthesized complexes along with their X-ray crystal structures, was investigated for their catalytic (co)polymerization ability toward various  $\alpha$ -olefin monomers.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Facile Method for the Large-Scale Synthesis of InPZnS Alloy Quantum Dots**

**강미재 김상욱**

아주대 분자과학기술학과

A novel and facile method for the large scale synthesis of InPZnS alloy quantum dots was developed, which control the optical properties according to the palmitic acid to 1-dodecanethiol ratio. The absorption and emission peaks showed a blue-shift when the amount of 1-dodecanethiol increased. The alloy structure was supported with TEM, ICP, XPS and XRD. The quantum yield of alloy quantum dots showed in the ranges 20% - 45% for all wavelengths and were overcoated with ZnS shell. Finally, a cadmium-free quantum dot yield was measured to be 2.74 g in a single reaction.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Carborane Photochemistry Triggered by Aryl Substitution: Carborane-Based Dyads with Phenyl Carbazoles

위경량 이종대<sup>1</sup> 강상욱

고려대 소재화학과 <sup>1</sup>조선대 화학과

Among three different isomers of carborane (C<sub>2</sub>B<sub>10</sub>H<sub>12</sub>), the 1,2-C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> (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.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electronic Optimization of Heteroleptic Ru(II) Bipyridine Complexes by Remote Substituents: Synthesis, Characterization, and Application to Dye-Sensitized Solar Cells

위경량 이종대<sup>1</sup> 강상욱

고려대 소재화학과 <sup>1</sup>조선대 화학과

We prepared a series of new heteroleptic ruthenium(II) complexes,  $\text{Ru}(\text{NCS})_2\text{LL}'$  (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 NMe<sub>2</sub> (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 NMe<sub>2</sub> 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 TiO<sub>2</sub> 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:  $\eta = 8.30\%$ ,  $JSC = 16.0 \text{ mA/cm}^2$ ,  $VOC = 717 \text{ mV}$ , and  $ff = 0.72$ . These values are better than N3-based device.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Simple environmentally friendly method for noble metal/graphene nanocomposites and their catalytic performance

김승현 김상욱<sup>1</sup>

아주대 분자과학기술학과 나노재료실험실 <sup>1</sup>아주대 분자과학기술학과

We synthesized the noble metal (Pd, Pt, Ag, and Au)/graphene nanocomposites using the hydrazine-free, and surfactant-free method. In our system, ascorbic acid and hot water are the co-reductant of noble metal salt and graphene oxide. In addition, we applied the prepared Pd/graphene nanocomposites to Suzuki coupling reaction as a catalyst.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Syntheses, Characterizations, Catalysis and Representative X-Ray Structures of Some Copper Complexes with Schiff-Base Ligands

shuranjan sarkar 이흥인

경북대 화학과

Schiff-base transition metal complexes have been extensively studied in the development of catalytic activities, photochemical reactions and medicinal chemistry. But in the modern chemistry, it is still a challenging task to design and synthesize multifunctional organic ligands/materials with desirable or predictable properties. We have synthesized several Schiff-base ligands which can form symmetrical and esthetic structures via selective interactions between the ligands and transition metals. Among the complexes, we present here some copper complexes showing catecholase activities. In this poster, we discuss the structures and characteristics obtained by a combination of elemental analysis, UV-vis spectroscopy, IR, EPR and x-ray crystallography. The catalytic reactions were initiated by adding hydrogen peroxide and 3,5-di-tert-butylcatechol into the solution of the complexes and monitored by UV-vis spectroscopy.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Tetrazole-Based Metallogel Induced with $\text{Ag}^+$ Ion and Its Silver Nanoparticle in Catalysis

이지하 이진용<sup>1</sup> 정종화

경상대 화학과 <sup>1</sup>성균관대 화학과

A tetrazole-based ligand forms a supramolecular metallogel in the presence of  $\text{Ag}^+$  in aqueous solution at basic condition. The silver-induced metallogel has been characterized by SEM, TEM, XRD, and rheometry. The metallogel exhibits a fiber structure. Upon standing, silver nanoparticles grow in the gel. TEM confirmed that the particles are exclusively formed in the gel fibers. The size of the silver nanoparticles formed onto the gel fibers are dependent to the concentration of silver during gel formation. The silver nanoparticles show a face-centered cubic crystalline structure. The silver nanoparticles can effectively catalyze reduction of 4-nitrophenol by sodium borohydride in aqueous solution. The formation of  $\text{Ag}^+$ -induced metallogel does not strongly depend on anions. According to DFT calculations, the two silver cations are coordinated to nitrogen at the tetrazole moiety. The other silver cation is coordinated to the nitrogen of the pyridine and coordinated to the oxygen of the amide moiety. Furthermore, the

rheological properties of the  $\text{Ag}^+$ -tetrazole-based metallogel were strongly dependent on the concentration of  $\text{AgClO}_4$ .



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발표코드: INOR.P-147

발표분야: 무기화학

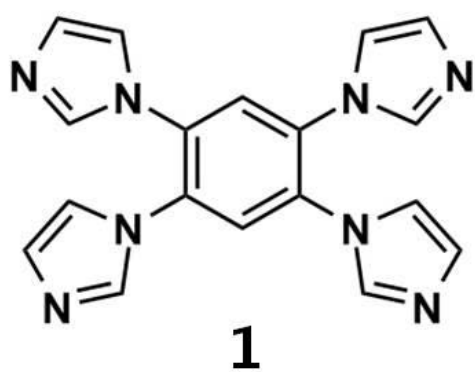
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Imidazole-Based Coordination Polymergel with $\text{Co}^{2+}$ ion

정성호 박선희 정종화

경상대 화학과

Compound 1 was synthesized which have four imidazole groups as a binding site for  $\text{Co}^{2+}$  ion. and evaluated the gel formation upon addition of transition metal ions in organic solvents. Compound 1 forms the gel with  $\text{Co}^{2+}$  salts. The color of  $\text{Co}^{2+}$  polymergel 1 shows the red color. On the other hand the red color of  $\text{Co}^{2+}$  polymergel 1 changed into blue color upon the addition of  $\text{CoBr}_2$ ,  $\text{CoCl}_2$ . In this conference, we will present the preparation, morphology, and chromism, of a imidazole-appended coordination polymergel incorporating  $\text{Co}^{2+}$  ions.



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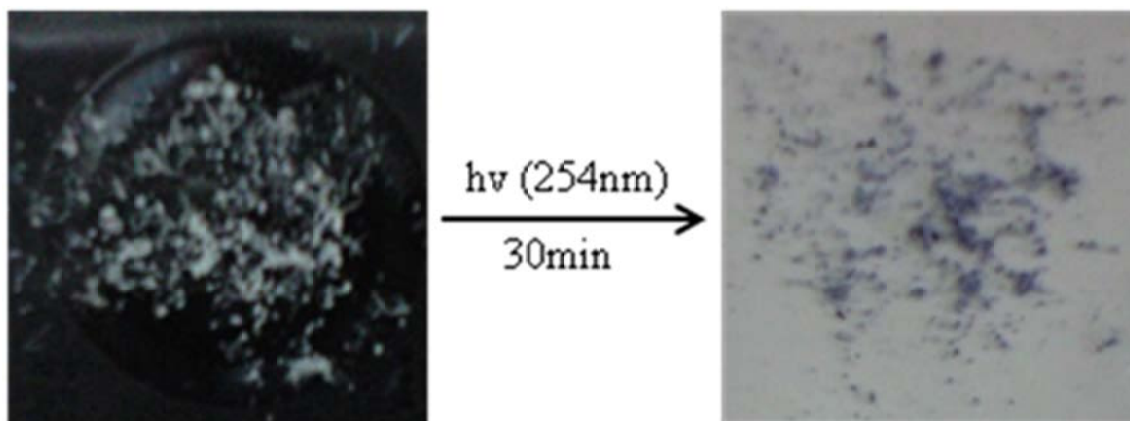
## The Gelation of Pyridine-Based Ligand Introduced Diacetylene and Its Characterization

최연원 서무룡 정종화

경상대 화학과

A pyridine-based ligand introduced diacetylene was synthesized using a few steps and gelled in water by heating. Interestingly, the ligand formed the metallogel in the presence of  $\text{Zn}^{2+}$  ions in DMSO. The hydrogel and the metallogel with  $\text{Zn}^{2+}$  were characterized by scanning electron microscopy (SEM), UV-vis spectroscopy and fluorophotometry. The hydrogel prepared at low concentration was made of micrometers-long nanofibrils as shown by SEM. On the other hand, the metallogel did not show nanofibrils but lumps. The fluorescence intensity of the gel in the presence of  $\text{Zn}^{2+}$  is quenched beside that of hydrogel which has no metal. When UV-vis was measured with pH-change, there wasn't any particular alteration in absorbance and wavelength, and it showed similar tendency in those of fluorescence measurement. The diacetylene introduced ligand which includes benzene instead of pyridine was prepared for reference test. This ligand changed its color from white to blue under UV irradiation and it suggests that the polymerization was occurred by covalent bond (Fig 1). The color change of

diacetylene-introduced ligand depends on the degree of polymerization reaction in the ligand. The blue phase signifies that the degree of polymerization is high. In this case, the color change to blue seems to originate from hydrogen bond between amide group and carbonyl group. Interestingly, the blue phase turned to red phase under high temperature. It means that the diacetylene-introduced ligand can be applied to thermo-sensitivity sensor. The ligand gelled in DMSO with  $\text{Cu}^{2+}$  ions.



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## Light-Induced Nitric Oxide Releasing from a Ruthenium Nitrosyl Complex : Spectroscopic Properties and Solvent Effects

조장훈 이흥인

경북대 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,  $[\text{Ru}(\text{ebpp})(\text{Cl})(\text{NO})]$ , where  $\text{H}_2\text{ebpp} = \text{N,N'-(ethylene di-} p\text{-phenylene)bis(pyridine-2-carboxamide)}$  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  $\text{Cl}^-$ . 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  $[\text{Ru-NO}]^6$  (Enemark-Feltham notation) electronic state of the complex becomes low-spin Ru(III) ( $d^5$ ,  $S=1/2$ ) state upon losing NO by photoactivation. We present here other evidences of photoactivated NO-releasing and other properties monitored by UV-VIS, EPR, ESI-MS, X-ray crystallography, and Cyclic Voltammetry (CV) at various conditions.





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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Preparation and X-ray Structure of Supramolecules Obtained from Macrocyclic Complex Having Carboxyl Side Chain at Different Reaction Condition**

**이재명 곽지훈**

순천대 화학과

The strategy for design and construction of the self-assembly structure with polyazamacrocyclic complex has been focused on tuning two-axial sites of the complexes with different auxiliary ligands. Also, the combination of coordination and hydrogen bonding approach has provided particularly interesting supramolecular systems in metal-organic hybrids. Recently, we have explored the development of a building block containing potentially coordination and hydrogen bonding sites as well to evaluate the role of coordination and hydrogen bonding in self-assembly of tetraaza donor macrocyclic complex. Here, we present the preparation and X-ray structure of two products from the reaction of macrocyclic complex of copper(II) containing carboxylic acids as side chain and tetracyanonickelate(II) at different reaction condition. We will discuss the effect of pH etc. on the crystal structure and assembly pattern of the obtained supramolecule.

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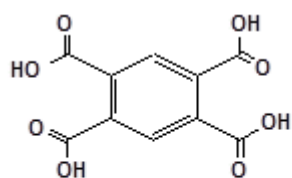
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design and Preparation of Supramolecules Obtained from the Combination of Macrocycles and Aromatic Polycarboxylates at Different Reaction Condition

Enkhzul Otgonbaatar 곽지훈

순천대 화학과

The use of multifunctional ligands for the preparation of metal organic compounds becomes of great interest. The compounds can contain 2-D and 3-D frameworks linked by organic ligands or hydrogen bonding. The current interest in multidimensional frameworks stems not only from their intriguing variety of architectures and topologies, but also their potential applications in luminescence, nonlinear optics, porous materials, gas storage and catalysis. Especially, aromatic polycarboxylate such as benzene tricarboxylic acid are reported in much cases for the building blocks to get the metal-organic frame works Here we report the network patterns obtained from the combination of copper(II) or nickel(II) complexes of macrocycles and 1,2,4,5-benzene tetracarboxylic acid at different reaction condition in detail.



1,2,4,5-benzene tetracarboxylic acid



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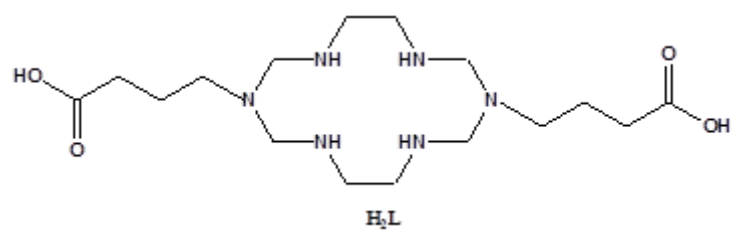
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Crystal Structure and Magnetic Properties of Cyano-Bridged Bimetallic Assembled $[\text{Cu}(\text{H}_2\text{L})]_3[\text{Fe}(\text{CN})_6]_2$

Enkhzul Otgonbaatar 곽지훈

순천대 화학과

Hexacyanomellates have been used as building blocks for the construction of a variety of coordination polymers with various interesting structures and properties. Cyano-bridged multiimetallic assembled moieties based on  $[\text{Fe}(\text{CN})_6]^{3-}$  building block, are attracted many attentions because of their interesting multi-dimensional structure and distinctive magnetic property as well. The bimetallic complex  $[\text{Cu}(\text{H}_2\text{L})]_3[\text{Fe}(\text{CN})_6]_2$  was obtained by the reaction of  $[\text{Cu}(\text{H}_2\text{L})](\text{ClO}_4)_2$  ( $\text{L}=3,10$ -bis(propylcarboxyl)-1,3,5,8, 10,12-hexaazacyclotetradecane) and  $\text{K}_3[\text{Fe}(\text{CN})_6]$  in water. This complex has been characterized by X-ray crystallography. The crystal structure of obtained exhibits a distorted octahedral geometry about copper atom. The complex  $[\text{Cu}(\text{H}_2\text{L})]_3[\text{Fe}(\text{CN})_6]_2$  shows a weak antiferromagnetic interaction between Cu(II) and Fe(III) ions with  $J = -1.73\text{cm}^{-1}$  and  $J = -1.01\text{cm}^{-1}$



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Metalloporphyrin Based Hexagonal MOF Particles and Their Use in Styrene Oxidation

김선돌 이다희 이영선 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 structural and functional interests. Metalloporphyrins are excellent building blocks for the construction of coordination polymers. 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 MOFs has been widely reported in latest years. Their properties are based on inherent characteristics of the size, morphology, and composition based on the organic building blocks. In here, we like to demonstrate the preparation of nano and micro-crystalline coordination polymer particles based on sever metalloporphyrins. Then we controlled morphology and

size from different reaction conditions such as solvent, reaction temperature and reaction time. In addition, we like to demonstrate their ability as heterogeneous catalysts.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## $\pi$ -Extended Zn-porphyrin derivatives for Single Crystalline TFT

최수정 채승현 이석중

고려대 화학과

There has been a considerable interest in synthesis of planar  $\pi$ -conjugated molecules for TFT (Thin Film Transistor) devices because  $\pi$ -conjugated system provide more efficient  $\pi$  orbital overlapping and high charge carrier mobility. In this presentation, we report the synthesis, characterization and transistor performance of various semiconductor materials based on Zn-porphyrin derivatives. These novel series of  $\pi$ -extend porphyrins have two phenyl and thiophene units to extend conjugation length. Particularly, TFTs using single crystals of porphyrin derivatives as active layers have been fabricated by slow solvent diffusion method. And their electrical, optical and charge transport properties are also demonstrated. Because porphyrin offers a variety of optical and electronic properties from the central metal and substituents, optimizing structural modification is crucial factor for improved high performance of organic thin film devices.



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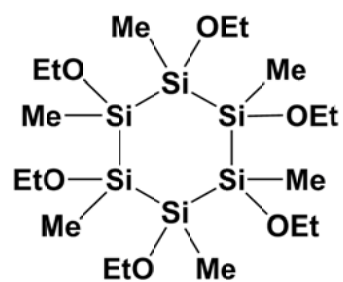
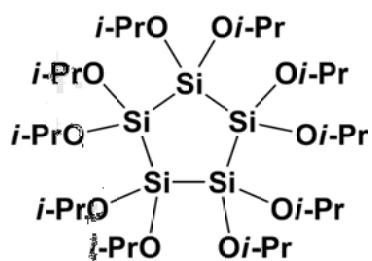
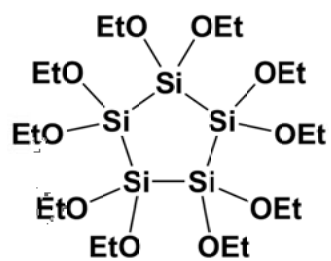
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Syntheses and Characterization of Alkoxycyclosilanes for New Precursors of Sol-Gel Reaction

박성진 조현모 이명의

연세대 화학및의화학과

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  $\sigma(\text{Si-Si})$  electron. These compounds are particularly preferred in application fields such as electronic materials. The cyclosilanes have been generally prepared by condensation reactions of diorganodihalosilanes. The synthetic yields of cyclic silanes depend on the choice of alkali metals and substituent groups of diorganohalosilanes. We synthesized four, five and six membered ring silanes from the reactions of dichlorodiorganosilane with reducing metals (Li, Mg). We also carried out nucleophilic substitution reactions of halogenated cyclosilanes with alcohols and amines. In this presentation, the syntheses and characterization of alkoxycyclosilanes will be discussed in detail.



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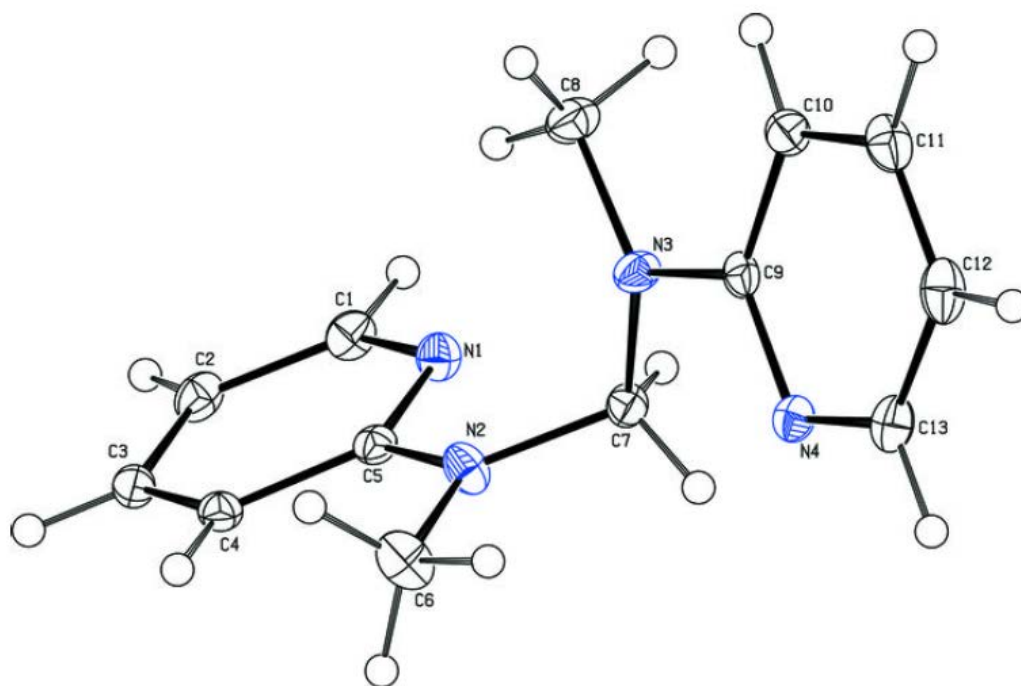
## Anion Sensing by a New Copper(II) Complex with a Pyridyl Amine

### Ligand

이문선 정현진 박경세<sup>1</sup> 이동현

전북대 화학과 <sup>1</sup>군산대 화학과

A colorimetric anion sensing utilizing coordination compounds continues to be major research efforts with environmental and biomedical relevance. Therefore, we report on the synthesis and characterization of Cu(II) complex of new ligand DPMA[DPMA=N,N'-Dimethyl-N,N'-bis(pyridin-2-yl)methanedi-amine]. A copper(II) complex of a different solvent(Methanol, Acetonitrile) was characterized by various spectroscopic methods. On the basis of these result, we tested the anion sensing ability towards Br<sup>-</sup>, Cl<sup>-</sup>, I<sup>-</sup>, SCN<sup>-</sup>, BF<sub>4</sub><sup>-</sup>, PF<sub>6</sub><sup>-</sup> and expected to utilize a chemical sensor through anion exchange.



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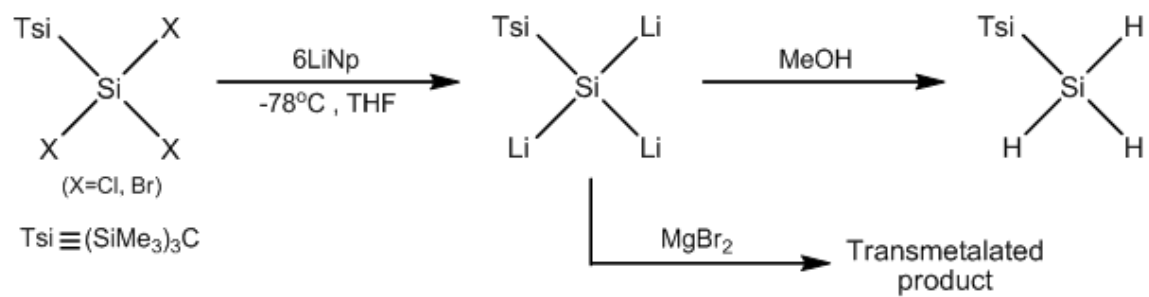
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Stability of Trianion species

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 ( $\text{TsiSiX}_3$ ,  $\text{Tsi}=\text{C}(\text{SiMe}_3)_3$ ,  $\text{X}=\text{Br}, \text{Cl}$ ) with more than 6 equivalents of lithium naphthalenide ( $\text{LiNp}$ ) in THF at  $-78^\circ\text{C}$  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  $\text{MgBr}_2$ ,  $^i\text{BuMgCl}$  and their thermal stability were also investigated. In this presentation, synthesis of trilithiosilane and its transmetalation will be discussed in detail.



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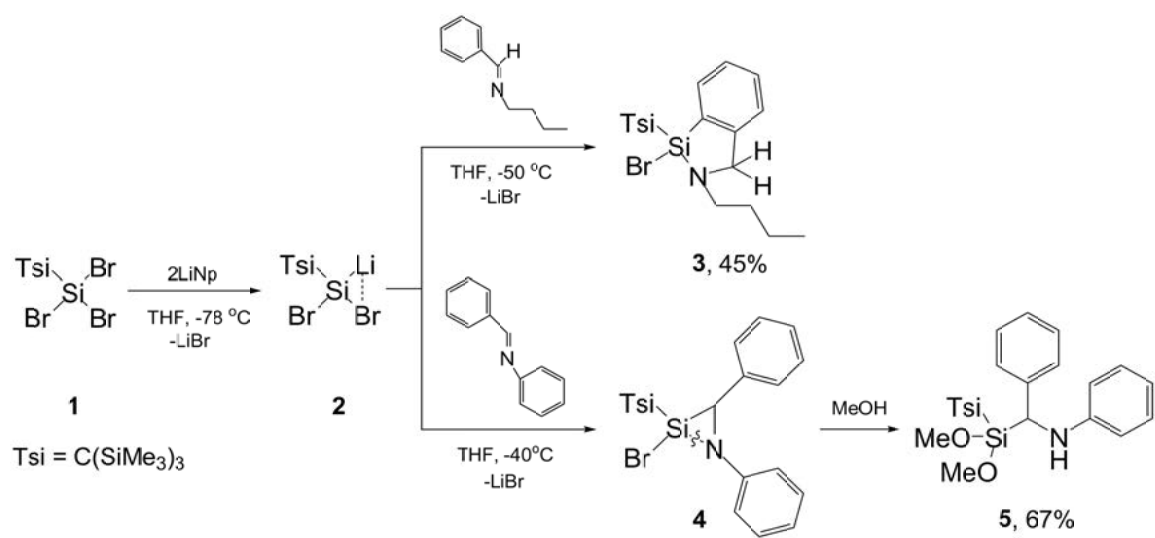
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Halosilylenoid Chemistry: Reactivities of Bromosilylenoid with Carbonyl Compounds

김승한 박서현 조현모 이명의

연세대 화학및의화학과

Over the past decade, a few novel silylenoids have been the subject of the extensive study. Silylenoid ( $R_2SiMX$ ) is a species which has an electropositive metal (M, alkali metal) and a leaving group (X, usually halogen) bound to the same silicon atom. Recently, we reported halosilylenoids, which were stable at room temperature. Bromosilylenoid 1, having the bulky substituent, Tsi (= trisyl, tris(trimethylsilyl)methyl group), was synthesized by the reduction of tribromotrisylsilane with 2 equivalent of LiNp (lithium naphthalenide). Using the bromosilylenoid, 1, we have studied its reactivity with various carbonyl, such as dimethylpentanone, adamantanone, cyclohexanone, and dimethylcyclohexanone. In the reaction of 1 with cyclohexanone, after an excess amount of cyclohexanone were added to bromosilylenoid, 1, the treatment of the reaction mixture with an excess of  $H_2O$ , MeOH and *i*-PrOH gave the corresponding products. In this presentation, we will discuss reactivities of bromosilylenoid with ketones in detail.





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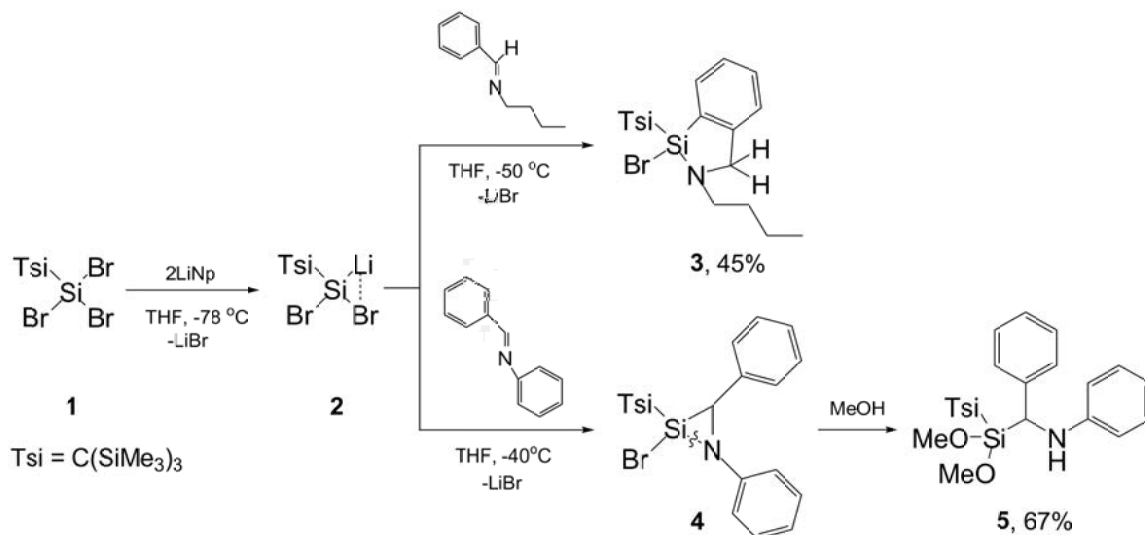
## Reactivities of Bromosilylenoid with Imines

박서현 조현모 이명의

연세대 화학및의화학과

Silylenoids are species containing an alkali metal (M) and a leaving group (X, usually halogen) bound to the same silicon atom, which makes them display amphiphilic properties. Reaction of a silylenoid with a compound containing a CN double bond has not been studied, whereas considerable experimental studies have been reported by several groups in case of silylenes which shared reaction characteristics with silylenoids. Herein, we report on reactions of a silylenoid with imines, such as *N*-butylphenylimine, *N*,1-di(phenyl)methanimine, which can be a new synthetic method for the synthesis of N, Si-containing heterocyclic compounds. Bromosilylenoid, **2** was prepared from the reaction of tribromo[tris(trimethylsilyl)methyl]silane, **1** with two equivalents of lithium naphthalenide in THF at -78 °C. Then, imines were added to resulting solution at same temperature. Interestingly, there was a great difference on results of reactions depending on imines. In case of reaction of **2** with *N*-butylphenylimine at -50 °C for 12 h, azaindane, **3** was synthesized through rearrangement in 45% yield. Compound **3** was characterized by multinuclear NMR spectroscopy and X-ray structural analysis. On the other hand,

silaziridine, **4** was synthesized from the reaction of **2** with *N*,1-di(phenyl)methanimine at -50 °C for 6 h, which was characterized by  $^{29}\text{Si}$  NMR spectroscopy. Ring cleavage of **4** was occurred by MeOH to give  $\alpha$ -silyl amine **5** in 67% yield. Compound **5** was characterized by GC/MS and multinuclear NMR spectroscopy. In this presentation, we will discuss the chemistry of bromosilylenoid with imines in detail.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Hydrogenation of Nitroarenes by Gold Nanoreactor with Conductive Shell

신혜선 허성

한국외국어대 화학과

Core-shell nanomaterials with a metallic core have been attractive themed issues over the past years in materials science. They are not only appealing in the structural point of view, but also very interesting in their characteristic functionalities that are originated from the confined architectures. In most cases, core-shell structured materials generally require more than two synthetic steps since they take either ‘inside-out’ route where core nanoparticles are made first or ‘outside-in’ route where outer shell structures are formed firstly. Herein, a novel in-situ synthesis of functionalized core-shell hybrid material is introduced with Au-core/layered conducting polymer-shell. The outer conductive polymer-shell exhibits an Ohmic behavior in electrical measurement and has distinctive cyano-functionality which presumably interacts with the Au-core. The Au-core shows high catalytic activities for the hydrogenation of various nitroarene compounds and which demonstrates the outer shell is readily accessible in chemical manner. The detailed

characterizations for the materials are further investigated by HR-TEM, SEM, FT-IR, PXRD, UV/vis spectroscopy, and XPS.



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## Sub-10nm Well-defined Pd-Pt Core-shell Nanoparticles with Enhanced Electrocatalytic Activity and Durability toward the Oxygen Reduction Reaction

최란 박준택<sup>1</sup> 한상우

KAIST 화학과 <sup>1</sup>한국기초과학지원연구원 원장실

The improvement of electrocatalytic activity toward oxygen reduction reaction (ORR) and durability of Pt-based catalyst with low Pt content is one of the important tasks to advance the performance of polymer electrolyte membrane fuel cells (PEMFCs). In this paper, we report on syntheses of sub-10 nm well-defined spherical Pd-Pt core-shell (Pd@Pt) nanoparticles (NPs) with various shell thicknesses and their electrochemical performances toward ORR as for cathode catalysts. Pd@Pt NPs were prepared by simple synthesis of *in-situ* heteroepitaxial growth of Pt on as-synthesized Pd NPs. As-prepared Pd@Pt NPs demonstrated the enhanced electrocatalytic activity toward ORR and improved durable stability compared to the commercial Pt catalyst. Moreover, a membrane electrode assembly (MEA) adopted Pd@Pt/C catalysts in a single PEMFC exhibited the nearly same performance to the commercial Pt/C catalyst in

spite of its lower Pt content. From the results, as-synthesized Pd@Pt/C catalysts facilitate low-cost and high-efficient automotive application of fuel cell.



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## Synthesis of Pd/SiO<sub>2</sub> Nanobeads for Use in Suzuki Coupling Reactions by Reverse Micelle Sol-gel Process

김아람 송현준<sup>1</sup> 박강현

부산대 화학과 <sup>1</sup>KAIST 화학과

Pd/SiO<sub>2</sub> nanobeads consisting of tiny Pd clusters with a diameter of about 2 nm were prepared via a sol-gel process for silica by using a water-in-oil microemulsion with Pd complexes and subsequent hydrogen reduction along with heat treatment. The Pd/SiO<sub>2</sub> catalyst was used as a high-temperature catalyst in Suzuki coupling reactions of various aryl bromides with phenylboronic acids. One important factor affecting the yield of the reaction is the superior chemical reactivity of the nanoparticles. The present result indicates that transition-metal nanoparticles can be used as catalysts for a wide variety of organic transformations.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Cu Nanoparticles in Ionic Liquid: An alternative catalytic system for Click Chemistry**

**Mohan Balaji 박강현**

부산대 화학과

In-situ prepared copper nanoparticles have been found to effectively catalyze the 1,3-dipolar cycloaddition of a variety of azides and alkynes furnishing the corresponding 1,2,3-triazoles in excellent yields. We have developed a new protocol to synthesize copper nanoparticles in Ionic Liquid structurally based on imidazolium as cation and tetrafluoroborate as anion and also found in-situ synthesized nanoparticles can catalyze click chemistry efficiently within short reaction time, low temperature and as well as inert atmosphere free conditions. The nanoparticles dispersed in Ionic Liquid can be recycled atleast four times without adding copper source and Ionic Liquid externally.



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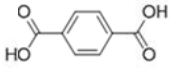
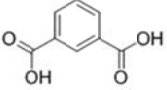
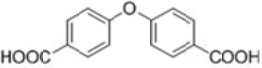
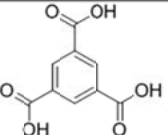
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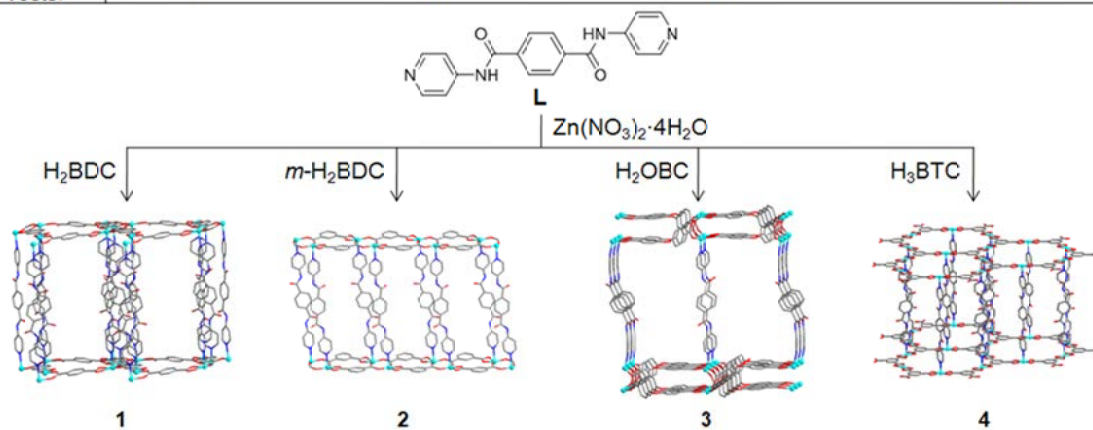
## Metal-Organic Frameworks based on Binary Ligands involving Bis(amidopyridine) and Carboxylic Acids with Different Coordination Vectors

이은지 박기민 이심성

경상대 화학과

Metal-organic frameworks 1-4 with 2-3D structures were prepared in the solvothermal reactions of transition metal ions with binary ligand system: bis(amidopyridine) ligand L and carboxylic acids ( $\text{H}_2\text{BDC}$ ,  $m\text{-H}_2\text{BDC}$ ,  $\text{H}_2\text{OBC}$  and  $\text{H}_3\text{BTC}$ ) with  $180^\circ$  or  $120^\circ$  coordination vector. Reaction of L with  $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  in the presence of  $\text{H}_2\text{BDC}$  afforded a 2-fold interpenetrated 3D polymeric array of formula  $\{[\text{Zn}_4(\text{L})_4(\text{BDC})_4]6\text{DMF}\}_n$  (1). Meanwhile, reaction of L with  $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  in the presence of  $m\text{-H}_2\text{BDC}$  gave a non-interpenetrated 2D array of formula  $\{[\text{Zn}_2(\text{L})_2(m\text{-BDC})_2]2\text{DMF}\}_n$  (2). In addition, reaction of L with  $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  in the presence of  $\text{H}_2\text{OBC}$  having longer  $120^\circ$  coordination vector afforded a 3-fold interpenetrated 3D polymeric array of formula  $\{[\text{Zn}_2(\text{L})(\text{OBC})_2]\text{DMA}\}_n$  (3). Treatment of L with  $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  in the presence of  $\text{H}_3\text{BTC}$  afforded a 3-fold interpenetrated 3D array of formula  $\{[\text{Zn}_3(\text{L})_3\text{BTC}_2]\text{DMA}\}_n$  (4). The photoluminescence and gas absorption properties are also discussed.

|                     |   |   |  |   |
|---------------------|---|---|--|---|
| Carboxylic Acids    |  |  |  |  |
|                     | H <sub>2</sub> BDC  | <i>m</i> -H <sub>2</sub> BDC  | H <sub>2</sub> OBC   | H <sub>3</sub> BTC  |
| Coordination Vector | 180°  | 120°  | 120°   | 120°  |



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발표분야: 무기화학

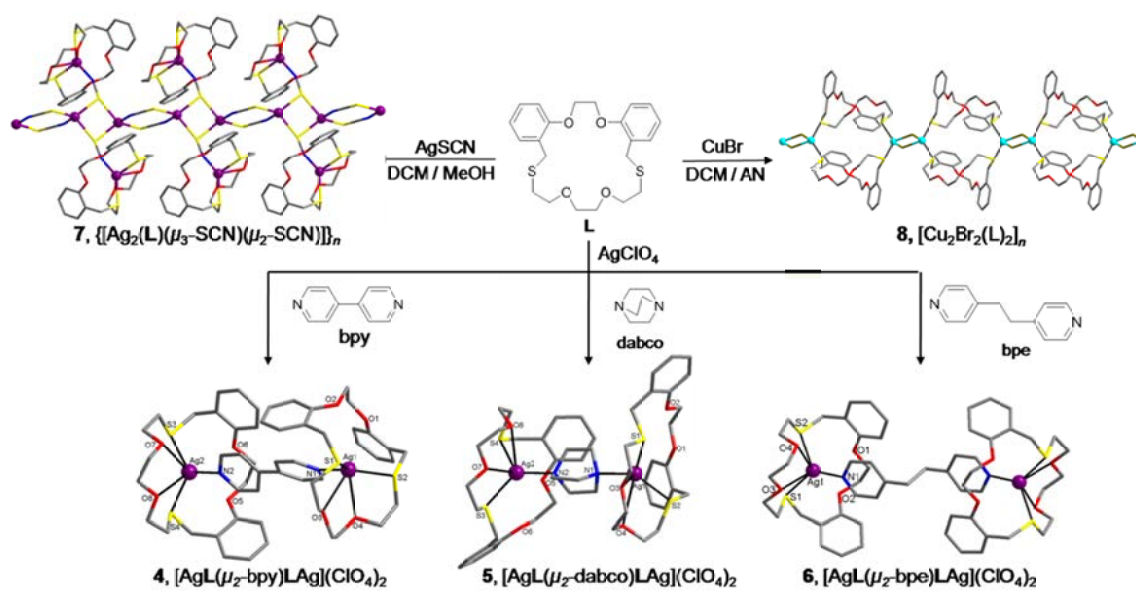
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-assembly of Soft Metal Supramolecular Complexes of an O<sub>4</sub>S<sub>2</sub>-Macrocycle with Different Coordination Modes

주희영 이심성

경상대 화학과

A range of thiophilic ( $\text{Ag}^+$ ,  $\text{Cu}^+$ ,  $\text{Hg}^{2+}$ , and  $\text{Pd}^{2+}$ ) mono-, di-, and multinuclear complexes (1-8) of the O<sub>4</sub>S<sub>2</sub>-donor macrocycle L with discrete (1-6) and continuous (7-8) forms were prepared and structurally characterized. First, reactions of L with  $\text{AgClO}_4$ ,  $\text{Hg}(\text{NO}_3)_2$ , and  $\text{K}_2\text{PdCl}_4$  afforded a typical endocyclic 1:1 complex  $[\text{Ag}(\text{L})]\text{ClO}_4$  (1) without anion binding,  $[\text{Hg}(\text{L})(\text{NO}_3)_2]$  (2), and  $[\text{cis-Cl}_2\text{Pd}(\text{L})]$  (3), respectively. Further, 1 can then be manipulated to provide the extended products. One-pot reaction of L with  $\text{AgClO}_4$  together with linker coligands ( $\text{L}'$ : bpy = 4,4'-bipyridine, dabco = 1,4-diazabicyclo[2.2.2]octane, and bpe = 1,2-bis(pyridyl)-ethane) afforded unique dumbbell-shaped complexes  $[\text{Ag}_2(\text{L})_2(\mu_2\text{-dabco})](\text{ClO}_4)_2$  (4),  $[\text{Ag}_2(\text{L})_2(\mu_2\text{-bpy})](\text{ClO}_4)_2$  (5), and  $[\text{Ag}_2(\text{L})_2(\mu_2\text{-bpe})](\text{ClO}_4)_2$  (6) with an LAg-L'-AgL pattern. Contrasting with the above discrete-type complexes, reactions of L with  $\text{AgSCN}$  and  $\text{CuBr}$  yielded the continuous 1D network complexes  $[\text{Ag}(\text{L})\text{SCN}]_n$  (7) and  $[\text{Cu}_2\text{Br}_2(\text{L})]_n$  (8), respectively.



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발표분야: 무기화학

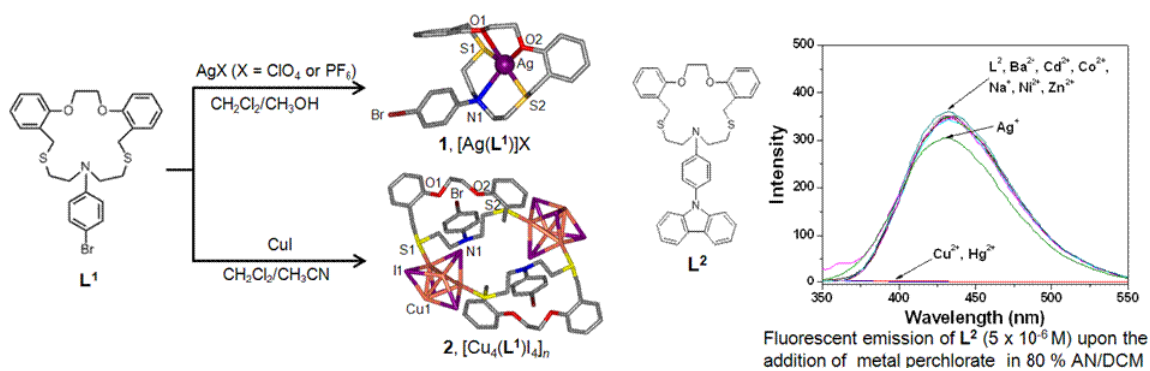
발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Carbazole-attached NO<sub>2</sub>S<sub>2</sub>-Macrocycle Exhibiting Hg<sup>2+</sup> and Cu<sup>2+</sup> Selectivity

이슬기 이심성

경상대 화학과

The NO<sub>2</sub>S<sub>2</sub>-donor macrocycle L<sup>2</sup> functionalized with fluorescent carbazole unit was synthesized by means of Buchwald procedure in good yield. The *N*-phenylated macrocycle precursor L<sup>1</sup> was synthesized by dithiol-dichloride coupling reaction of corresponding dichloride with *N*-dithiol, using Cs<sub>2</sub>CO<sub>3</sub> in DMF. In the metal-induced photoluminescence experiment, a selective chelation enhanced fluorescence quenching (CHEQ) effect was observed upon addition of mercury(II) and copper(II) perchlorates into L<sup>2</sup>, although a relatively small CHEQ effect was observed with silver(I). In addition, the silver(I) and copper(I) complexes of L<sup>1</sup> were obtained and crystallographically characterized. An endo-dentate 1:1 monosilver(I) complex 1, [Ag(L<sup>1</sup>)]X; (X = ClO<sub>4</sub> or PF<sub>6</sub>) which show isomorphous structures were obtained from the reactions of L<sup>1</sup> with silver(I) salts. Meanwhile, reaction of L<sup>1</sup> with copper(I) iodide afforded a 1-D coordination polymer 2 linked with Cu<sub>4</sub>I<sub>4</sub> cluster unit which shows yellow photoluminescence at 555 nm. For L<sup>2</sup>, the investigation of the related complexation is in progress.



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발표코드: INOR.P-167

발표분야: 무기화학

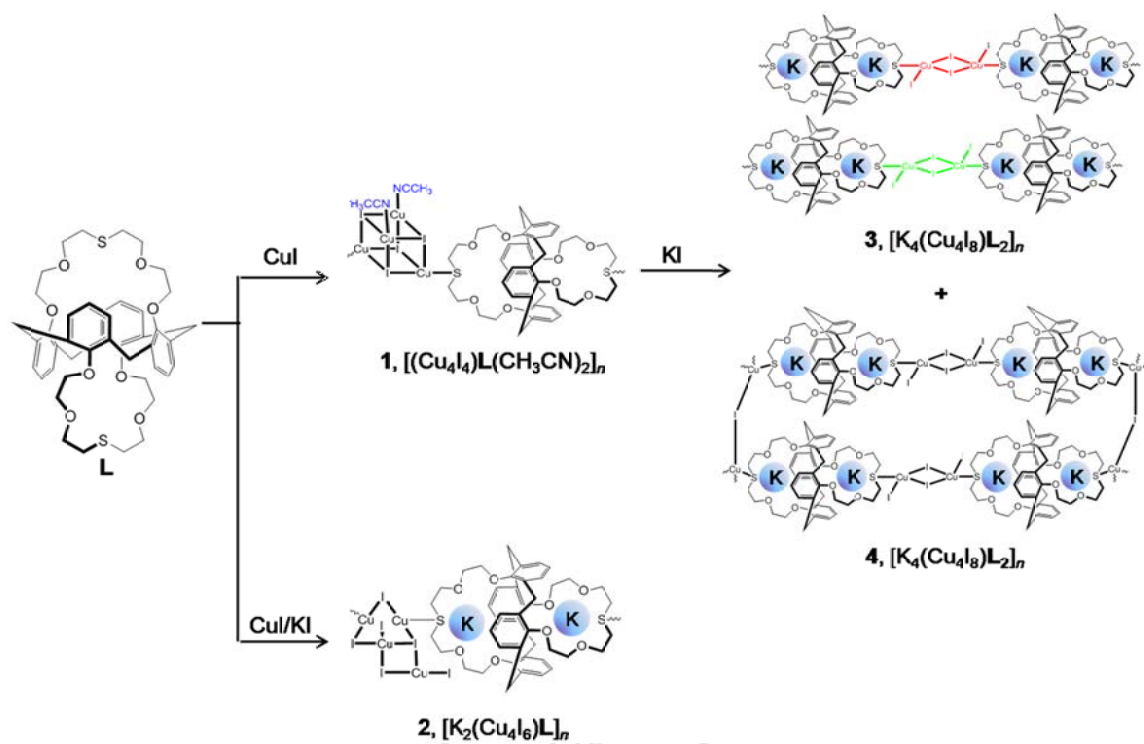
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Influence of Potassium(I) on the Networking of Calix[4]-bis-monothiacrown with Soft Metal Ions

김자연 이재영<sup>1</sup> 이심성

경상대 화학과 <sup>1</sup>건양대 나노바이오화학과

In the extension of our previous work<sup>1</sup> on the exocyclic coordination polymer 1 exhibiting a photoluminescence switching behavior, the influences of potassium(I) on the networking of calix[4]-bis-monothiacrown (L) with copper(I) iodide are reported. First, one-pot reaction of L with CuI/KI afforded a 1-D coordination polymer 2, of a formula  $[K_2(Cu_4I_6)L]_n$ , exhibiting the endocyclic dipotassium complex units are linked by exocyclic scoop-type  $Cu_4I_6^{2-}$  clusters via Cu-S bonds. On the other hand, stepwise reaction of 1 with KI gave a mixture of 3,  $[K_8(Cu_8I_{16})(L_4)]_n$  and 4,  $[K_4(Cu_4I_8)(L_2)]_n$ , which show 1-D and 2-D structures linked with rhomboidal  $Cu_2I_2$  clusters, respectively, encapsulating two potassium(I) ions inside the cavity in each case. Further study on the endo/exo complexation and networking is in progress. 1. J. Y. Lee, H. J. Kim, J. H. Jung, W. Sim, S. S. Lee, *J. Am. Chem. Soc.* 2008, 130, 13838.





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장소: 일산KINTEX

발표코드: INOR.P-168

발표분야: 무기화학

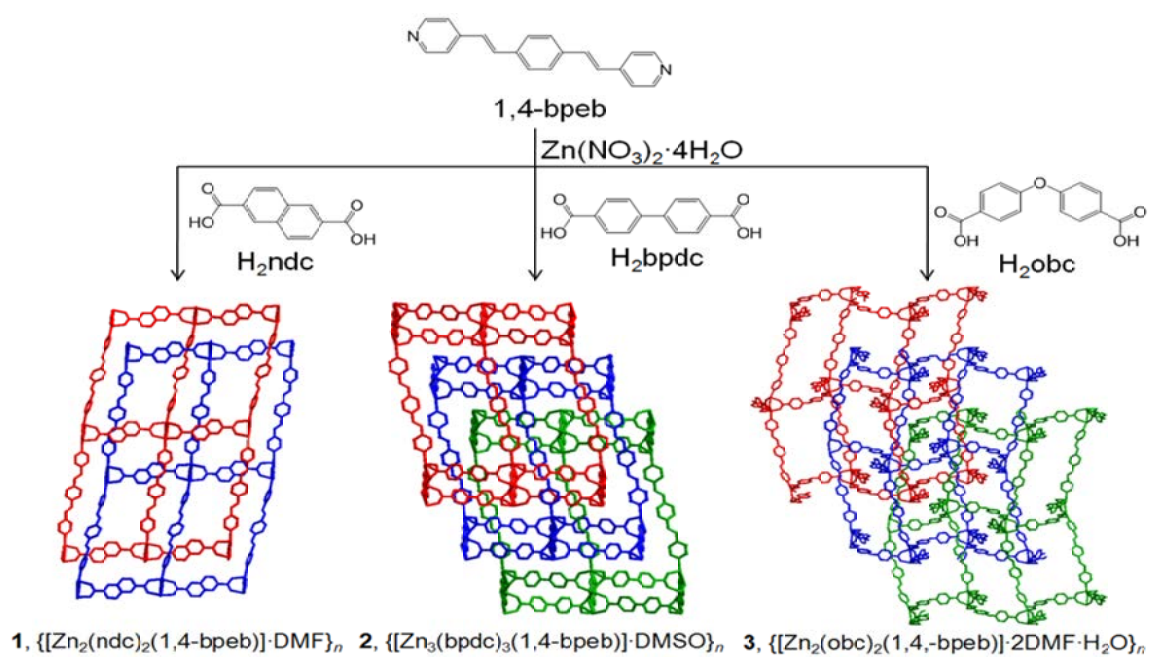
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-assembly of 3D Zinc(II) Coordination Polymers based on Dipyridine Derivative (1,4-bpeb) and Dicarboxylic Acids

박인혁 Jagadese J. Vittal<sup>1</sup> 이심성

경상대 화학과 <sup>1</sup>Department of Chemistry, National University of Singapore

1,4-bis[2-(4-pyridyl)ethenyl]benzene (1,4-bpeb) having two C=C bonds was prepared as a candidate for [2+2] photodimerization to link through one or two cyclobutane units. Solvothermal reaction of 1,4-bpeb with three kinds of dicarboxylic acids (H<sub>2</sub>ndc, H<sub>2</sub>bpdc and H<sub>2</sub>obc) and zinc(II) nitrate in the presence of NaOH solution enabled the isolation of 3D metal-organic frameworks (MOFs) (1-3). For example, 1,4-bpeb and H<sub>2</sub>ndc afforded the 2-fold interpenetrated 3D coordination polymer, {[Zn<sub>2</sub>(ndc)<sub>2</sub>(1,4-bpeb)]·DMF}<sub>n</sub> (1). On the other hand, 1,4-bpeb and H<sub>2</sub>bpdc yielded the 3-fold interpenetrated 3D coordination polymer {[Zn<sub>3</sub>(bpdc)<sub>3</sub>(1,4-bpeb)]·DMSO}<sub>n</sub> (2). In case of 1,4-bpeb and H<sub>2</sub>ndc, again 3-fold interpenetrated 3D coordination polymer {[Zn<sub>2</sub>(obc)<sub>2</sub>(1,4-bpeb)]·2DMF·H<sub>2</sub>O}<sub>n</sub> (3) was isolated. The photophysical properties such as solid-state photoluminescence and TGA are also discussed.



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발표분야: 무기화학

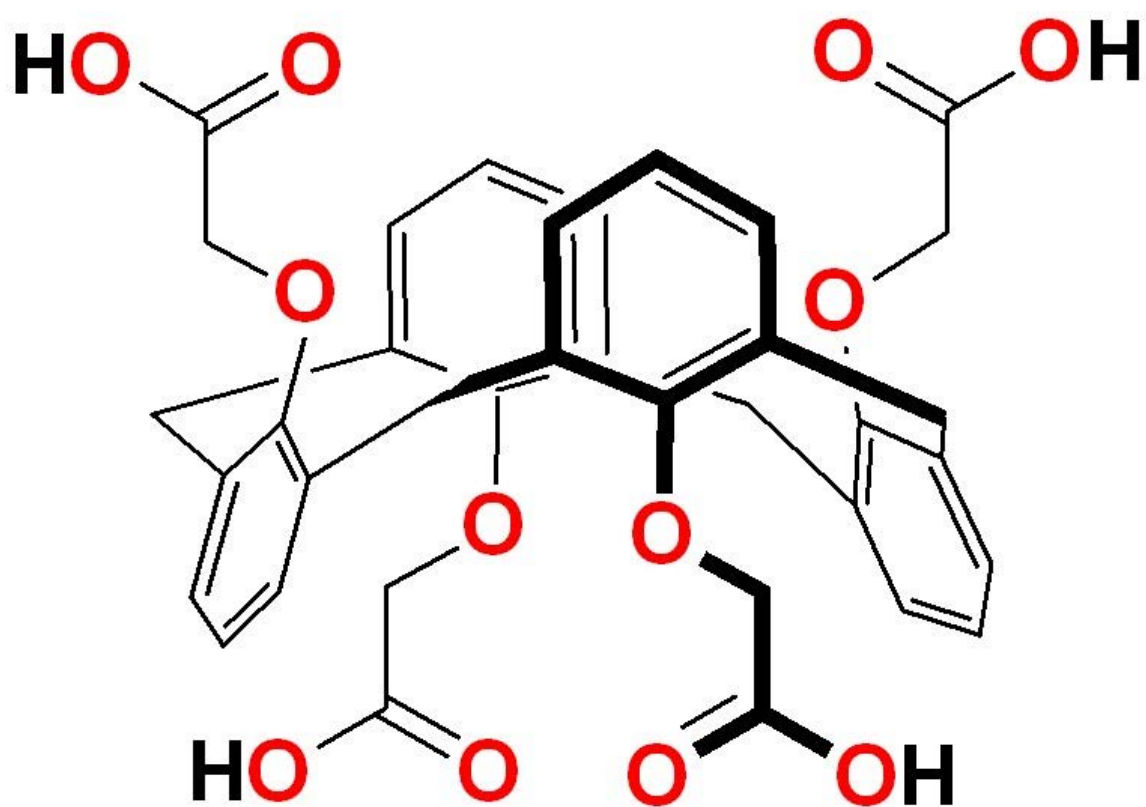
발표종류: 포스터, 발표일시: 수 18:00~21:00

### 3-D Nanoporous Coordination Polymers Based on Calix[4]arene Tetraacetate

박기민 이은지 이심성

경상대 화학과

Porous coordination networks have been extensively developed because of their potential applications. A calix[4]arene derivative H<sub>4</sub>CTA (= Calix[4]arene TetraAcetic acid) is a good candidate for the preparation of various three-dimensional nanoporous coordination polymers because it has four carboxylic pendent arms as coordination sites. Using the solvothermal reaction, we prepared four 3D nanoporous coordination polymers: {[Pb<sub>2</sub>(CTA)]·2DMF}<sub>n</sub>, [Cd<sub>2</sub>(CTA)(DMF)<sub>3</sub>]<sub>n</sub>, {[Zn<sub>2</sub>(CTA)(bpy)(DMF)]·nDMF}<sub>n</sub> and {[Cu<sub>2.5</sub>(μ<sub>3</sub>-OH)(K@CTA)(H<sub>2</sub>O)<sub>0.5</sub>]<sub>n</sub>DMF}<sub>n</sub>. Herein, we report crystal structures and physical properties of the obtained three-dimensional nanoporous coordination polymers based on H<sub>4</sub>CTA.



**H<sub>4</sub>CTA**



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발표코드: INOR.P-170

발표분야: 무기화학

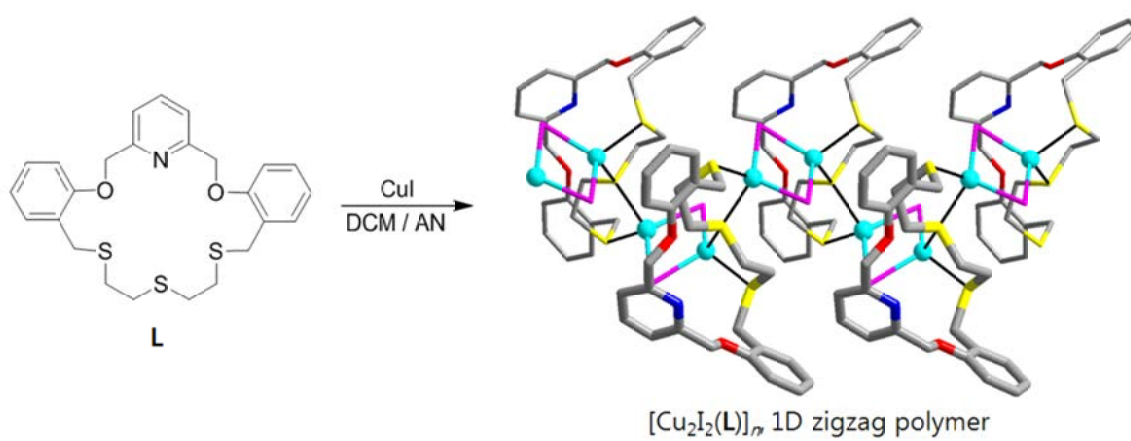
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Coordination Polymer with Thiaoxaaza-Macrocycle

이형환 이심성

경상대 화학과

The pyridine-containing thiaoxaaza-macrocycle (L) was synthesized by dithiol-dichloride coupling reaction of corresponding dichloride with a dithiol, using  $\text{Cs}_2\text{CO}_3$  in DMF under high dilution condition. L was confirmed by  $^1\text{H}$ -NMR,  $^{13}\text{C}$ -NMR and ESI-MS. In addition, crystal structure of L was structurally characterized by single-crystal X-ray crystallography. L forms an exo-type coordination polymer 1 with copper(I) iodide via  $\text{S}_3$ -donor atoms. In 1, the ligand L was linked by  $[\text{Cu}_2\text{I}_2(\text{L})]_n$  with  $\text{Cu}_2\text{I}_2$ -rhomboid to give a zigzag type polymeric chain.



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발표코드: INOR.P-171

발표분야: 무기화학

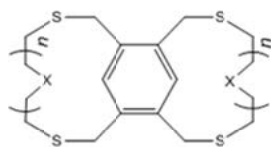
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Bis-thiamacrocycles and their Supramolecular Complexes

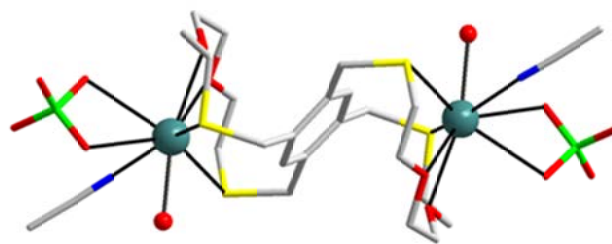
DEUKAM SIEWE ARLETTE 이심성

경상대 화학과

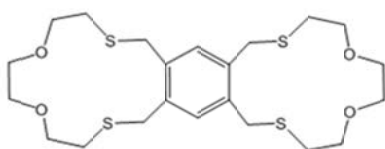
Since first bis-thiamacrocyclic  $L^1$  was reported by Loeb group<sup>1</sup>, no bis-thiamacrocyclic system has been reported till now. In this work, we report the synthesis of new series of the bis-thiamacrocycles and their complexes with supramolecular structures.  $L^1$ - $L^3$  were synthesized by 1,3-bis-cyclization between tetrabromide and corresponding dithiol in the presence of  $Cs_2CO_3$  under high dilution condition. In preparing  $L^2$ , 1,2-bis-cyclization product  $L^{2a}$  as an isomer was also isolated as a minor product by recrystallization. From the reaction of thiophilic metal salts with  $L^1$ - $L^3$ , several complexes were obtained and structurally characterized. For example, a dilead(II) complex 1, with a formula  $[Pb_2(L^2)(CH_3CN)_2(H_2O)_2(ClO_4)_2](ClO_4)_2$ , and a zigzag-type 1-D coordination polymer 2 with a formula  $[Ag(L^2)]_n(PF_6)_n$  were isolated. In 2, the silver(I) which links the  $L^2$  via exocyclic Ag-S bonds is four-coordinated with a distorted tetrahedral geometry. 1. S. J. Loeb, G. K. H. Shimizu, *Inorg. Chem.* 1993, 32, 1001-1006.



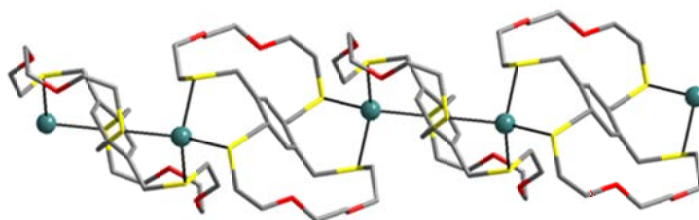
$L^1$ :  $X=O$ ,  $n=1$   
 $L^2$ :  $X=O$ ,  $n=2$   
 $L^3$ :  $X=NH$ ,  $n=1$



1, dilead(II) complex of  $L^2$



$L^{2a}$



2, 1-D silver(I) coordination polymer of  $L^{2a}$





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장소: 일산KINTEX

발표코드: INOR.P-172

발표분야: 무기화학

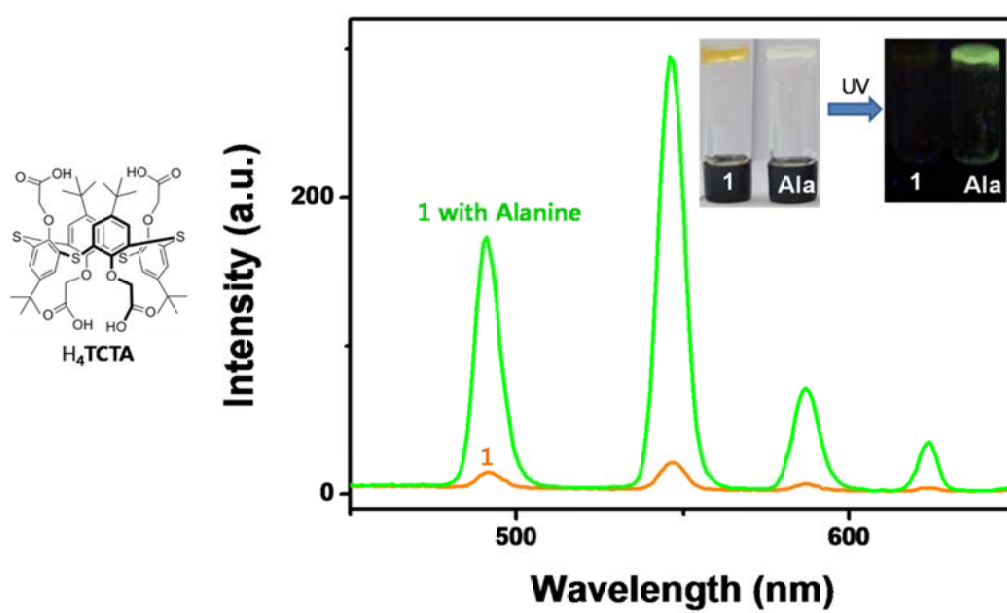
발표종류: 포스터, 발표일시: 수 18:00~21:00

## H<sub>4</sub>TCTA-Based Coordination Polymer Gel for Detection of Alanine

박선희 김가영 정종화

경상대 화학과

We synthesized the *p-tert*-butyl-thiacalix[4]arene tetraacetic acid (H<sub>4</sub>TCTA). H<sub>4</sub>TCTA forms yellow gel (1) upon addition of Tb<sup>3+</sup> ion in DMF/0.1M NaOH (6:1 v/v) mixed solvents at 110 °C. A variety of amino acids were added to the 1 in order to investigate the molecular recognition ability of 1. Interestingly, The addition of alanine to gel 1 exhibited the strong emission. In addition, the yellow color of gel H<sub>4</sub>TCTA with Tb<sup>3+</sup> was changed to the white color. The results are due to change of coordination number of Tb<sup>3+</sup> ion with alanine. To probe the fluorescence and the color change of H<sub>4</sub>TCTA with Tb<sup>3+</sup> upon the addition of the alanine, we have attempted the preparation of the crystalline complex of H<sub>4</sub>TCTA, such as a 3-D coordination polymer {[Tb(TCTA)<sub>3/4</sub>(H<sub>2</sub>O)<sub>2</sub>]·H<sub>2</sub>O}<sub>n</sub>.



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발표코드: INOR.P-173

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Biological toxicity study for aminoacids capped ZnS:Mn nanocrystals

**박상현 황청수**

단국대 화학과

aminoacids-capped water-dispersible ZnS:Mn nanocrystals were synthesized and their biological effects on the growth of *E. coli* were investigated. Particle sizes of these ZnS:Mn-aminoacids nanocrystals were found from their HR-TEM images. In addition, their solution photoluminescence spectra showed similar broad emission peaks around 600 nm. Among the aminoacids capped ZnS:Mn nanocrystals, ZnS:Mn-His significantly suppressed the growth of *E. coli* at 100  $\mu\text{g/mL}$  and 1  $\text{mg/mL}$  concentrations, something not observed for ZnS:Mn-Cys.

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발표코드: INOR.P-174

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Growth of Uniformly Oriented Silica MFI and BEA Zeolite Films on Substrates

Pham Cao Thanh Tung 김현성<sup>1</sup> 윤경병<sup>1</sup>

서강대 나노물질연구소 <sup>1</sup>서강대 화학과

Zeolite films are widely used in various fields such as molecular sieve membranes, membrane reactors, hosts for nonlinear optical (NLO) molecules, low dielectric (low  $k$ ) materials. For these purposes, perfect zeolite films featured with uniform orientations of crystal axes have been expected to give best performances. However, no methods have been available for the last 30 years. We will present a novel method to grow pure silica MFI and BEA zeolite films with all the channel systems are open from the top to the bottom of the films and uniformly oriented regardless of the film thicknesses. We will also present marked improvements in their performances during their applications for second-order NLO materials and xylene mixture separation.

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장소: 일산KINTEX

발표코드: INOR.P-175

발표분야: 무기화학

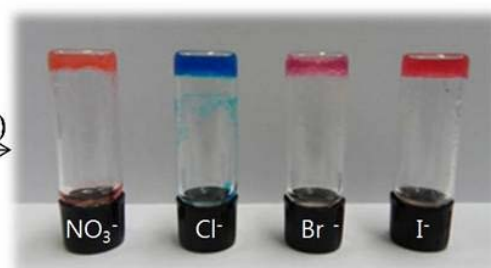
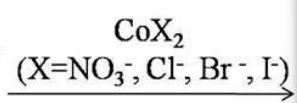
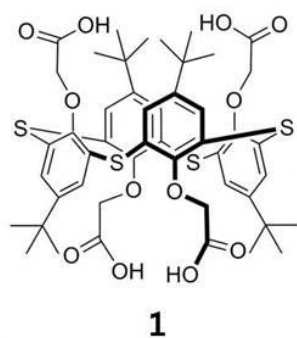
발표종류: 포스터, 발표일시: 수 18:00~21:00

## H<sub>4</sub>TCTA-Based Metal-Organic Framework Gel as Chemosensor for Chlorine Gas

김가영 박선희 정종화

경상대 화학과

We chose simple *p-tert*-butyl-thiacalix[4]arene tetraacetic acid (H<sub>4</sub>TCTA) as the framework to which to attach ligands because of its well-defined and extensively developed in metal-organic framework (MOF) chemistry. Thus, we synthesized the H<sub>4</sub>TCTA(**1**). **1** forms the gel upon addition of Co<sup>2+</sup> ion in DMF/H<sub>2</sub>O. Interestingly, the red color of Co<sup>2+</sup> coordination polymeric gel **1** was changed into the blue color by addition of gases containing chloride atoms such HCl, SOCl<sub>2</sub>, (CO)<sub>2</sub>Cl<sub>2</sub>, and COCl<sub>2</sub>. These results are due to change of coordination numbers of Co<sup>2+</sup> by chloride atoms. In this conference, we will detail present on the preparation of Co<sup>2+</sup> coordination polymer gel and its application as a chemosensor for gases containing chloride atoms.



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발표코드: INOR.P-176

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

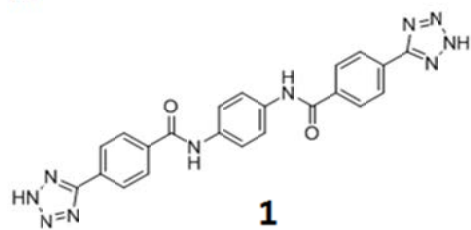
## Preparation of Tetrazole-Based Metal-Coordination Polymeric Hydrogel

최희경 이지하 안진호 정종화

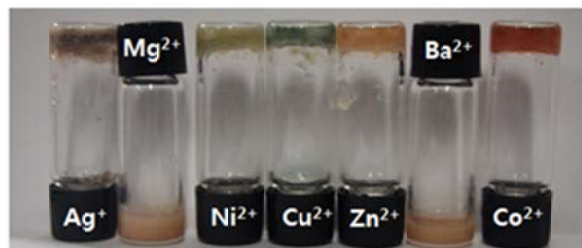
경상대 화학과

Compound **1** was synthesized and its gelation ability was evaluated in the absence and the presence of metal ions such as  $\text{Mg}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ag}^+$ ,  $\text{Ba}^{2+}$ , and  $\text{Ni}^{2+}$  in water. Interestingly, **1** formed gel in the presence of  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ag}^+$  and  $\text{Co}^{2+}$  ions. The gels in the presence of  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ag}^+$  and  $\text{Co}^{2+}$  were also characterized by SEM, UV/vis spectroscopy, and fluorescent spectroscopy. The gel **1** with  $\text{Ni}^{2+}$  showed the fiber structure with 290 length and 50nm diameter. The gelation of compound **1** with  $\text{Ni}^{2+}$  is due to formation of coordination polymeric structure by coordination bonds. The rheological property of  $\text{Ni}^{2+}$  coordination polymer gel **1** was measured. In this conference, we will present on the gel formation of ligand **1** with  $\text{Ni}^{2+}$  and its physical properties.

(A)



(B)





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장소: 일산KINTEX

발표코드: INOR.P-177

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and characterization of acrylated $\text{TiO}_2@\text{SiO}_2$ core shell nanoparticle

안진호 정성호 이지하 정종화

경상대 화학과

The  $\text{TiO}_2@\text{SiO}_2$  core shell type nanoparticles were prepared by sol-gel reaction and characterized by SEM, TEM and powder XRD. The  $\text{TiO}_2@\text{SiO}_2$  nanoparticle shows the spherical structure with 700~800nm diameter. After calcination, the diameter of  $\text{TiO}_2$  was shrunk. In addition, we attached the acrylate moiety onto the surface of  $\text{TiO}_2@\text{SiO}_2$  nanoparticle. The acrylate group attached onto  $\text{TiO}_2@\text{SiO}_2$  nanoparticle acted as a functional group to the synthesis of polymer.

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발표코드: INOR.P-178

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Metallogel of Three Pyridine Derivative with $\text{Cd}^{2+}$ Ion

이효희 박선희 정성호 정종화

경상대 화학과

We synthesized compound 1, which has three pyridine groups as a binding site for  $\text{Cd}^{2+}$  ion. Compound 1 could gelate with  $\text{Cd}^{2+}$ . The metallogel 1 in the presence of  $\text{Cd}^{2+}$  shows the fiber structure with 50 nm diameter by observation of SEM. In addition the single crystall structure of 1 with  $\text{Cd}^{2+}$  was obtained.

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발표코드: INOR.P-179

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Large scale synthesis of pure VSH-1 and its characterization

Shuvo Jit Datta 윤경병<sup>1</sup>

서강대 나노물질연구소 <sup>1</sup>서강대 화학과

A method to produce pure VSH-1 in large quantities (~20 g) was developed. Analyses of the diffuse-reflectance UV-Vis spectra of  $M^{n+}$ -VSH-1 ( $M^{n+} = K^+, Na^+, Ca^{2+}, Pb^{2+}, \text{ and } Zn^{2+}$ ) revealed that the bands that appear in the 200-400 nm region arise due to the D-A-A triad charge-transfer (CT) interaction among the  $V^{4+}$ ,  $O^{2-}$ , and  $M^{n+}$ , and the 447, 590, and 879 nm bands arise due to the d-d transition of  $V^{4+}$ . The measured atomic magnetic moment ( $\mu$ ) was 1.73 BM, indicating that all the V atoms exist in  $V^{4+}$ . The ESR spectrum of VSH-1 showed a strong signal due to  $V^{4+}$  with the g value of 1.959 with  $\Delta H_{pp}$  value of 131 G. The Raman spectra of  $M^{n+}$ -VSH-1 revealed the existence of strong V=O stretching at  $955\text{ cm}^{-1}$ , and other peaks at 373 (weak), 453 (weak), 534 (weak), 620 (medium), 800 (weak), and  $1072\text{ cm}^{-1}$ . The V=O stretching band shifted to a higher energy region upon increasing the Sanderson's electronegativity of  $M^{n+}$ . The thermogravimetric (TGA) analysis showed that VSH-1 is thermally stable up to  $550^\circ\text{C}$  and above which the oxidation of  $V^{4+}$  occurs and the structure collapse.

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장소: 일산KINTEX

발표코드: INOR.P-180

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-assembly of M12L6 nanocages composed of homochiral salen building blocks

조건형 설창훈 허정석

충남대 화학과

나노미터 크기의 동공을 가지는 나노주머니 (nanocage) 착화합물은 물질 분리, 분자 센서, 약물 전달 등 유용한 특성이 기대되어 그 합성 및 응용에 관한 연구가 활발하다. 정사면체 형태의 비교적 큰 동공을 가지는 나노주머니 화합물을 합성하기 위하여 양 말단에 pyrimidyl 작용기가 치환된 chiral salen 유기 분자와 palladium(II) 착화합물을 자기조립하여 homochiral M12L6 타입의 nanocage 화합물을 합성하였다. 나노케이지의 안정성을 높이기 위하여 platinum(II) 착화합물과 고온에서 반응하여 동일한 정사면체 형태의 나노케이지 또한 합성하였다. 케이지 입구의 입체장애를 조절하기 위하여 새로운 salen building block 을 고안하여 다양한 나노케이지 화합물을 합성하였다. 나노케이지 화합물의 합성 및 용액 상에서의 host-guest chemistry 결과를 자세히 보고하겠다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-181

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A porous coordination polymer composed of fluorescent building blocks

설창훈 조건형 허정석

충남대 화학과

선택적인 물질 흡착, 분리 및 센싱을 비롯한 다양한 응용을 위해 배위 고분자 화합물에 대한 연구가 활발히 진행되고 있다. 특히, 화학센서로 활용하기 위해서는 유용한 발색단을 포함하는 배위 고분자 화합물의 합성이 요구된다. 우리는 강한 형광을 띄는 H<sub>2</sub>FODC(9-fluorenone-2,7-dicarboxylic acid)발색단을 빌딩 블록으로 하여 3 차원 네트워크 구조를 가지는 새로운 Metal-Organic Framework 화합물을 합성하였다. 이 경우 2 층으로 interpenetration 된 구조를 형성함을 X-ray 결정구조 분석을 통하여 확인하였다. 배위 고분자 화합물의 자세한 X-ray 결정구조, 광학특성 및 표면적 분석 결과를 보고하겠다.

일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: INOR.P-182

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of New Strontium Complex

조지쉐비메리 박보근 김창균 정택모

한국화학연구원 화학소재연구본부

A new strontium complex was synthesized by treating corresponding ligands in 1:1 ratio with  $\text{Sr}(\text{btsa})_2$  to yield desired complex. This complex was crystallized from the hexane solution upon cooling. The compound was characterized using NMR spectroscopy, FT-IR and Elemental Analysis. The crystals grown from the parent solution were studied by single crystal X-ray diffractometer which reveals that complex crystallized in triclinic space group. The thermo gravimetric analysis was carried out to measure the decomposition character and volatility of the complex.

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발표코드: INOR.P-183

발표분야: 무기화학

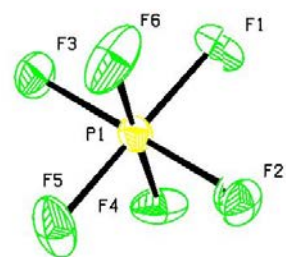
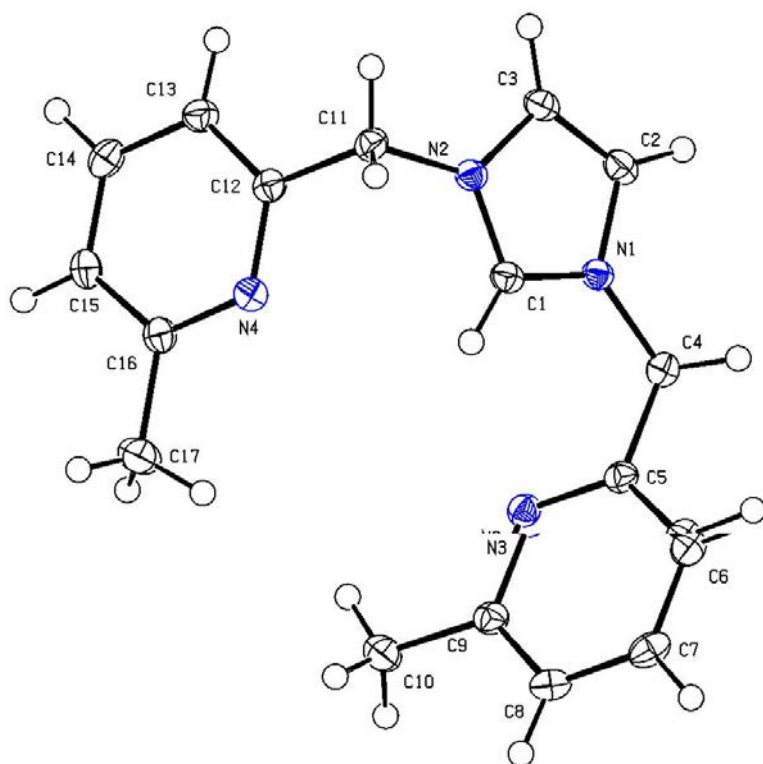
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Carbene Transfer Reactivities of Silver(I)- *N* -Heterocyclic Carbene Complexes

정현진 배호연 이수연 이동현

전북대 화학과

Recently, transition-metal complexes of *N* -heterocyclic carbenes(NHCs) have attained tremendous research interest due to the unique properties of them. Particularly the NHC complexes of Ag(I) are very simple to prepare and frequently utilized as carbene-transfer reagents. Here we report on the syntheses and characterization of silver(I) complex of new pyridine substituted NHC ligands. Silver NHC complexes are very useful precursors for NHC complexes of other metals. The silver complex was synthesized by the treatment of N-heterocyclic chelates, 1,3-bis[(6-methyl-2-pyridyl)methyl]imidazolium hexafluorophosphate and 1,3-Bis[(6-methyl-2-pyridyl)]-imidazolium hexafluorophosphate with Ag<sub>2</sub>O. The molecular structures of the complexes have been elucidated by single-crystal X-ray crystallography. Other NHC-metal complexes have been synthesized by carbene transfer reaction with the corresponding metal precursors.





일시: 2012년 4월 25~27일(수~금) 3일간

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

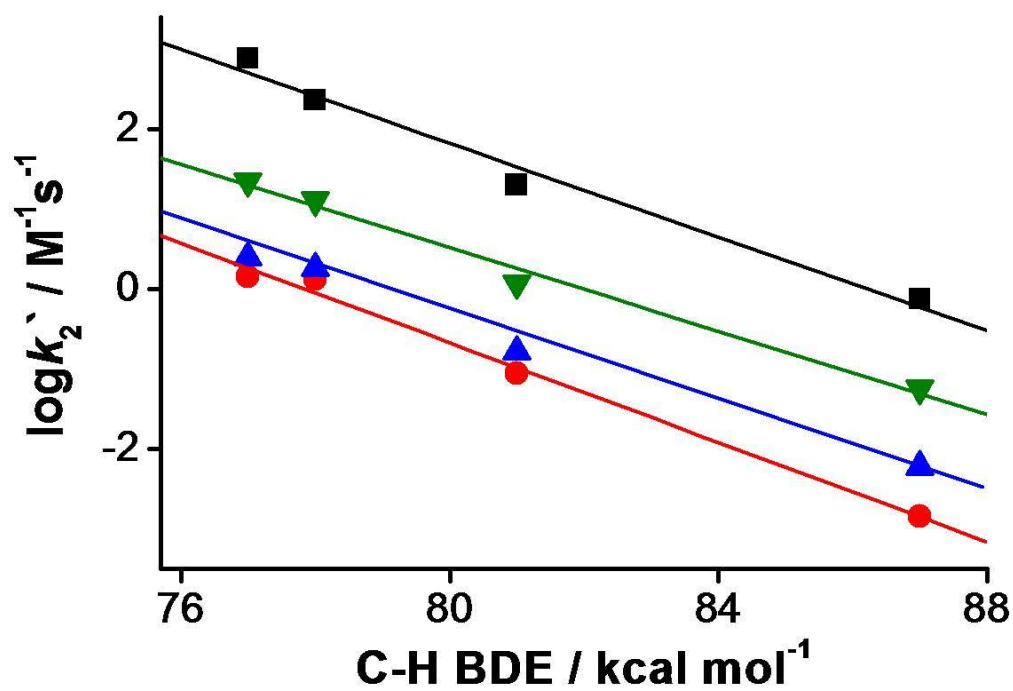
## Reactivity Comparison of Four Nonheme Iron(IV)-Oxo Species in C-H Bond Activation and Electron Transfer Reaction

김은정 서미숙 김진화 Jan-Uwe Rohde<sup>1</sup> 남원우<sup>2</sup>

이화여대 바이오융합과학과 <sup>1</sup>The University of Iowa, Iowa City <sup>2</sup>이화여대 화학과

We have recently reported a highly reactive mononuclear nonheme iron(IV)-oxo complex,  $[(\text{Me}_3\text{NTB})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$  in both C-H bond activation and oxygen-atom transfer reactions. This intermediate is more reactive than iron(IV)-oxo porphyrin  $\pi$ -cation radical (i.e., a model of cytochrome P450, compound I). To date, it has been reported as the most reactive species among synthetic nonheme iron(IV)-oxo complexes and shows extremely low activation barrier in C-H bond activation of cyclohexane according to density functional theory (DFT) studies. To try to pinpoint the underlying factors determining the reaction rate, we have studied the C-H bond activation (Fig 1.) and kinetic isotope effects of four nonheme iron(IV)-oxo complexes,  $[(\text{L})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$  (L =  $\text{Me}_3\text{NTB}$ , L2, L1 and TPA). We also studied electron-transfer (ET) properties to determine the reduction potential of  $[(\text{L})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$  by adapting a series of ferrocene derivatives as one-electron reductants. Fig.1 Plot of  $\log k_2$  of  $[\text{Fe}^{\text{IV}}(\text{O})(\text{Me}_3\text{NTB})]^{2+}$  (■),  $[\text{Fe}^{\text{IV}}(\text{O})(\text{L2})]^{2+}$  (▼),  $[\text{Fe}^{\text{IV}}(\text{O})(\text{L1})]^{2+}$  (▲) and  $[\text{Fe}^{\text{IV}}(\text{O})(\text{TPA})]^{2+}$  (●) against C-H

BDE of substrates. Second-order rate constants,  $k_2$ , were determined at  $-40^\circ\text{C}$  and then adjusted for reaction stoichiometry to yield  $k_2'$  based on the number of equivalent target C-H bonds of substrates.



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발표분야: 무기화학

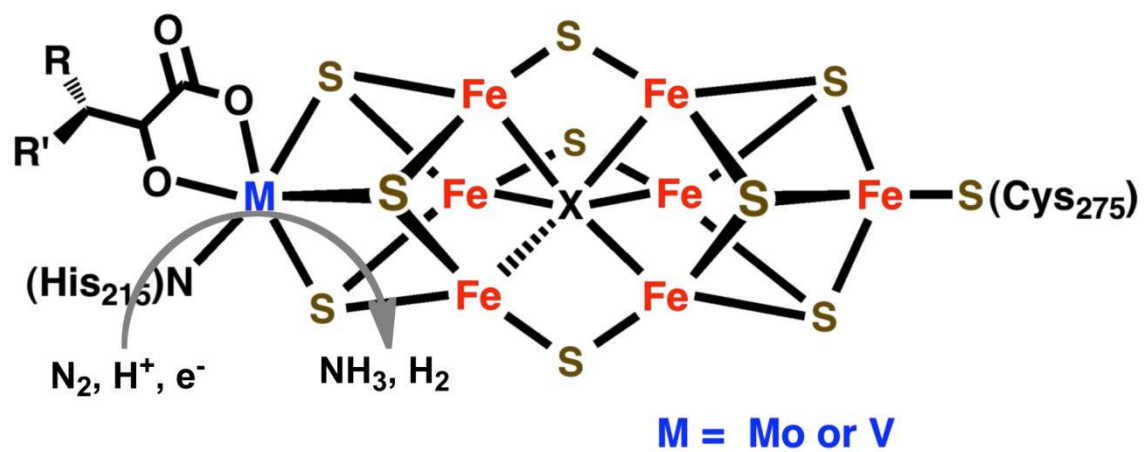
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Vanadium Complexes for Studying the Reduction of Dinitrogen

김진 박고은 유창호 이윤호

KAIST 화학과

Utilization of the 1st row transition metals for developing molecular catalysts is essential in current energy research topics. A specific system for Haber-Bosch process to produce ammonia from dinitrogen and dihydrogen at ambient conditions is a particular interest of our research. A biological dinitrogen fixation catalyzed by nitrogenase enzymes demonstrates a methodology to utilize such transition metals to work on the activation of dinitrogen. We are motivated by the active site chemistry of the enzyme to develop a synthetic catalyst revealing  $N_2$  activation at ambient conditions. We will discuss a series of vanadium complexes supported by tripodal tetradentate  $PEP_2$  ligand ( $E = P$  or  $N$ ) for describing the syntheses, characterization and the reactivity study particularly toward dinitrogen. Tridentate  $PEP$  ( $E = P$  or  $N$ ) vanadium complexes will be also described to compare the reactivity pattern regarding the effects of geometric and electronic variations.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and X-ray Crystal Structure of Zinc(II) and Cadmium(II) Complexes Bearing N, N-bis(1-pyrazolyl)methyl Aniline Derivatives

이효선 김성훈<sup>1</sup> 이하진<sup>2</sup>

경북대 자연과학대학 화학과 <sup>1</sup> 경북대 화학과 <sup>2</sup> 한국기초과학지원연구원 전주센터

Together with the facile and high yielding formation of [Nbpma], [Nbpmmm], and [Nbdpm] ligands, for example, [Nbpma] is N,N-Bis{(1-H-Pyrazole-1-yl)methyl}aniline, a new series of air-stable Zn(II) complexes, [Nbpma]ZnCl<sub>2</sub> (1a), [Nbpmmm]ZnCl<sub>2</sub> (2a), and [Nbdpm]ZnCl<sub>2</sub> (3a) has been synthesized. In addition, the complexation with CdBr<sub>2</sub>·4H<sub>2</sub>O gave very air stable dibromo-bridged binuclear cadmium (II) species, [(Nbpma)Cd(??Br)Br]<sub>2</sub> (1b), mononuclear [Nbdpm]CdBr<sub>2</sub> (2b). All complexes are characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, UV, IR spectroscopy, elemental analysis and X-ray crystallography. Especially, the X-ray structure determination of 1b revealed that the geometry at each cadmium center is best described as trigonal bipyramid with two equivalent half molecules in an overall C<sub>2</sub>-symmetric framework. However, X-ray crystallography of monomeric 2b indicated that it has connecting aniline's nitrogen with cadmium metal center.

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발표코드: INOR.P-187

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Tungsten Precursors for WO<sub>x</sub> Thin Films

여소정 박보근<sup>1</sup> 김창균<sup>1</sup> 정택모<sup>1</sup>

충북대 화학과 <sup>1</sup>한국화학연구원 화학소재연구본부

Tungsten oxide (WO<sub>x</sub>) is an important inorganic material with a number of key properties (electrochromism, photochromism, photocatalysis) that have translated to a diverse range of applications. The monomeric novel tungsten precursors were synthesized from W(N<sup>t</sup>Bu)<sub>2</sub>Cl<sub>2</sub>(py)<sub>2</sub> and bidentate ligands. The new compounds were fully characterized by NMR, IR, and mass spectroscopy, thermogravimetric analysis (TGA), differential thermal analysis (DTA), as well as elemental analysis. It is thought that the compounds are suitable as a CVD/ALD precursor to tungsten-based oxide thin films.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-188

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Novel Indium Sulfide Complexes

박주현 김창균<sup>1</sup> 정택모<sup>1</sup> 박보근<sup>1</sup>

충북대 화학과 <sup>1</sup>한국화학연구원 화학소재연구본부

Metal chalcogenide chemistry is an attractive subject due to intergrating properties of classical electronics, optical and semiconductor materials associated with unique topological structures, and the potential application as catalysts or as superconductors. Indium sulfide is an important material for optoelectronic and photovoltaic application. We have synthesized novel indium precursors for indium sulfide thin films deposition using ALD/CVD process. All compounds have been characterized by means of NMR, FT-IR, elemental analysis, and thermogravimetric analysis (TGA).

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발표코드: INOR.P-189

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **X-ray crystal structures including a three-wing propeller structure and photoluminescence properties of Cu(I) coordination polymers based on N/S mixed ligands**

천상훈 김태호 전영은 김진은

경상대 화학과

N/S mixed donor ligands ( $L^1$ ,  $L^2$ ,  $L^3$ )  $C_{13}H_{19}NS$ ,  $C_{11}H_{17}NS$ ,  $C_{14}H_{15}NS$  are synthesized. Reaction of  $L^1$ ,  $L^2$ ,  $L^3$  with CuI afforded the four types of complexes in stoichiometry (ligand : metal). All ligands yielded 1:1 complexes and  $L^2$  gave a new 3:7 complex. Structures of 1:1 complexes are 1D loop chains with  $Cu_2I_2$  unit, and 3:7 complex looks like three-wing propeller. Structures of coordination polymers were determined by single-crystal X-ray diffraction. TGA/DTA data and photoluminescence spectra were also measured.



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발표코드: INOR.P-190

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of Photoluminescent Cu( I ) Coordination Polymers Based on N/S Doner Ligands with Various Length of Alkyl Chain

김태호 천상훈 전영은 김진은

경상대 화학과

In recent years, copper(I) chemistry has attracted increasing attention because of diverse structures and photophysical properties of the complexes as well as potential applications such as electroluminescent displays. We have explored a number of coordination polymers based on dithioether ligands and  $(\text{CuI})_x$ . As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we synthesized N,S donor ligands,  $L^1$ ,  $L^2$ , and  $L^3$  with various length of alkyl chain to change chemical/physical properties of coordination polymers. Three Cu(I) coordination polymers 1, 2 and 3 based on the ligands were prepared. The polymers are composed of rhomboidal  $\text{Cu}_2\text{I}_2$  nodes, which emit skyblue light. Results of our investigation including syntheses, structural characterization, thermal and photoluminescent properties of three new Cu(I) coordination polymers are presented.

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발표코드: INOR.P-191

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Structures of Photoluminescent Cu( I ) Coordination Polymers Based on N/S Doner Ligands

전영은 김태호 천상훈 김진은

경상대 화학과

N/S mixed donor ligands ( $L^1$ ,  $L^2$ ,  $L^3$ ),  $C_{12}H_{18}N_2S$ ,  $C_{13}H_{11}N_2S$ ,  $C_{10}H_{16}N_2S$  were synthesized. Reaction of the ligands with CuI afforded two types of complexes in stoichiometry (L:CuI=1:1 and 1:2), such as,  $[Cu_2I_2L^1]_n$  (1),  $[CuIL^2]_n$  (2),  $[Cu_2I_2L^2]_n$  (3), and  $[Cu_2I_2L^3]_n$  (4). Structures of the polymers are 2D network structures based on rhomboid  $Cu_2I_2$  clusters. Luminescence spectra of the polymers 1, 3 and 4 exhibit emission peaks at about 603 nm at room temperature. Polymer 2 shows emission peak at 540 nm. TGA and DTA curves show that structural transformations of complexes 1 and 2 occur at 131 °C and 122 °C, respectively.

일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: INOR.P-192

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Alkylmagnesium Amino-alkoxide Complexes as Precursors for MgO

김효숙 박보근<sup>1</sup> 정택모<sup>1</sup> 김창균<sup>2</sup>

성균관대 화학과 <sup>1</sup>한국화학연구원 화학소재연구단 <sup>2</sup>한국화학연구원 화학소재연구본부

Magnesium oxide (MgO) thin films have attracted great scientific and technological interest in recent decades. Because of its distinguished properties such as a wide band gap (7.2 eV), a low dielectric constant (9.8), a low refractive index, an excellent chemical and thermal stability (melting point=2900°C), it is widely used as inorganic material in diverse areas such as fire resistant construction materials, optical materials, protective layers in plasma display panels, buffer layers of multilayer electronic/photonics devices, and perovskite ferroelectric thin films. In this study, magnesium complexes have been synthesized by the reaction of Grignard reagent and aminoalkoxide and characterized by means of NMR spectrometry, FT-IR, and elemental analysis. Their molecular structures were defined by single-crystal diffraction and the thermal properties were studied by thermogravimetric analysis (TGA).

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발표코드: INOR.P-193

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of novel Tantalum precursors using ALD/CVD

신수정 정택모<sup>1</sup> 김창균<sup>2</sup> 박보근<sup>1</sup>

고려대 화학과 <sup>1</sup>한국화학연구원 화학소재연구단 <sup>2</sup>한국화학연구원 화학소재연구본부

Tantalum nitride (TaNx) films have been attractive candidates as a diffusion barrier, gate electrode for capacitors used in memory devices because of their high thermal, mechanical, chemical stability, and good electrical conductivity. Also Tantalum carbo-nitride (TaCN) films have been studied as a gate electrode in the next generation nano-CMOS (complementary metal oxide semiconductor) technology for its low resistivity, proper work function and high reliability. We have synthesized novel Tantalum complexes as precursors for TaN and TaCN thin films using ALD/CVD process. All compounds have been characterized by means of NMR spectrometry, FT-IR, elemental analysis, and TGA.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: INOR.P-194

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design of rigid porous coordination networks

이길령 Yakiyama Yumi Masaki Kawano

포항공과대 첨단재료과학부

Porous coordination network is a class of porous polymeric materials, consisting of metal ions linked by organic bridging ligands. The syntheses of porous coordination networks attracted much attention in terms of many potential applications such as gas storage, catalyst, sensors, ion exchange and drug delivery and so on. Recently, we have newly designed and synthesized a nitrogen-modified hexaazaphenalenyl-based highly symmetrical ligand having three pyridyl groups. Furthermore, we have synthesized several network structures with this ligand and several metal sources. Interestingly, some of them showed unique properties such as epitaxial-like structure transformation. Here, we report the preparation of newly designed ligands having carboxylic groups and its network formation with metal ions.

일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: INOR.P-195

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design 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.

일시: 2012년 4월 25~27일(수~금) 3일간

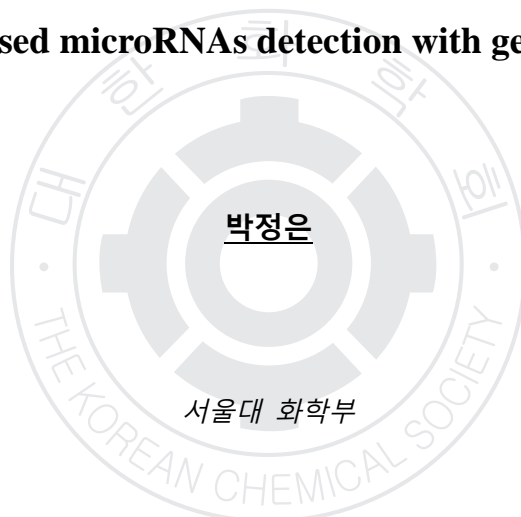
장소: 일산KINTEX

발표코드: INOR.P-196

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Bio-barcode-based microRNAs detection with gel electrophoresis



MicroRNA (miRNA) is a short non-coding RNA, consisting of very few nucleotides, average of 22. A miRNA binds to target messengerRNA (mRNA), resulting in translational repression or target degradation. Thus, they can act as negative gene regulators. Several miRNAs have been found to related with various types of diseases, especially cancer and diabetes. The most widely used miRNA detection method is Northern blotting, which is considered as the standard of miRNA detection methods. This method, however, is time-consuming and has low sensitivity. For theses reasons, we developed the miRNA detection method which is simple, fast, and sensitive, "double-helix bio-barcode assay with gel electrophoresis". We chose three different miRNAs as lung cancer biomarker. Using magnetic microparticle and gold nanoparticle, we detected these miRNAs in one solution. Based on this bio-barcode method, non-enzymatic, cost-effective and multiplexed detection of target miRNAs could be possible with a conventional gel electrophoresis platform.

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장소: 일산KINTEX

발표코드: INOR.P-197

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Comparison of Cu(II)-TTF Complexes: One with [2,6-bis(carboxyl)tetrathiafulvalene] and One with [2,7-bis(carboxyl)tetrathiafulvalene]**

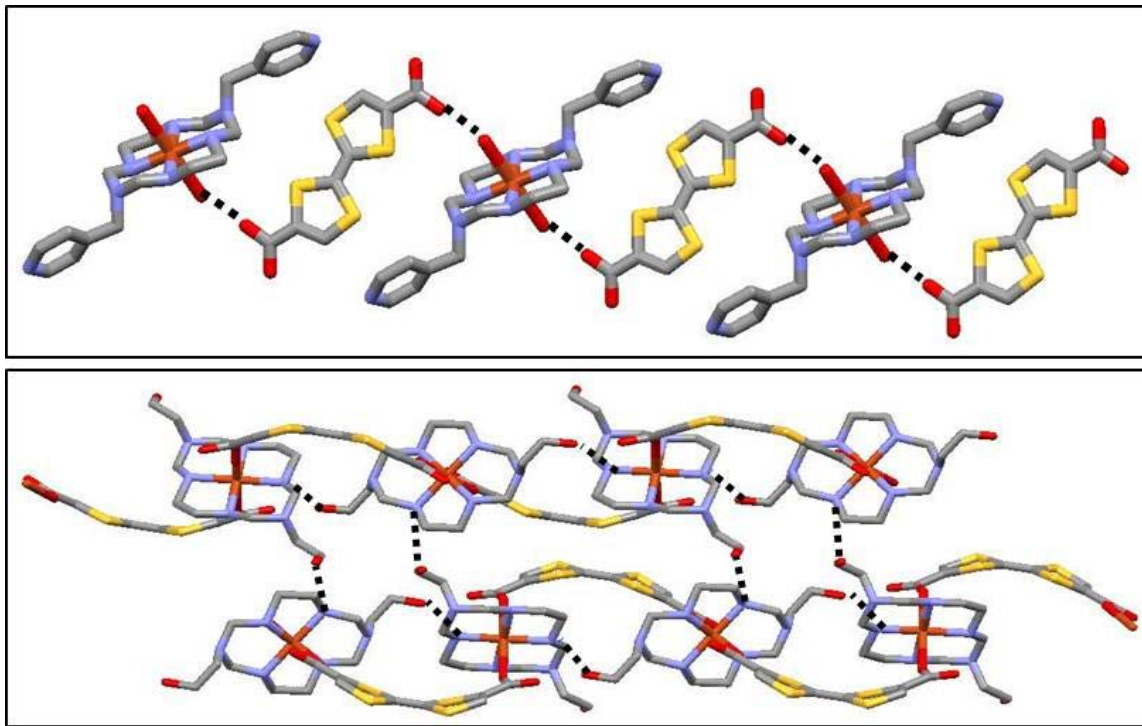
이주은 이홍인

경북대 화학과

Metal complexes containing TTF (tetrathiafulvalene) exhibit interesting electric and magnetic properties. In the line of searching the bond-forming ability between transition metal ions and carboxylate-functionalized TTF derivatives, we have synthesized copper(II) complexes with hexaaza-macrocyclic ligands, one with pyridine functional groups (L1) and the other with OH functional groups (L2), and compared their abilities of forming complexes with two carboxylate-functionalized TTF isomers, *trans*-2COO-TTF [2,6-bis(carboxyl)tetrathiafulvalene] and *cis*-2COO-TTF [2,7-bis(carboxyl)tetrathiafulvalene]. X-ray crystallographic studies found that Cu(II)(L1) and *trans*-2COO-TTF gave a 1-dimensional chain through the hydrogen bonds between the axial water ligand of Cu(II)(L1) and *trans*-2COO-TTF. In case of Cu(II)(L2) and *cis*-2COO-TTF, *cis*-2COO-TTF bridges two Cu(II)(L2) to form a 1-dimensional coordination polymer. This coordination polymer is further



extended to a 2-dimensional sheet through the hydrogen bonds between the hydroxyl oxygens and the nitrogens of the macrocyclic ligands of the adjacent 1-dimensional coordination polymer. In this poster, we discuss the characteristics of the complexes investigated by various analytical methods including X-ray crystallography, EA (Elemental Analyzer), EPR (Electron Paramagnetic Resonance), IR, and MPMS.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, luminescence, and magnetic properties of transition metal compounds with organic ligand including 4,4'-dipyridylamine units

신종원 김승휘 민길식<sup>1</sup>

경북대 화학과 <sup>1</sup> 경북대 사범대학 화학교육과

New supramolecular solids whose topologies depend on the cation and counterion  $[L_{0.5}Zn_{0.5}(H_2O)_{0.5}](NO_3) \cdot 6H_2O$  (1),  $[L_{0.5}Cd_{0.5}(H_2O)](NO_3) \cdot 2H_2O \cdot 2CH_3OH$  (2),  $[LCu(CH_3COO)_2] \cdot 1.5CH_3OH$  (3), have been prepared by the self-assembly of  $MX_2$  ( $M = Cd, Zn, Cu$ ,  $X = NO_3^-, CH_3COO^-$ ) with *N,N,N',N'*-tetra-4-pyridyl-methaneamine (L, t4p). Compounds 1 and 2 display three-dimensional brick-like coordination polymers due to the geometry of metal (Zn and Cd) ions with four pyridine groups in t4p ligand, while compound 3 shows one dimensional helical chain structure along the a axis because one pyridine group did not bind to adjacent copper(II) ion. 1 exhibits a blue color luminescence under the UV-Vis lamp, whereas 2 do not show the luminescence in the same condition. In this poster, we will present the detailed preparation of the ligand and metal compounds, crystal structure, magnetic properties, and luminescent behaviors.

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발표코드: INOR.P-199

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Selective encapsulation of meta-stable sulfur by porous coordination network and its structure analysis with powder X-ray diffraction

최완욱 Hiroyoshi Otsu Masaki Kawano

포항공과대 첨단재료과학부

Porous coordination network has been used for many studies such as gas separation/storage, catalysis, molecular recognition, conductivity, and so on. However, the usage of pores for chemical reaction is still under development. Especially there is no example of trapping unique reactive species in a porous material based on clear structural evidences. Elemental sulfur has many reactive unstable allotropes like S<sub>6</sub> and S<sub>7</sub>. Therefore, we investigated sulfur encapsulation to the porous network system. We succeeded in trapping an unprecedented small unstable sulfur compound in the network by gas phase diffusion to the porous coordination network. Nevertheless, this sulfur allotrope is usually unstable, porous coordination network allowed this compound can be stable in ambient condition because of a pore effect. The structure of encapsulated sulfur was determined by ab initio XPRD analysis, and characterized by elemental analysis and TG-DSC. Moreover, the chemical reactivity of encapsulated sulfur with acetylene gas was investigated.

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장소: 일산KINTEX

발표코드: INOR.P-200

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

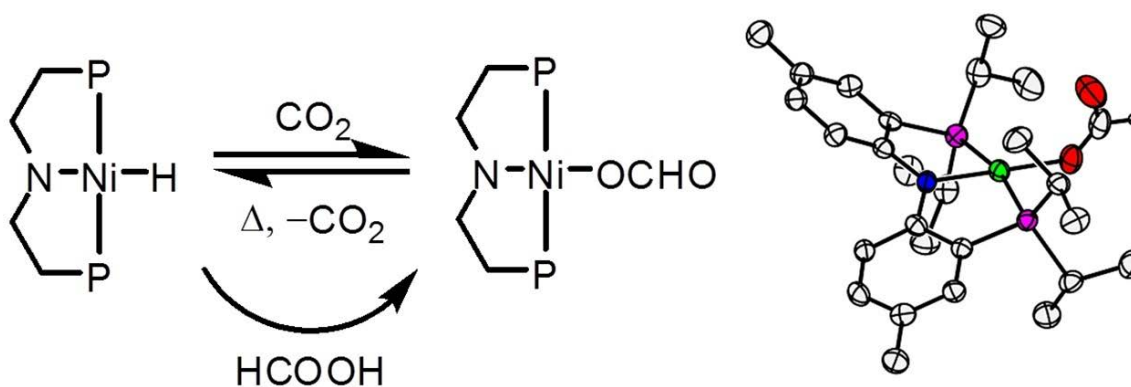
## CO<sub>2</sub> activation on a PNP Nickel center

유창호 방현석 김진 이윤호

KAIST 화학과

Activation of CO<sub>2</sub> is a one of the crucial research topics in terms of reducing one of the greenhouse gases and utilizing carbon dioxide as an abundant and cheap C1 source for various chemicals and fuel. In nature, carbon dioxide is captured and utilized by a biological process known as CO<sub>2</sub> fixation. Especially, some microbes such as *Rhodospillum Rubrum* manipulate CO<sub>2</sub> to produce CO catalyzed by CODH; Carbon monoxide dehydrogenase. Recently, X-ray crystal structure of CODH reveals the nature of the active site where CO<sub>2</sub> is located in a nickel center in square planar environment. Thus, studying nickel complex in square planar geometry can be fine strategy for activating CO<sub>2</sub>. Meanwhile, PNP pincer ligand has been reported to form square planar geometry with nickel. Here, Activation of carbon dioxide has been explored with [PNP]NiH species utilizing tridentate amidodiphosphino pincer ligand (PNP = N[2-P(CHMe<sub>2</sub>)-4-methylphenyl]<sub>2</sub>). At ambient condition, [PNP]NiH reacts with CO<sub>2</sub> to give nickel formate complex, which was separately prepared by the reaction of [PNP]NiH with formic acid. Another nickel

complex with a tetradentate ligand,  $\text{NP}_3 = \text{N}[2\text{-P}(\text{CHMe}_2)\text{-4-methylphenyl}]_3$ , will be also discussed for describing the synthesis and reactivity toward carbon dioxide.



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장소: 일산KINTEX

발표코드: INOR.P-201

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Tin Precursors for SnO<sub>2</sub>Thin Films Deposition

정은애 박보근 김창균 정택모

한국화학연구원 화학소재연구본부

The wide variety of electronic and chemical properties of metal oxides makes them exciting materials for basic research and for technological applications alike. 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 structures of the compounds were studied by single crystal diffraction.

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장소: 일산KINTEX

발표코드: INOR.P-202

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Regioselective Edge Effect of 2-Dimensional Layered Nanocrystals

정소희 천진우

연세대 화학과

Properties of nanoscale materials can heavily depend on the local environments, especially for 2-dimensional layered nanomaterials such as transition metal chalcogenide (TMC) and graphene. For example, the electronic structures of graphene nanodevice are experiencing significant influence from the edge structures. We have discovered that an external stimulus can trigger selective chemical transformation phenomena in 2-D layered nanomaterials. These transformations are characteristically driven by the 2-D anisotropy of these layered materials. The regioselective edge reactions, hetero-epitaxial transformative growth and ion migration generate a centrally void single crystalline, double-convex toroidal nanocrystal. The unique anisotropic characteristics of the 2-D layered nanocrystal are the key for this unusual chemical transformation. This phenomenon seems to be general as we observe similar transformative processes in the presence of other cation stimuli. The principles of using 2-D layered templates for building toroidal nanocrystals seem to be broadly applicable.

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발표코드: INOR.P-203

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Structural Studies of Metal(II)-Dicarboxylate Complexes with 1,10-phenanthroline

구본권

대구가톨릭대 생명화학과

Three new metal(II) complexes,  $[\text{Mn}(\text{dpa})(\text{phen})(\text{H}_2\text{O})_2]_n$  (1) (dpa = dephenate, phen = 1,10-phenanthroline),  $[\text{Ni}_2(\text{nda})(\text{phen})_2(\text{H}_2\text{O})_6](\text{nda})(\text{H}_2\text{O})$  (2) (nda = 2,6-naphthalene dicarboxylate), and  $[\text{Ni}_2(\text{dpa})(1,10\text{-phen})_2(\text{H}_2\text{O})_6](\text{dpa})(3)$ , have been synthesized and characterized by elemental analysis, infrared spectroscopy, thermogravimetric analysis, and single crystal X-ray diffraction. In complex 1, Mn(II) ion is six-coordinated, and Mn(II) ions are bridged by dpa ligands into 1D chains. Both complexes 2 and 3 are dimers and two Ni(II) ions are bridged by one nda/dpa ligand cooperated with the terminal ligand phen. In each complex, the dicarboxylate ligand is coordinated to metal(II) ions as a bismonodentate.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Solution processable using fluorinated small molecule in organic solar cell

백상현 조나라 임남우<sup>1</sup> 이재관<sup>2</sup> 고재중

고려대 소재화학과 <sup>1</sup>고려대 세종캠퍼스 소재화학과 <sup>2</sup>조선대 화학교육학과

Organic solar cells (OPV) have been widely investigated recently due to their potential for light-weight, low-cost, and large-scale roll-to-roll processing. Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. Solution processable small molecule-based donor material has been also attempted as attractive alternative of donor in organic solar cell due to its facile synthesis, purification, and low batch-to-batch variation compared to polymeric materials. Here, we designed and synthesized three compound using fluorinated benzothiadiazole moiety in small molecule organic solar cells. The difluorinated compound gave high efficiency of 4.35% with a short circuit photocurrent density (Jsc) of 10.76, an open circuit voltage (Voc) of 0.9, a fill factor 0.45.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Efficient Small Molecule Photosensitizer containing Bis-dimethylfluorenyl Amino Benzo[b]thiophene for High Open Circuit Voltage in High Efficiency Solution Processed Organic Solar Cell**

**김주영 임기민 임남우<sup>1</sup> 이재관<sup>2</sup> 고재중**

고려대 소재화학과 <sup>1</sup>고려대 세종캠퍼스 소재화학과 <sup>2</sup>조선대 화학교육학과

Solution processed organic solar cells (OSCs) fabricated by means of versatile printing techniques such as doctor blade, inkjet, and roll-to-roll can provide the most attractive advantages of device such as low cost, light weight, solution processability. To now, solution processed small molecule organic solar cells (SMOSCs) based on small molecule photosensitizer and PCBM BHJ materials have exhibited promising PCEs of above 6 % as attractive alternatives to polymer solar cell (PSC). In this paper, the new small molecule photosensitizer, bisDMFA-BTTh-MMN having benzothiophene donor moiety exhibited the high power conversion efficiency of 4.01% with high open circuit voltage of 0.95 V in solution processed small molecule organic solar cells.

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발표코드: INOR.P-206

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Correlating the photovoltaic performance of alumina modified dye-sensitized solar cells with the properties of metal-free organic sensitizers

최혜주 김철우 백상현 고재중

고려대 소재화학과

Low photovoltage for metal-free organic dye-sensitized solar cells (DSSCs) has been restricting them surpassing the equivalent cells based on ruthenium complex sensitizers (typically N719). In this study, an alumina ( $\text{Al}_2\text{O}_3$ ) layer was employed to cover on the titania ( $\text{TiO}_2$ ) surface before dye loading in order to improve the photovoltage of the organic dye based DSSCs. The open-circuit voltage ( $V_{oc}$ ) of the solar cell was found to increase by 0.02~0.06 V for a variety of organic sensitizers by the presence of the  $\text{Al}_2\text{O}_3$  overcoat, while the photocurrent ( $J_{sc}$ ) was observed highly dependent on the property of the sensitizer. Results show that for the sensitizers with a low Low-Unoccupied-Molecular-Orbital (LUMO) level or a large molecular size, the DSSC yielded a decreased  $J_{sc}$  due to two factors, (i) an insufficient driving force for electron injection due to the upshift of the conduction band level of the  $\text{TiO}_2/\text{Al}_2\text{O}_3$  electrode, and (ii) a decrease of dye adsorption amount for the  $\text{TiO}_2/\text{Al}_2\text{O}_3$  electrode in comparison with

the referenced TiO<sub>2</sub> electrode because of the reduced pore size and porosity by Al<sub>2</sub>O<sub>3</sub> coating. However, for the sensitizers with a high (more negative) LUMO level and a small molecular size, the J<sub>sc</sub> of the DSSCs based on the TiO<sub>2</sub>/ Al<sub>2</sub>O<sub>3</sub> electrode was very close to that composed of only TiO<sub>2</sub> electrode. Using such organic dyes sensitizing on the TiO<sub>2</sub>/ Al<sub>2</sub>O<sub>3</sub> electrode, over 8% in the efficiency of the DSSCs was easily attained and particularly an efficiency of 8.72% was obtained for a cocktail solar cell with two organic dyes.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Push-Pull Organic Semiconductors Comprising of Bis-dimethylfluorenyl Amino Benzo[b]thiophene Donor and Nitro Acceptor for Solution Processed Small Molecule Organic Solar Cells**

송주만 조나라 임남우<sup>1</sup> 이재관<sup>2</sup> 고재중

고려대 소재화학과 <sup>1</sup>고려대 세종캠퍼스 소재화학과 <sup>2</sup>조선대 화학교육학과

Solution processed organic solar cells (OSCs) 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 (BHJ) materials comprising of low-bandgap semiconducting polymers and [6,6]-phenyl-C61 (or 71)-butyric acid methyl ester (C61 (or 71)-PCBM). New efficient push-pull organic semiconductors comprising of the bis(9,9-dimethyl-9H-fluoren-2-yl)aniline (bisDMFA) and the N,N-(6-bis(9,9-dimethyl-9H-fluoren-2-yl)amino-benzo[b]thiophen (bisDMFABT) as electron donor having nitro acceptor were easily synthesized. And their photovoltaic characteristics were investigated in solution processed small molecule organic solar cells (SMOSCs). The organic semiconductor having NO<sub>2</sub> acceptor exhibited

the best power conversion efficiency of 2.70 % with short circuit current of 8.19 mA/cm<sup>2</sup>, fill factor of 0.40, and open circuit voltage of 0.83 V in SMOSC devices with TiO<sub>x</sub> thin layer.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Facile Synthesis of Fluorine-Substituted Benzothiadiazole-Based Organic Semiconductors and Its Use in Solution Processed Small Molecule Organic Solar Cell**

**조나라 김주영<sup>1</sup> 김철우 이재관<sup>2</sup> 고재중**

고려대 소재화학과 <sup>1</sup>고려대 화학과 <sup>2</sup>조선대 화학교육학과

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-C<sub>61</sub> (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. This fluorine atom often affords its unique features that when integrated into bulk heterojunction composite with PCBM boost the intermolecular charge transfer through C-F-H interaction, affecting the performance characteristics. For these reasons, we have interested in the more reinforced ICT from small molecule organic semiconductor through substitution of electron withdrawing atom,

especially fluorine onto the efficient push-pull semiconductor backbone for solution processed small molecule organic solar cell. A facile new synthetic protocol for the iodinated compounds of the fluorinated benzothiadiazole was successfully performed as key step to produce the fluorinated benzothiadiazole motifs. And these fluorinated benzothiadiazole-based organic semiconductors, bis[TPA-diTh]-MonoF-BT and bis[TPA-diTh]-DiF-BT as efficient p-type organic semiconductor exhibited the power conversion efficiency of 2.95 % with high open circuit voltage of 0.85 V in solution processed small molecule organic solar cell.





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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Spherical polypyrrole nanoparticles as a highly efficient counter electrode for dye-sensitized solar cells

김철우 도광석 고재중

고려대 소재화학과

Discrete spherical polypyrrole (PPy) nanoparticles with a uniform diameter of 85 nm and electrical conductivity of  $10 \text{ S cm}^{-1}$  were fabricated by chemical oxidative polymerization within micelles composed of myristyl trimethyl ammonium bromide (MTAB) and decyl alcohol as the nanoreactors. A methanol-based colloidal dispersion containing 5 wt% PPy was dropcast directly onto fluorine-doped tin oxide (FTO) glass to use as counter electrodes (CEs) in dye-sensitized solar cells (DSSCs). The surface resistivity of the PPy layer on the FTO glass decreased from 624 to  $387 \text{ } \Omega \text{ sq}^{-1}$  after post-doping with concentrated HCl vapor for 1 min. The DSSCs made of PPy/FTO and HCl-doped PPy/FTO CE exhibited power conversion efficiencies of 5.28 and 6.83%, respectively under standard AM 1.5 sunlight illumination. The post-doped and highly oxidized PPy allowed the electrons to move into the PPy layer readily and facilitated the electrocatalytic reaction of the

I3 —————/I ————— redox couple, giving enhanced cell performance. Moreover, the cell efficiency was enhanced to 7.73% with further fine tuning of the electrolyte composition, which is comparable to the value (8.2%) using conventional Pt CEs.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New type of organic sensitizers with a planar amine unit for efficient dye-sensitized solar cells

도광석 김철우 임기민 임남우<sup>1</sup> 고재중

고려대 소재화학과 <sup>1</sup>고려대 세종캠퍼스 소재화학과

Novel organic sensitizers comprising donor, electron-conducting, and anchoring groups were engineered at a molecular level and synthesized for sensitization of mesoscopic titanium dioxide injection solar cells. The organic sensitizers JK-72, JK-97, and JK-98 anchored onto TiO<sub>2</sub> and were tested in dye-sensitized solar cell with a volatile electrolyte. The monochromatic incident photon-to-current conversion efficiency of these sensitizers is above 85%, and JK-98-sensitized solar cells yield a short-circuit photocurrent density of 16.78 mA/cm<sup>2</sup>, an open-circuit voltage of 745 mV, and a fill factor of 0.70, corresponding to an overall conversion efficiency of 8.71% under standard AM 1.5 sun light. This result is affected by the suppression of dark current owing to the blocking effect of a long alkyl chain at donor.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, structure and luminescence properties of silver(I) complexes with *N,N,N',N'*-tetra-4-pyridyl-methaneamine (t4p)

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경북대 화학과 <sup>1</sup> 경북대 사범대학 화학교육과

Novel supramolecular solids whose topologies depend on the counteranions, [Ag(t4p)](NO<sub>3</sub>)·CH<sub>3</sub>OH (1) and [Ag(t4p)](CF<sub>3</sub>COO)·CH<sub>3</sub>OH (2), have been prepared by the self-assembly of AgX (X = NO<sub>3</sub><sup>-</sup>, CF<sub>3</sub>COO<sup>-</sup>) with *N,N,N',N'*-tetra-4-pyridyl-methaneamine (t4p). Compound 1 displays three-dimensional brick-like coordination polymer due to the geometry of silver(I) ions connected with four pyridines of t4p, while compound 2 shows two-dimensional framework structure with honeycomb motif along the *ac* plane. 1 exhibits a strong visible light emission ranging from violet to red wavelengths, whereas 2 shows a strong violet emission at around 390 nm and a weak visible emission at around 490 nm. In this poster, the detailed preparation of t4p ligand and compounds, crystal structure and luminescence properties will be described.

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## Distribution Pattern of Length, Length Uniformity, and Density of $\text{TiO}_3^{2-}$ quantum wire in an ETS-10 Crystal Revealed by Laser-Scanning Confocal Polarized Micro-Raman Spectroscopy

최도영 Shuvo Jit Datta<sup>1</sup> 윤경병

서강대 화학과 <sup>1</sup>서강대 나노물질연구소

ETS-10 is a molecular sieve which contains  $\text{TiO}_3^{2-}$  quantum wires (QWs) running along the [110] and [1-10] directions, respectively. Due to a large number of inherent defects, the lengths and local densities of  $\text{TiO}_3^{2-}$  QWs are expected to vary significantly within the crystal interiors. However, there have been no methods to analyze the distribution pattern of their relative lengths, length homogeneities, and local densities within a crystal. In this work we will present that the laser scanning confocal polarized micro-Raman (LSC-PMR) spectroscopy is a highly useful tool for the analysis of the distribution pattern of the length, length uniformity, and density of the  $\text{TiO}_3^{2-}$  quantum wire within a crystal, and the novel fact that the above three physical values are not evenly distributed within the crystals but distributed in a symmetrical manner according to an interesting pattern. LSC-PMR will also serve as a very useful tool for the elucidation of many important features of other zeolites and zeolite-encapsulated molecules.

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## Chiral imprinting of helical graphene nanotube by using helical silica nanotube as a template

문승진 안진호 정성호 정종화

경상대 화학과

The single layered sheet of the graphene(SSG) was prepared by Hummer method. To prepare chiral structure of the graphene, the chiral silica nanotubes were used as a template. SSG was immobilized onto the silica nanotubes by the electrostatic interaction. SSG immobilized silica nanotubes(SSG-SNT) were characterized by SEM, TEM, AFM and FT-Raman. According to TEM and SEM observations, SSG were well-immobilized onto the silica nanotube. SNT@SSG was observed the chirality in the presence of organic compound. The right handed SNT@SSG showed the right helicity with the organic compound. Whereas the left handed SNT@SSG showed the left helicity with the organic compound.

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## Chemosensor of Salicylimine-based Fluorophore for Aluminum Ions and Application to Bioimaging

김수진 강희경 노진영<sup>1</sup> 김철<sup>2</sup> 김진흥

이화여대 화학·나노과학과 <sup>1</sup>서울과학기술대 정밀화학과 <sup>2</sup>서울과학기술대 정밀화학과 친환경  
소재제품센터

In this study, an assay to quantify the presence of aluminum ions using a salicylimine-based receptor was developed utilizing turn-on fluorescence enhancement. Upon treatment with aluminum ions, the fluorescence of the sensor was enhanced at 510 nm due to the formation of a 1:1 complex between the chemosensor and aluminum ions at room temperature. As the concentration of  $\text{Al}^{3+}$  was increased, the fluorescence gradually increased. Other metal ions, such as  $\text{Na}^+$ ,  $\text{Ag}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Hg}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Fe}^{3+}$ , and  $\text{In}^{3+}$ , had no such significant effect on the fluorescence. In addition, we show that the probe could be used to map intracellular  $\text{Al}^{3+}$  distribution in live cells by confocal microscopy.

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## Visible Light-Driven Photochemical Production of NADH Using Cobaloxime Catalysts

이정하 김수진 김진홍

이화여대 화학·나노과학과

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  $\text{NAD}^+$  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,  $\text{NAD}^+$ , 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  $\text{CO}_2$  was carried out in the presence of formate dehydrogenase using the NADH photochemically generated using the cobaloxime/eosin/TEOA system.



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## Electrocatalytic Oxidation of Oligonucleotides Adsorbed on Different Sized Au Nanoparticles

Wu Qiong 강희경 Nie Xiaohui 김진흥

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  $\text{Ru}(\text{bpy})_3^{2+}$  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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## Indium Coordination Polymer particles of 1,2-Bis(5-carboxy-2-methylthien-3-yl)cyclopentene

소혜경

연세대 화학과

Metal-organic coordination polymer particles (CPPs) constructed by metal centers and various organic linkers has been produced with gas storage, selective separation, magnetic and nonlinear optical characters. Recently, the development of photoresponsive materials based on metal-organic CPPs complexes has attracted increasing attention. Photochromic materials give a reversible color change in response to light irradiation. The aim of this study is synthesis of Indium coordination polymer particles constructed by Indium and 1,2-Bis(5-carboxy-2-methylthien-3-yl)cyclopentene and analysis of properties by control of shapes and sizes.

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## Syntheses of Porous Aromatic Frameworks

강은영 오유진 노경규<sup>1</sup> 노영수 김자현

숭실대 화학과 <sup>1</sup>숭실대

A Porous Aromatic Framework (PAF), PAF-1 is synthesized from tetrakis(4-bromophenyl)methane(TBPM) by a Yamamoto-type Ullmann C-C coupling reaction, and its surface area is greater than 4000 m<sup>2</sup>/g. Despite our repeated trials at different reaction conditions, the products resulted in reduced BET surface areas smaller than 3300 m<sup>2</sup>/g, which is ascribed to difficulties in removing Ni metal particles completely from the products. A Suzuki-Miyaura reaction also worked for the synthesis of PAF-1 through cross-coupling of tetrakis(4-bromophenyl)methane and tetrakis(4-phenylboronic acid pinacol ester)methane. Although the produced amorphous powder gave a much smaller surface area (630 m<sup>2</sup>/g), the cross-coupling method seems to be more suitable for making other PAFs based on our further exploration of expanded tetrahedral building units.

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## **Anisotropic Photoluminescence in uniformly oriented Fluorophore-Incorporating zeolite-L crystals by contact sliding method**

최성은 이진석

숙명여대 화학과

Development of the methods to organize zeolite microcrystals into uniformly aligned monolayers on various substrates have been pursued viewing microparticles as a novel class of building blocks. It is therefore necessary to develop methods for organizing them into larger organized entities and to explore practical applications of the organized entities. Here, we present a new and simple strategy for the alignment of hexagonal columnar zeolite L crystals by using contact sliding method. Line patterned PR/Si wafer were used as substrates. The use of patterned PR/Si has also an advantage since the PR layer can be removed after assembly of zeolite crystal without disassemble of zeolite crystals. Suspension of fluorophore-containing zeolite crystals was dropped on the patterned PR/Si substrate and slide glass was located top of patterned PR/Si substrate. When the slide glass was slowly slid, fluorophore-containing zeolite crystals were aligned parallel to substrate along the pattern. Depend on the width of line pattern,

degree of alignment was changed and the photoluminescences of the monolayers of aligned zeolite crystals are highly anisotropic.



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## Effect of a Surfactant to the Hydrothermal Synthesis of CdS Sub-micrometer Spheres

강수민 전영진

건국대 응용화학과

The morphological control of semiconductor nanomaterials has been extensively carried out because semiconductor nanomaterials exhibit many interesting properties which originate from their shape and size. As reported before, we successfully synthesized submicrometer-sized CdS particles under hydrothermal condition by judicious choice of reaction conditions such as solution pH. However, in order to obtain the CdS particles with narrow size distribution, it requires rather long time, i.e., 3d. Therefore, we used a nonionic surfactant, Pluronic F127 to shorten the reaction time. The synthesis, reaction condition, and detailed characterization by using various spectroscopic techniques will be presented.

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## Synthesis of Mesoscale Metal Chalcogenide Nanoparticles from Selenium Templates

박세호 송현준<sup>1</sup> 박준택<sup>2</sup>

KAIST 화학과 <sup>1</sup>KAIST 화학과 <sup>2</sup>한국기초과학지원연구원 원장실

We studied that meso-sized Ag<sub>2</sub>Se nanoparticles could be synthesized by controlling Se precursors at low temperature (263 K) and the cation exchange reactions were used as generic approach to transform Ag<sub>2</sub>Se to CdSe, ZnSe and PbSe nanoparticles. Recently, many studies in this area focused on selenium particles over 100 nm or less than 10 nm in size because Se templates tend to crystallize and grow up into nonspherical shapes. In this study, the use of viscous ethylene glycol (EG) allowed for leading to monodispersed particles and poly(vinyl pyrrolidone) (PVP) was added to prevent any possible agglomeration. A solution of SeCl<sub>4</sub> and PVP in EG was introduced to NaBH<sub>4</sub> solutions at 263 K. NaBH<sub>4</sub> solutions were used to reduce Se<sup>+</sup> to Se precursors. And then the reaction vessel was quickly transferred into an oil bath heated at 333 K. When AgNO<sub>3</sub> solutions were added, Ag<sup>+</sup> was reduced to Ag by NaBH<sub>4</sub>. Synthesized Ag was easily reacted with Se precursors, and Ag<sub>2</sub>Se nanoparticles were produced. Cation exchange reactions were used to synthesize CdSe, ZnSe and PbSe from mesoscale Ag<sub>2</sub>Se nanoparticles.

The products were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and UV-Vis spectroscopy. The results of XRD and TEM analyses demonstrated that the products were spherical in mesoscale with orthorhombic (Ag<sub>2</sub>Se), hexagonal (CdSe, ZnSe), and cubic (PbSe) structures. This approach for Ag<sub>2</sub>Se, CdSe, ZnSe and PbSe nanoparticles is efficient and simple to synthesize mesoscale metal calcogenide nanoparticles from selenium templates.





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## Synthesis of $\text{Cu}_2\text{ZnSnS}_4$ nanoparticles through a simple sonochemical method

송미연 정원목 이원영 김항근 심일운

중앙대 화학과

$\text{Cu}_2\text{ZnSnS}_4$ (CZTS) has attracted much attention as a potential photovoltaic material because of its excellent properties. CZTS have suitable band gap energy of 1.4-1.5eV and large absorption coefficient. Synthesis of CZTS nanoparticles through a simple sonochemical method were tried in various solvents under the multibubble sonoluminescence (MBSL) conditions. For the their thipycal synthesis, we used  $\text{CuCl}_2$ ,  $\text{ZnCl}_2$ ,  $\text{SnCl}_2$ , and TAA(thioacetamide). Methanol was used as solvent. Prepared  $\text{Cu}_2\text{ZnSnS}_4$  nanoparticles were examined by XRD, ICP, UV-vis spectrophotometer, and HR-TEM.

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**In-situ generation of a well-dispersed MWCNTs / syndiotactic polystyrene composite using pentamethylcyclopentadienyltitanium trimethoxide anchored to MWCNTs**

고민정 이휘현 박가현 김영조<sup>1</sup> 이준승

전남대 화학과 <sup>1</sup>충북대 화학과

A wall-dispersed multiwall carbon nanotube/ syndiotactic polystyrene composite was prepared by simple in-situ polymerization of styrene using pentamethylcyclopentadienyltitanium trimethoxide attached to the shortened and functionalized MWCNT(f-MWCNT).  $\text{Cp}^*\text{Ti}(\text{OMe})_3$  attached to pristine MWCNT in the presence of methylaluminoxane(MAO) did not produce PS, whereas  $\text{Cp}^*\text{Ti}(\text{OMe})_3$  attached to f-MWCNT showed a high catalytic activity for the syndiospecific polymerization of styrene under the same polymerization conditions.

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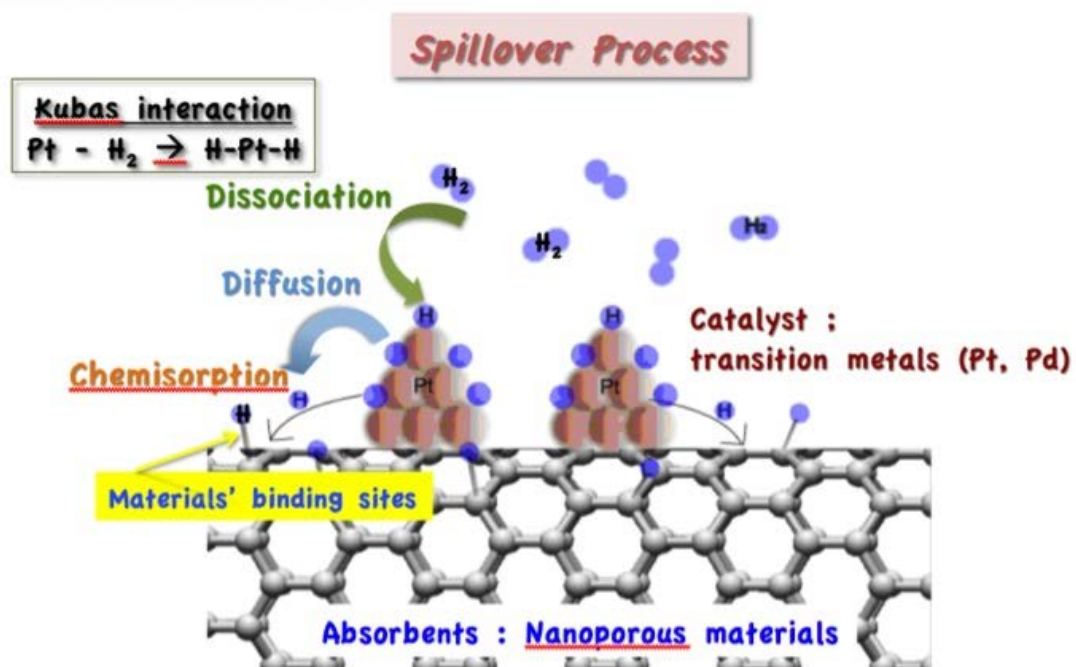
## Investigation of the Hydrogen Spillover in Pt-sputtered Zeolites

이희주 조인화<sup>1</sup> 강승기<sup>1</sup> 최용남 윤경병<sup>2</sup>

한국원자력연구원 중성자과학연구부 <sup>1</sup>한국원자력연구소 중성자과학연구부 <sup>2</sup>서강대 화학과

Hydrogen storage is still a bottleneck for the utilization of hydrogen as an energy source for fuel-cell vehicles. Sorption in solid sorbents via physisorption or chemisorption pathways is being extensively investigated. Nevertheless, no material or method has been able to satisfy the gravimetric uptake target set by DOE, which is 6wt% for 2010. One of the most promising pathways for hydrogen adsorption utilizes the so-called spillover mechanism. A very important attribute of this mechanism is that it is operative at ambient temperature as opposed to storage of H<sub>2</sub> by physisorption, which requires very low temperatures. However, despite decades of studies and applications of the spillover effect in the catalysis field, the root of reason of controversy of spillover process in the research community is that the spillover mechanism in hydrogen storage materials is still very poorly understood. One fundamental assumption of the spillover mechanism is that hydrogen molecules can be dissociated by the doped metal cluster (Pd, Pt) on the absorbnt [MOFs, zeolites, carbon materials], and the resulting hydrogen atoms can diffuse away from the metal clusters and bind to the surface of the porous materials as shown Fig. 1. In this study, in-situ

neutron diffractions were carried out to investigate the hydrogen spillover of two kinds of Pt-sputtered zeolites, a cation rich system (Na-X > Na-Y) and the opposite system (ZSM-5), by measuring the diffraction patterns at 4 K. To support these data, we measured the inelastic neutron scattering (INS) and spectra at same sample environment and Raman spectroscopy.



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## Low temperature EPR of $\text{Cu}^{2+}$ in Cu-X zeolite and HKUST-1 with $\text{H}_2$ adsorption

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Nanoporous materials are considered as candidates of hydrogen storage materials at low temperature:  $\text{H}_2$  molecules can be adsorbed onto their surface by Van der Waals force. Among them Cu-X Zeolite and HKUST-1 ( $[\text{Cu}_3(\text{TMA})_2(\text{H}_2\text{O})_3]\text{n}$ ) have  $\text{Cu}^{2+}$  ions and we assume the ions acts as adsorption sites of  $\text{H}_2$  molecules. We measured EPR of  $\text{Cu}^{2+}$  at several low temperatures (4~150K) in order to elucidate the effect of adsorbed  $\text{H}_2$  to  $\text{Cu}^{2+}$  in Cu-X Zeolite and HKUST-1 at low temperature. After  $\text{H}_2$  load at 150K, EPR signal increased compared with one in vacuum. In addition, the effects of excitation by visible light of samples at 4K were measured and analyzed.

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## Effect of Water on the Behavior of Semiconductor Quantum Dots in Zeolite Y: Aggregation with Framework Destruction with H-Y and Disaggregation with Framework Preservation for $\text{NH}_4^+$ -Y

김현성 윤경병

서강대 화학과

Treatment of dry  $\text{M}^{2+}$ -exchanged zeolite Y ( $\text{M}^{2+} = \text{Cd}^{2+}$ ,  $\text{Mn}^{2+}$ , and  $\text{Zn}^{2+}$ ) with dry  $\text{H}_2\text{S}$  leads to the formation of isolated, ligand-free, subnanometer metal sulfide quantum dots (QDs) in zeolite Y without framework destruction and with  $\text{H}^+$  as the counter cation. Treatment of the dry  $\text{H}^+$ /CdS QD-incorporating zeolites Y with dry  $\text{NH}_3$  leads to the neutralization of  $\text{H}^+$  to  $\text{NH}_4^+$ . During this process, the framework structure remains intact. However, small amounts of interconnected CdS QDs were formed within the zeolite Y by coalition of isolated CdS QDs at the windows. With  $\text{H}^+$  as the counter cation, isolated CdS QDs rapidly aggregate into interconnected and mesosized QDs with accompanying destruction of ~50% of sodalite cages leading to the framework rupture. With  $\text{NH}_4^+$  as the counter cation, however, the isolated QDs and zeolite framework remain intact even after exposure to the moist air for 4 weeks. Interestingly, the interconnected QDs that were formed during neutralization of  $\text{H}^+$  with  $\text{NH}_3$  disintegrate

into isolated QDs in the air. Similar results were obtained from ZnS and MnS QDs generated in zeolite Y. Thus, ligand-free, naked, subnanometer QDs can now be safely preserved within zeolite pores under the ambient conditions for long periods of time. This finding will expedite the generation and dispersion of various QDs in zeolite pores, their physicochemical studies, and applications.



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## Concentration of Plasmonic Nanoparticles on Fluidic Surface

이영광 남좌민<sup>1</sup>

서울대 화학과 <sup>1</sup>서울대 화학부

The plasmonic coupling of metal nanoparticles enables tuning the interaction between electromagnetic waves and metallic nanostructures, which gives rise to many of unprecedented physical consequences including light concentration in a nanometeric volume for improving fluorescence, Raman scattering and single molecule detection. Nanogap engineering between metal nanostructures is a highly straightforward method to couple and tune localized surface plasmons. Active tuning of plasmonic nanogap is, nevertheless, still challenging. Here, we present a straightforward strategy to engineer inter-particle gaps by concentrating plasmonic particles on two-dimensional fluidic lipid bilayer surface. This lateral manipulation allows for active, reversible coupling of surface plasmon resonances and this is quantitatively evaluated by dark-field microscopy-correlated spectroscopy.



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## Flower-like Magnesium Oxide Growth via Common Ion Effect

유현웅 김남운<sup>1</sup>

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The shape and size of inorganic nanostructures have great influence on their optical, electrical and physical properties. In particular, magnesium oxide (MgO) is an exceptionally important material in a variety of fields such as catalysis, toxic waste remediation, reinforcing reagent and as additives in refractory, paint and superconductor products. As MgO is a typical wide bandgap insulator with its excellent thermodynamic stability, low dielectric constant, and low refractive index, it has been widely used for growing various thin film materials. For this application, it is worth developing suitable growth method for MgO nanostructure. In this study, the optimum hydrothermal process to fabricate flower-like Mg(OH)<sub>2</sub> spheres was investigated using SEM, XRD and FT-IR for a simple and well controllable process. Hydrolysis and pH control on the final morphology are also studied.

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## Photovoltaic Effects of the CdS and PbS Quantum Dots Encapsulated in Zeolite Y

김현성 윤경병

서강대 화학과

Photovoltaic (PV) effects of the CdS and PbS quantum dots (QDs) encapsulated in zeolite-Y were studied. For this, zeolite-Y films with the thicknesses between 350 and 2,500 nm were grown on ITO glass and into which 3.2, 4.3, and 6.3 CdS and 3.4, 4.6, and 6.7 PbS per unit cell, respectively, were loaded. They are denoted as  $(\text{CdS})_n\text{Y}_f$  and  $(\text{PbS})_n\text{Y}_f$ , respectively, where  $n$  denotes the loaded amount. At higher loadings of CdS or PbS the films underwent crack formation.  $(\text{CdS})_n\text{Y}_f$  showed a novel PV effect with Pt-coated ITO glass as the counter electrode in the electrolyte solution consisting of  $\text{Na}_2\text{S}$  (1 M) and  $\text{NaOH}$  (0.1 M). In contrast,  $(\text{PbS})_n\text{Y}_f$  showed a negligible PV effect. The PV effect increased with increasing the loaded amount ( $n$ ) of CdS and increasing the film thickness. In the case of  $(\text{CdS})_{6.3}\text{Y}_f/\text{Pt}$ , the short circuit current ( $I_{sc}$ ), open circuit voltage ( $V_{oc}$ ), fill factor ( $FF$ ), and the efficiency ( $\eta$ ) were  $0.3 \text{ mA cm}^{-2}$ , 423 V, 28, and 0.1%, respectively, under the AM 1.5,  $100 \text{ mW cm}^{-2}$  condition. The efficiency decreased by only 10% after 18 days of continuous measurements. The PV efficiency of  $(\text{CdS})_{6.3}\text{Y}_f$  increased by three

times when it was coupled to (PbS)<sub>6.7</sub>Y<sub>f</sub>. Under this condition the IPCE value at 398 nm was 42% and the APCE value was 82% at 405 nm. In the case of (CdS)<sub>6.3</sub>Y<sub>f</sub>, the volume fraction of CdS in (CdS)<sub>6.3</sub>Y<sub>f</sub> is only 2.2% and the minimum edge-to-edge distance between the photoactive QDs was 5.6 nm. The negatively charged framework, the charge-balancing cations, and the strong electric fields produced by them are proposed to be responsible for the very long distance carrier mobility in (CdS)<sub>6.3</sub>Y<sub>f</sub>.



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## Increase of 3<sup>rd</sup>-Order Nonlinear Optical Activity of PbS Quantum Dots in Zeolite Y by Increasing Cation Size

김현성 윤경병

서강대 화학과

The 3<sup>rd</sup>-order nonlinear optical (3-NLO) activity of PbS quantum dots (QDs) encapsulated in zeolite Y has been expected to sensitively change upon changing the counter cation of the zeolite host. However, the ion exchange of the pristine counter cation, H<sup>+</sup>, with other cations has not been possible because the framework decomposes and the QDs aggregate immediately upon exposure of the PbS QDs-incorporating zeolite Y with H<sup>+</sup> as the counter cation to the atmosphere. We now report that when H<sup>+</sup> was transformed to NH<sub>4</sub><sup>+</sup>, the framework of PbS QD-containing zeolite Y does not undergo decomposition and the PbS QDs do not undergo aggregation to larger QDs during the aqueous ion exchange of NH<sub>4</sub><sup>+</sup> with alkali metal (M<sub>A</sub><sup>+</sup>) ions, where M<sub>A</sub><sup>+</sup> = Li, Na<sup>+</sup>, K<sup>+</sup>, and Rb<sup>+</sup>. The 3-NLO activity of the M<sub>A</sub><sup>+</sup>-exchanged PbS QD-incorporating zeolite Y film increases with increasing the size of M<sub>A</sub><sup>+</sup>. The stabilization of the surface-bound exciton by the electron rich framework oxide and electron poor cation is proposed to be responsible for the increase. This is a first example to show a method to systematically increase the 3-

NLO activity of QDs dispersed in a dielectric matrix by systematically changing its property, which will serve as a guideline for future researches. These results will also promote applications of QD-incorporating zeolites in various fields.



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**입체성이 매우 큰 Terphenyl에 근거한 리간드를 이용한  
Hydroxide로 연결된 Cubane 형태의 전이금속 화합물들의 합성  
및 분석**

**김남석 윤성호 박규순<sup>1</sup>**

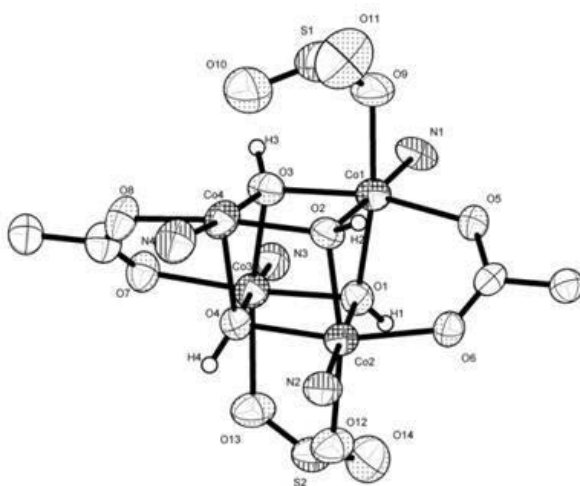
국민대 생명나노화학과 <sup>1</sup>국민대 화학과

최근 Photosystem II 의 Water Oxidation Center(WOC)<sup>(1)</sup>의 활성화 자리에서 관찰되는 Mn 을포함하는 Cubane-type core 는 광합성 작용에서 매우 중요한 역할을 하는것으로 인식되어 많은 연구의 대상이 되고 있다. 더불어 이러한 Cubane-type 전이금속 화합물은 독특한 자기적 성질을 나타내는 Single Molecule Magnet(SMM)<sup>(2)</sup>으로 작용할 가능성이 있어 무기화학의 주 연구 분야의 하나로 각광을 받고 있다. 하지만 현재까지 보고된 cubane 의 대부분은 alkoxo bridged cubane 으로 자연계에 존재하는 hydroxo bridged cubane 과는 상당한 구조적 차이를 보이고 있다. 본 발표에서는 sterically hindered terphenyl-based carboxylate

리간드를 이용하여 그림에 나타낸 것과 같이  $[\text{Co}_4(\mu_3\text{-OH})_4(\mu\text{-O}_2\text{CAr}^{4\text{F-Ph}})_2(\text{-OTf})_2](1)$ ,  $[\text{Ni}_4(\mu_3\text{-OH})_4(\mu\text{-O}_2\text{CAr}^{\text{Tol}})_2(\mu\text{-OTf})_2]$  (2), 그리고  $[\text{Cu}_4(\mu_3\text{-OH})_4(\mu\text{-O}_2\text{CAr}^{4\text{tBu-Ph}})_2(\mu\text{-OTf})_2]$  (3)의 합성과 결정구조등의 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 **1** 화합물 중심부의 50% anisotropic ellipsoid를 나타낸 ORTEP 그림.

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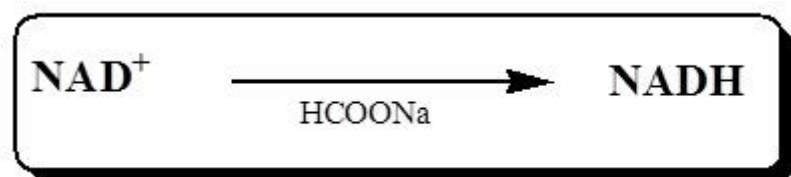
## Synthesis and Catalytic Activity of a Rhodium Complex for the Conversion of $\text{NAD}^+$ to NADH

D.Sivanesan 윤성호<sup>1</sup>

국민대<sup>1</sup> 국민대 생명나노화학과

The regeneration of the co-enzyme 1,4-NADH, the reduced form of nicotinamide adenine dinucleotide ( $\text{NAD}^+$ ), has continued to be high in the field of biocatalysis, where enzymatic reduction reactions are important for the synthesis of chiral organic compounds. The rhodium complexes are known for their conversion of  $\text{NAD}^+$  to NADH by the chemical and the electrochemical method. Addition to the regeneration of co-enzyme, recently it has been reported that rhodium complexes can act as an electrocatalyst for the  $\text{CO}_2$  reduction in an aqueous organic medium. To improve the catalytic properties of reported catalyst including the turn over number, the new rhodium complex was synthesized. Herein, we report the synthesis, electrochemical properties and catalytic effect of rhodium complex. Acknowledgement: This research was supported by the Converging Research Center program through the National research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2010K001153).





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## Single Nanoparticle Attached AFM tip for Tip Enhanced Raman Spectroscopy

김웅 박준원

포항공과대 화학과

Tip enhanced Raman spectroscopy (TERS), analytical technique to detect a single molecule, records a specific fingerprint of chemical bond. Through picking of attached on a single DNA to hybridize a gold nanoparticle, a single gold nanoparticle is attached with edge of AFM tip for TERS. Various silver staining conditions were controlled by silver shell thickness (10nm~50nm) of gold attached with edge of AFM tip. Less than 5 nm thickness of gold coating is placed as the protective silver layer. Through TERS tip on nanoparticle, we will strongly use single-molecule's characteristic, bioassay. This tip can measure more precisely TERS mapping than ever before.

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## Co based MOFs as electrode for supercapacitor

이덕연 안도영 한성환

한양대 화학과

We explore the cobalt based metal-organic-frameworks (Co-MOF) as a promising material for supercapacitors. The doctor bladed Co-MOF film exhibits a good pseudocapacitor behaviour with the specific capacitance up to 206.76 F g<sup>-1</sup>. The electrochemical redox switching is reversible perfectly for a long run which leads to the loss of only 1.5% in capacitance for 1000 electrochemical life cycle stability test.

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## Enhancement of carrier mobility of ZnO conducting channel via photoinduced charge transfer

김은경 한성환

한양대 화학과

We build organic-inorganic hybrid film devices which consist of a compact dense inorganic n-type active layer and organic p-type electron donor materials on the conducting channel of the device, by simple solution process. Poly (3-hexylthiophene) (P3HT) was chosen as electron donor p-type material and ZnO nano-particle was as n-type active layer. The modified n-channel thin-film phototransistor, wherein, n-ZnO as electron collector and hole-blocking layer, extracts and grounds the photo-generated electrons, and p-P3HT as absorbs and electron pumping material, thereby increasing the electron concentration and mobility in the conducting channel hole density via electron transfer.

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## **Preparation, characterization and application of CoS thin film using chemical bath deposition for supercapacitor**

**임이슬 수프리야 한성환**

한양대 화학과

CoS thin film was simply deposited on ITO glass with chemical bath method. It is very simple method to make films and control the morphology of film. The morphology of CoS film is examined by scanning electron microscopy and UV-Vis spectroscopy. The supercapacitance of CoS film is investigated by cyclic voltammetry. The results show that film of CoS forms a uniform film of around 300 nm thickness on ITO glass. The CoS thin film exhibit a specific capacitance of 131 F g<sup>-1</sup> in 1M KOH electrolyte. The surface reaction between CoS and electrolyte was inferred from redox active site.

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## Anodic Tin Oxide Based Super capacitors

Dipak V. Shinde 안도영 한성환

한양대 화학과

Anodization is widely used to make self assembled structures in case of metals like Ti, W, Fe, Al etc. It produces well ordered, mesoporous 1-D structures which are used in variety of devices like Li-ion batteries, solar cells, super-capacitors, gas sensors, biosensors etc. Tin oxide is wide band gap (3.6 eV) semiconductor used in variety of fields, wherein performance is always affected by its size and morphology. It has been previously utilized in super-capacitors but the capacitance value remained low due to non porous nature of the films. Herein we report on the fabrication of highly porous, self assembled structures of Tin oxide by anodizing tin metal plates in weak organic acids like oxalic acids and phosphoric acid. The obtained structures are highly porous and when utilized in supercapacitor gave a specific capacitance of 274 F/g which is the highest value reported so far, for tin oxide based capacitors.

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## Crystal Structures and Physical Properties of Eu(III) and Tb(III) Complexes with Diphenate and Picolinate Ligands

심용석 강성권

충남대 화학과

Lanthanide trivalent ions are effective for luminescent materials because of their excellent quantum efficiency. In particular, lanthanide trivalent complexes show intense absorption bands in the UV region. Both Eu(III) and Tb(III) complexes have been characterized by X-ray single crystal studies. Metals are nine-coordinated to oxygen and nitrogen atoms of diphenate, 6-hydroxypicolinate, and/or 6-methylpicolinate ligands. The geometries around metals are capped square antiprism or square antiprism. We will discuss the structural features and spectroscopic properties of UV and PL spectra of these complexes.

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## Dual-Tridentate Fe(III) Complexes Containing Bidentate Tetrazole Ligand For Selective binding with Alkali Metal

이휘현 박가현 고민정 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 ( $LH_2$ ) and 2,2'-bipyrimidine(bpym) in  $H_2O$ , high dimensional mixed metal coordination polymers,  $[Li_3(bpym)_{1.5}FeL_3(H_2O)_6]_n$  (1a),  $[Na_3(bpym)_{1.5}FeL_3(H_2O)_7]_n$  (2a),  $[K_3(bpym)FeL_3(H_2O)_7]_n$  (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 ( $FeL_3^{3-}$ ) 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  $[Li_3FeL_3(H_2O)_3]$  (1b), 2-D  $[Na_3FeL_3(H_2O)_7]$  (2b) and  $[K_3FeL_3(H_2O)_7]$  (3b) were



synthesized and coordination between alkali metal ion and iron fragment ( $\text{FeL}_3^{3-}$ ) was stronger than bpym contained species. In particular, due to lack of binding sites, potassium binds to TzOH ligands with  $\sigma$  and  $\pi$  character in complex 3b



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## The dimension-controlled zinc imidazolate frameworks via different molar ratio

방원주 홍창섭

고려대 화학과

Since the initial inspiration for realizing metal-organic frameworks (MOFs) with zeolitic structures, considerable effort has been made towards novel approaches to construct zeolitic metal-organic frameworks by using tetrahedral metal imidazolates. We have synthesized two types of imidazolate frameworks by mixing zinc nitrate and 2-methylbenzimidazole (H-mim) with a different molar ratio via conventional solvothermal reaction. One of these is a 3D framework, while the other is a 2D layered framework. The former has 4-zinc nodes connected by nitrogens of imidazole ligands. There are no solvent accessible channels, but DMF solvent molecules are located in inner spaces of the framework. The later is comprised of stacked layers which consist of 2-zinc nodes linked by imidazoles. The DMF molecules are positioned into the interlayers. We'll present the structures, sorption properties of these two compounds in details.

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## Crystal-to-amorphous transformation in the azide-bridged Mn(II) and

### Ni(II) compounds

임광수 홍창섭

고려대 화학과

New compounds,  $[M(\text{PBMDPO})(\text{N}_3)(\text{H}_2\text{O})_2](\text{N}_3)$  [ $M = \text{Mn}(1\text{a}), \text{Ni}(2\text{a})$ ;  $\text{PBMDPO} = 1,1'-(1,4\text{-phenylenebis(methylene))dipyridinium-4-olate}$ ] have been produced by slow evaporation method and characterized by elemental analysis, infrared spectroscopy, and single crystal X-ray diffraction. Compounds 1a and 2a can be described as a 2-D coordination sheet in which 1-D  $[M(\text{N}_3)]_n$  chains are interlinked by PBMDPO ligands. Heating at  $130^\circ\text{C}$  for 10 h under vacuum, the crystalline compound 1a lost  $\text{H}_2\text{O}$  molecules, resulting in an amorphous phase. The desolvated sample,  $[\text{Mn}(\text{PBMDPO})(\text{N}_3)](\text{N}_3)$  (1b) recovered its original crystallinity after exposure to water vapor. However, compound 2 did not exhibit a water-induced reversible crystal-to-amorphous transformation. Detailed structural and magnetic studies will be given in the presentation.

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## Magnetic Nanoparticles-Activated Intracellular Signaling

이은정 조미현<sup>1</sup> 이재현<sup>1</sup> 유동원<sup>1</sup> 천진우<sup>1</sup> 신전수<sup>2</sup>

연세대 나노메디컬학과 <sup>1</sup>연세대 화학과 <sup>2</sup>연세대 의과대학 미생물학교실

Regulation of cellular activities has opened new and exciting areas of research in the fields of basic cell biology and biomedical science. Among various kinds of cellular activity regulators, magnetic nanoparticles are becoming important tools for controlling microscopic behaviors of the cell metabolism. Because these particles can be coupled with magnetic field to produce enough force to initiate the actuation of biological objects with high target specificity, this magnetic stimulation system can switch the cellular activity on and off by focusing magnetic field. By employing nanoparticles, precisely controlled mechano-actuators of biological processes are possible due to not only their small sizes but also their versatility for multi-valencies in functional group attachments. In this study, we demonstrate that magnetic triggering of membrane receptor clustering-mediated intracellular signaling is possible in cellular system. This new magnetic actuator can provide non-invasive and remote controllability with maximum manipulation efficiency of cellular functional groups and minimizing cell destructions.

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## 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, a characteristic stretching in the force-distance curve showing single unbinding force was observed due to the elasticity of the protein. Also, an adhesion force map was obtained. With these approaches, unambiguous sorting the specific unbinding event, and observing hydrodynamic behavior of CB[6] based on a BSA substrate were possible.

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**Single DNA-tailored Au-Ag core-shell dimer with a narrow  
distribution of large enhancement factors in surface-enhanced Raman  
scattering**

이정훈

서울대 화학부

Generating plasmonic nanogap nanostructures with highly strong and quantitative surface-enhanced Raman scattering (SERS) signals with a narrow distribution of high SERS enhancement factors (EFs) is of significant importance in nanomaterials, plasmonics and Raman communities, especially for wider and more practical chemical and biological sensing applications. Here, we designed and synthesized two different dimeric GSND probe systems ; GSND-I that can systematically vary nanometer gap with the same Au core size and GSND-II that can tune Au core size with a fixed sub-nanometer interparticle gap ? to extensively study relationships between single-molecule SERS intensity, EF distribution over many particles, interparticle distance, particle size/composition and excitation laser wavelength.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cytocompatible Encapsulation of Living Chlorella Cells within SiO<sub>2</sub>-TiO<sub>2</sub> Nanocomposite Shells

고은혜 최인성

KAIST 화학과

The artificial shells of hard inorganic nanocomposites on individual living cells would protect the cells against thermal stress, and control cell division. These emerging properties could be combined with cell-surface functionalizations for applications to cell-based biosensors and assays as well as for fundamental studies on single-cell based biology. In this work, individual Chlorella cells were encapsulated within silica/titania nanocomposite shells in a biocompatible method that utilized a designed peptide. The cell viability was maintained, and the division of the encapsulated Chlorella cells was controlled. The cell viability was enhanced compared with the previous work, TiO<sub>2</sub>-only shell formation. Furthermore, SiO<sub>2</sub>-TiO<sub>2</sub> in our system effectively dissipated heat energy and maintained the cell viability about 7-fold better than the unencapsulated one. For the cell manipulation, magnetic nanoparticles were successfully embedded in the shell. In addition, the incorporation of TiO<sub>2</sub> to the shell made it possible to anchor the ligands of interest to the shell via catechol chemistry. All in all, the combination of biological SiO<sub>2</sub> and

abiological  $\text{TiO}_2$  for the shell formation gave more tunability of the artificial shells compared with the  $\text{SiO}_2$  or  $\text{TiO}_2$  shells only.





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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ethylene Polymerization using graphene composite

최백합 박성진<sup>1</sup> 이경석<sup>2</sup> 최인성

KAIST 화학과 <sup>1</sup>인하대 화학과 <sup>2</sup>한국표준과학연구원 분석화학표준센터

Metallocene, which has transition metal atoms sandwiched by aromatic rings, is one of the representative systems for organometallic catalysts. Group 4-based metallocene catalysts have been most commonly used for the production of polyolefins, which have great world-wide markets in the real life. Graphenes and carbon nanotubes (CNTs) were composed of extended  $sp^2$  carbon networks, showing high electron mobility as well as have extremely large steric bulkiness relative to metal centers. A few example of chemically modified graphenes (CMGs) showed interesting performances as a catalysts or as a supporter in catalytic reactions. In this work, a reduced graphene oxide (RGO) was attached on a zirconocene and separately, on a titanocene. Resulting hybrid systems showed excellent catalytic performances for ethylene polymerizations and produced polyethylenes (PEs) with extremely increased molecular weights relative to free catalytic systems without graphene materials.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

**Novel Tm-Ni Heterobimetallic Complex**  
 **$\{(H_2O)_2(DMF)_{10}Tm_2[Ni(CN)_4]_3\}_\infty$  including O-H...N-C Hydrogen**  
**Bond**

**박대영 유철휘<sup>1</sup> 정장훈<sup>2</sup>**

명지대 화학과 <sup>1</sup>호서대 일반대학원 그린에너지공학과 <sup>2</sup>명지대 자연과학대학/화학과

A novel Tm-Ni heterobimetallic complex  $\{(H_2O)_2(DMF)_{10}Tm_2[Ni(CN)_4]_3\}_\infty$  was obtained via metathesis reaction of 2:3 molar ratio of  $Tm(NO_3)_3 \cdot 6H_2O$  with  $K_2[Ni(CN)_4] \cdot 6H_2O$  in DMF at room temperature. The molecular structure of the complex was determined by a single crystal X-ray diffraction analysis. The crystal system is a triclinic. R1 and wR2 are 0.040 and 0.062, respectively. This structure is an extended chain consisting of alternating Tm and Ni complexes. Within a chain, each Tm atom is bonded to five DMF molecules, one water molecule, and two  $Ni(CN)_4$  and each  $Ni(CN)_4$  complex is bonded to two Tm complexes. There is a  $Ni(CN)_4$  complex off by itself (with the Ni on an inversion center), and this complex is involved in hydrogen bonding with the water molecule bonded to Tm. Hence this  $Ni(CN)_4$  complex, by virtue of its inversion center, serves as a link between two extended chains

through this hydrogen bonding. The other hydrogen atom of this water molecule is involved in a hydrogen bond with a nitrile group in a neighboring extended chain.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## The size and shape effect on amyloid $\beta$ assemblies

김유나 남좌민

서울대 화학부

Alzheimer's disease (AD) is a progressive neurodegenerative disorder affecting large number of the aging population. The major clinical manifestation of AD is memory loss resulting in behavioral deficits, disorientation in time and space, and impairments in language skills. It is widely accepted that AD results from amyloid- $\beta$  accumulation in extracellular regions and neurofibrillary tangles in neurons. In the presence of amyloid- $\beta$  accumulation surrounded by degenerating neurites, these abnormal deposits would be the source of some neurotoxic effect. Here, we designed and realized a model system that allows a systematic study on amyloid  $\beta$  deposition and its toxicity to neuron cells. In this system, the supported lipid layer (SLB) was used as a substrate that mimics in-vivo-like neuron cell membrane environment. On the SLB, amyloid- $\beta$  assemblies were induced by injecting spherical Au nanoparticles (AuNPs) and Au nanorods (AuNRs), and then neuroblastoma cells were seeded for the neurotoxicity test. The size and shape (aspect ratio for AuNRs in this case) effects on the formation of various amyloid  $\beta$  aggregates were studied on this template using dark-field light scattering from Au nanostructures.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

**New derivatives of TE2A with enhanced stability for Cu(II) ions; a better option for TE2A as a bifunctional chelator**

**AJIT V. DALE DARPAN N.PANDYA 김정영<sup>1</sup> 이호춘<sup>2</sup> 하영수 김종희 이윅희 안광일<sup>1</sup>**

유정수

경북대 의과대학 분자의학교실 <sup>1</sup>한국원자력의학원 방사성의약품연구팀 <sup>2</sup>대구경북과학기술원  
에너지시스템공학

Importance of bifunctional chelators (BFCs) has increased over last decade, due to their potential application in the field of radiopharmaceuticals. In order to be successful, a BFC should form stable complexes with metal ions. Cyclam with two acetate pendant arms, TE2A was found to be a better chelator for Cu(II) ions than widely used TETA. In order to check the effect of methyl substitutions on two remaining secondary amines of TE2A backbone with respect to their stability with Cu(II) ions, we synthesized mono and di substituted TE2A (MM-TE2A and DM-TE2A) in five and four steps in good overall yield. The Cu(II) complexes of MM/DM-TE2A were synthesized in high yields. Acidic decomplexation and cyclic voltammetry experiments were carried out for Cu(II) complexes to evaluate

their kinetic stability. Cu-TE2A was used for the comparison studies. The degradation pattern of Cu(II) complexes was monitored using a HPLC system. Cu-DM-TE2A showed higher stability than Cu-MM-TE2A. Cyclic voltammetry studies showed quasi irreversible reduction potential for both Cu-MM- and Cu-DM-TE2A. MM- and DM-TE2A were quantitatively radiolabeled with  $^{64}\text{Cu}$  using  $^{64}\text{CuCl}_2$ . Both  $^{64}\text{Cu}$ -MM/DM-TE2A did not show any sign of decomplexation for up to 24 h in the serum stability test. LogP studies confirmed that  $^{64}\text{Cu}$ -DM-TE2A was more lipophilic than  $^{64}\text{Cu}$ -MM-TE2A. Biodistribution studies revealed that both  $^{64}\text{Cu}$ -MM- and  $^{64}\text{Cu}$ -DM-TE2A showed rapid clearance from body. To conclude, methyl substitutions on TE2A on remaining secondary amine of cyclam backbone resulted in more stable Cu(II) complexation than TE2A.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhanced isosteric heats of H<sub>2</sub> adsorption by post-synthetic cation exchange in anionic metal-organic frameworks

최명호 박혜정 백명현

서울대 화학부

We have synthesized anionic metal-organic frameworks that contain ammonium cations in the pores. The post-synthetic cation exchange of ammonium ions with Ca<sup>2+</sup> and Fe<sup>2+</sup> increases significantly the isosteric heats (Q<sub>st</sub>) of the H<sub>2</sub> adsorption as well as the H<sub>2</sub> storage capacities.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ruthenium<sup>II</sup>(bpy)<sub>3</sub> and Nickel<sup>II</sup> Based 3D Framework

전승안 백명현

서울대 화학부

A 3D metal-organic framework exhibiting redox active properties was prepared using a Ru<sup>II</sup>(bpy)<sub>3</sub> and a Ni<sup>II</sup> bis-macrocyclic complex. It contains voids of up to 42.8% of the cell volume. Although the framework shows a broad absorption band over the entire visible range in the solid state, it did not evolve H<sub>2</sub> gas upon irradiation with artificial sunlight in various buffer solutions. When the 3D framework was immersed in separate aqueous solutions of AgNO<sub>3</sub> and NaAuCl<sub>4</sub> · 2H<sub>2</sub>O, Ag and Au nanoparticles, respectively, were formed. The presence of these nanoparticles was confirmed by HRTEM images and EPR spectra.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhancement of Isothermic Heat of H<sub>2</sub> Adsorption by Inclusion of Crown Ethers in a Porous Metal-Organic Framework

박혜정 백명현

서울대 화학부

We have demonstrated by the experimental and theoretical studies that the inclusion of 18-Crown-6 or 15-Crown-5 in a porous MOF significantly increases isothermic heat ( $Q_{st}$ ) of the H<sub>2</sub> adsorption. The increase of  $Q_{st}$  value is much greater than that by the inclusion of alkali metal or alkali earth metal ions, and comparable to that by the presence of accessible metal sites in the MOF. Our results indicate that 18-Crown-6 has a greater effect than 15-Crown-5 on the enhancement of  $Q_{st}$ .

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Colloidal SnSe<sub>2</sub> Nanoplate-graphene composites as anode materials for high performance lithium ion batteries

진재원 최재원 손성욱

성균관대 화학과

SnSe<sub>2</sub> nanoplates were synthesized using SnCl<sub>2</sub> with imidazoline-2-selenone in oleylamine at 220 °C for 2h. Their graphene composites were prepared by reduction of graphene oxide in presence of SnSe<sub>2</sub> nanoplates and characterized through TEM, SEM, XRD and XPS studies. Coin-type electrochemical cells were fabricated using SnSe<sub>2</sub> nanoplates, graphenes and SnSe<sub>2</sub> nanoplate-graphene composites. SnSe<sub>2</sub> nanoplate-graphene composites had the improved electrochemical performances and stabilities due to the enhanced conductivities and buffering role of graphene. In this work, we will show that 2D nanomaterial-graphene composites can be good candidate as stable electrode materials for high capacity lithium ion batteries.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Shape-controlled synthesis of SnSe nano-columns for energy device applications

장권호 juanxu 최재원 진재원 손성욱

성균관대 화학과

By a single precursor approach based on  $[\text{Sn}\{\text{Si}(\text{CH}_3)_2(\text{NC}_4\text{H}_9)_2\}(\text{u-Se})]_2$ , assembled SnSe nano-columns were phase-selectively prepared. Heating of the single precursor in the presence of oleylamine resulted in formation of the assembled SnSe nano-columns, which were characterized by SEM, TEM, EDS, PXRD, UV-VIS and XPS analysis. The SnSe nano-columns showed discharge capacities of 505 - 473 mAh/g and stability as anode materials in lithium ion batteries. In addition, they had direct band-gap 0.98 eV, indirect band-gap 0.93 eV determined by a reflectance UV-VIS, so they can be used in opto-electric devices.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Organometallic approach for synthesizing new amorphous SnFexSyOz plates and application of their -graphene composites for lithium ion batteries

juanxu 장권호 최재원 진재원 손성욱

성균관대 화학과

Unprecedented colloidal SnFexSyOz(SFSO) nanoplates were synthesized by organometallic approach and characterized by TEM, HR-TEM, EDS, PXRD, and XPS. The graphene-like SFSO plates have amorphous character, and can be considered as meta-stable intermediate materials in the formation of iron-tin alloy materials. Their widths and thicknesses were 1 - 5  $\mu\text{m}$  and 1.2 - 1.8 nm respectively. The SFSO-graphene composites showed high discharge capacities of 736 - 727 mAh/g and excellent stabilities as anode materials.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Columnarly assembled Colloidal In<sub>2</sub>S<sub>3</sub> nanoplates on Graphene as anode materials for high performance lithium ion batteries

최재원 진재원 이제호<sup>1</sup> 손성욱

성균관대 화학과 <sup>1</sup>성균관대 에너지과학과

This study shows that heat-treatment of colloidal inorganic nanoplates with columnar assembly under argon is a good strategy for development of anode materials. The heating of colloidal In<sub>2</sub>S<sub>3</sub> nanoplates under argon resulted in the formation of film-like materials through interconnection of plates side by side because the plates had a strong preference for growth in the vertical direction to the basal plane. When the columnarly assembled colloidal In<sub>2</sub>S<sub>3</sub> plates were heated at 400 °C under argon for 2 hours on graphene, more efficient anode materials with smaller diameters were obtained. Interestingly, the heat-treated columnarly assembled In<sub>2</sub>S<sub>3</sub> plates on graphene had a layered structure, which was attributed to the possible existence of carbon materials between plates formed by the heat-treatment of surfactant under argon. The heat-treated graphene-In<sub>2</sub>S<sub>3</sub> composites showed enhanced discharge capacities, up to 716-837 mAh/g as well as excellent stabilities. In addition, the materials showed promising columbic efficiencies and rate performances. We believe that, based on the strategy in this work, diverse graphene-inorganic

nanomaterial composites with a layered structure can be prepared and applied as new anode materials in lithium ion batteries.



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**Refinement of the electrophilic DMSO/ $\text{POCl}_3$  reaction with meso-aryl BODIPY systems: implications for biological ROS sensing and neurodegenerative disease research**

**전태홍 D.G.Churchill**

KAIST 화학과

We report a synthetic, optical, biological, structural, study where ROS fluorescent/optical probing capacity in sulfur containing 4,4-difluoro-1,3,5,7-tetramethyl-8-(2/3-thienyl/furyl)-4-bora-3a,4a-diaza-s-indacene-based systems is elucidated. Importantly, a recently published  $\text{POCl}_3/\text{DMSO}$  reaction mentioned the 2-chloro-6-methylsulfide derivative as the exclusive product (Kim, T. I.; Park, S.; Choi, Y.; Kim, Y. Chem. Asian J. 2011, 6, 1358-61). However, here, via the same protocol, related co-products were isolated and characterized including the 2,6-disulfido and 2,6-dichloro species. The 8-meso tail group modifies product type and distribution slightly. MeS-containing products undergo a time-dependent “off-on” response with NaOCl (10 equiv), etc. This was reported previously by Kim et. al. for the 2-chloro-6-methylsulfide species. Compounds 4b and 2b enter the cytosol of SH-SY5Y neuroblastoma and accumulate in the juxtannuclear region; cell toxicity was determined to be very low. Cheminformatics c

log p values were obtained on all species including ones where the sulfur is oxidized. Compounds were characterized by NMR spectroscopy and X-ray diffraction.





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## 유기태양전지의 전자주개층 물질로써 dipyrrin 유도체의 합성과

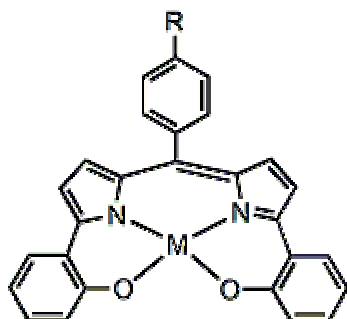
특성분석

전여진 윤성호

국민대 생명나노화학과

최근 세계 각국의 태양광발전 연구방향은 저가이고 flexible 한 유기물 기반 광발전 시스템으로 이동 중이며 그 중 차세대 태양전지로 주목받고 있는 유기태양전지(OPV)는 크게 고분자 타입과 단분자 타입으로 나눌 수 있다. 단분자 태양전지는 고분자 태양전지에 비해 현재 에너지변환효율이 다소 낮고 진공 증착 설비 등이 필요한 단점이 있지만, 재료개발 및 정제가 용이하고 유도체 합성에 의한 잠재적 물질 후보군이 많다는 장점을 가지고 있다. 단분자 유기태양전지의 전자주개층 물질로는 현재까지 주로 프탈로시아닌(Pc)계 화합물만이 알려져 있다. 최근 low bandgap 물질인 DCV3T, DCV5T, TDCV-TPA 등이 연구되고 있지만 사용되고 있는 유기물의 종류는 매우 제한적이라 할 수 있다. 이러한 물질 후보군으로 개발한 dipyrrin 기반의 다양한 유도체 합성 방법과

특성분석에 대하여 발표하고자 한다 (그림). 특히 이러한 물질의 UV-vis 흡수 분광 분석 결과 기존의 Pc 계열 물질에 비해 매우 높은 흡광계수를 보여주어 새로운 전자주개층 물질로 기대되고 있다. 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 (MEST) (KRF-2008-C00146)



R = H, OMe, COOH

M = Al<sup>3+</sup>, B<sup>3+</sup>, Fe<sup>3+</sup>, Mn<sup>3+</sup>, Co<sup>3+</sup> and etc



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## **$^2\text{H}$ and $^7\text{Li}$ Solid-State MAS NMR Study of Local Environments and Lithium Adsorption on the Iron(III) Oxyhydroxide, Akaganeite ( $\beta\text{-FeOOH}$ )**

김종식 신지현<sup>1</sup> 정혜윤

동아대 화학과 <sup>1</sup>동아대 자연과학대학

$^2\text{H}$  and  $^7\text{Li}$  MAS NMR spectroscopy have been applied to characterize the surface and bulk hydroxyl groups and  $\text{Li}^+$  sorption on the iron oxyhydroxide akaganeite ( $\beta\text{-FeOOH}$ ), a common soil mineral with a large surface area and uptake capacity for toxic cations and anions. The formation of both inner and outer-sphere complexes on the surface of akaganeite was confirmed, the former giving rise to  $^7\text{Li}$  NMR signals with large  $^7\text{Li}$  hyperfine shifts. The concentrations of these complexes was determined as a function of pH and possible  $\text{Li}^+$  binding modes and sites are proposed based on their  $^7\text{Li}$  hyperfine shifts. The binding is compared with those of the other  $\text{FeOOH}$  polymorphs, goethite and lepidocrocite. The modes of binding are similar to those of goethite, except that sites at the entrances to the tunnels become available for binding, particularly for nanosized akaganeite particles.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

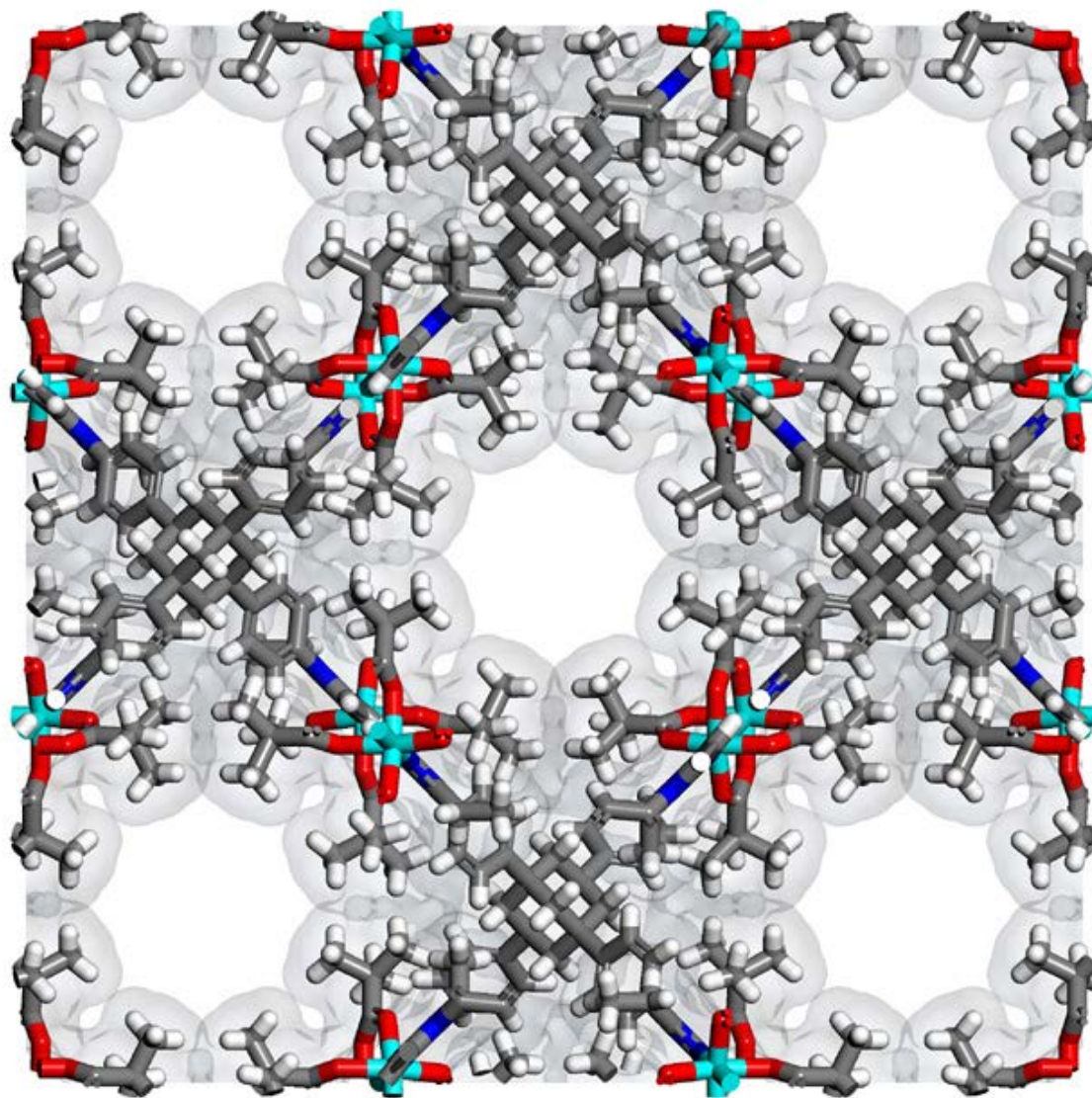
## Flexible Metal-Organic Framework with Hydrophobic Pores

Xie Lin-Hua 백명현

서울대 화학부

In recent years, metal-organic frameworks (MOFs) have been intensively studied as a new type of porous materials due to their promising application potential for gas storage and separation, chemical sensor, catalysis, fabrication of metal nanoparticles, etc. An obstacle for their applications is moisture sensitivity of the porous frameworks. Here, we present a new MOF with one-dimensional channels with a diameter of about 6.5-7.0 angstroms lined by the hydrophobic tert-butyl groups. After activation with supercritical CO<sub>2</sub>, PXRD patterns revealed that the structure was severely shrunk. Gas sorption studies revealed that the activated compound was able to adsorb most common gases (N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub> and CH<sub>4</sub>). In particular, stepwise adsorption and hysteretic desorption behaviors, which must be related with the breathing effect of the framework, were observed for N<sub>2</sub>, O<sub>2</sub> and CO<sub>2</sub> gases. However, no water uptake was observed even under the saturated water-vapor pressure at room temperature. PXRD patterns also indicated that this hydrophobic material was stable even after exposure to saturated water vapor or immersion in liquid water for a week. In contrast, the as-synthesized phase turned to be amorphous shortly after being

immersed in water. Besides, Grand Canonical Monte Carlo simulations for water adsorption for framework of the as-synthesized phase revealed the presence of hydrophilic sites on its pore surface. These results demonstrated that the structural shrinkage of the framework upon guest removal profoundly changed the pore surface and enhanced its hydrophobicity.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication and characterization of copper sulfide surface by hydrothermal method**

**김종욱 진종성 정의덕**

한국기초과학지원연구원 부산센터

Surface modification of copper plate has been used to obtain better interaction with other materials such as organic polymers. Copper sulfide incorporation onto the surface of copper plate have been hydrothermally fabricated at 140 °C for various reaction time with sodium dodecyl benzene sulfonate (SDBS) as surfactant. The morphological structure of surface was characterized by scanning electron microscopy (SEM), energy dispersive spectrometer (EDS) and transmission electron microscopy (TEM). The crystal structure was confirmed by X-ray diffraction (XRD) and the chemical bonding states was measured by X-ray photoelectron spectroscopy.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

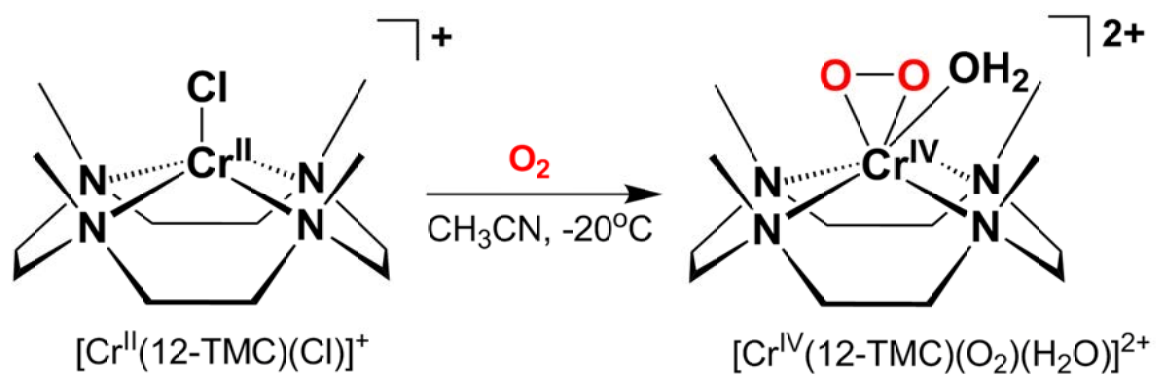
## **A Mononuclear 'side-on' Chromium(IV)-Peroxo Complex : Crystallographic and Spectroscopic Characterization and Reactivity**

**한정은 조재흥<sup>1</sup> 남원우<sup>2</sup>**

이화여대 바이오융합과 <sup>1</sup>이화여대 나노과학부 <sup>2</sup>이화여대 화학과

Metal dioxygen adducts, such as metal-superoxo and -peroxo species, are key intermediates detected in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. The synthesis and spectroscopic characterization of an end-on Cr(III)-superoxo complex with a 14-membered macrocyclic ligand and its reactivity in C-H bond activation (e.g., electrophilic reactivity) was reported previously. In this work, Cr(IV)-peroxo complex,  $[\text{Cr}^{\text{IV}}(12\text{-TMC})(\text{O}_2)(\text{Cl})]^+$  (12-TMC=1,4,7,10-tetramethyl-1,4,7,10-tetraazacyclododecane), was synthesized by changing ring size of the macrocyclic ligand, and characterized with X-ray crystallography and spectroscopic methods such as UV-vis absorption, electrospray ionization mass, EPR, resonance Raman. In contrast to the end-on Cr(III)-superoxo complex, the Cr(IV)-peroxo complex was not reactive in electrophilic reactions but was capable of deformylating aldehydes via nucleophilic reaction. These results indicate the significance of supporting

ligands in tuning the geometric and electronic structures and reactivity of metal-O<sub>2</sub> intermediates that have been shown to have biological as well as synthetic usefulness in biomimetic reactions.





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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Residual acetone produces explosives during the production of graphite oxide

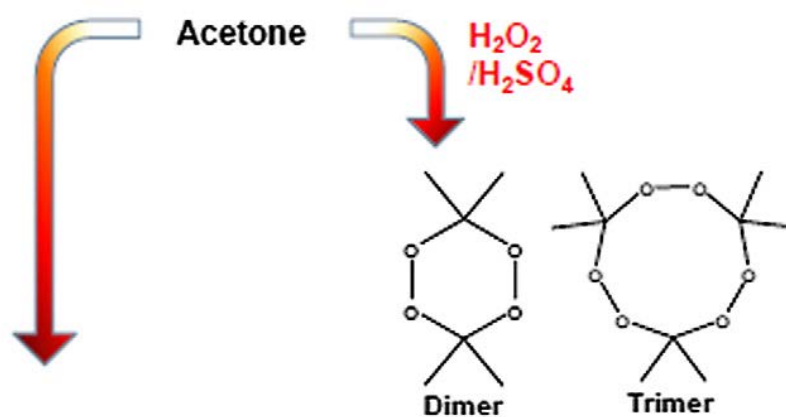
이승준 박성진 오정훈

인하대 화학과

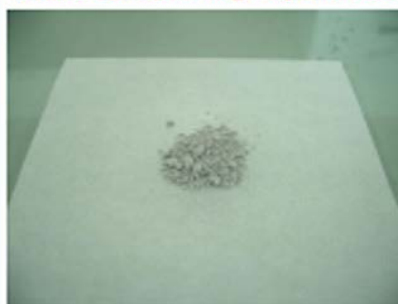
Chemically modified graphenes (CMGs) are promising candidates for a wide range of applications. Graphite oxide (GO) is most commonly used to produce CMGs. We note that residual acetone can produce dangerous explosives during the synthesis of GO. Addition of acetone produced acetone peroxides via a reaction with  $\text{H}_2\text{O}_2$  and  $\text{H}_2\text{SO}_4$ , which are used in the Hummers/modified Hummers methods of making GO. The use of  $\text{Na}_2\text{S}_2\text{O}_3$  instead of  $\text{H}_2\text{O}_2$  yielded GO without making explosives.

### Hummers/modified Hummers method

1. Graphite
2.  $\text{H}_2\text{SO}_4$
3.  $\text{KMnO}_4/\text{NaNO}_3$
4. Excess water
5.  $\text{H}_2\text{O}_2$



Mixture including explosives



Acetone peroxide



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발표코드: INOR.P-264

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization, and Crystal Structures of Intramolecularly Stabilized Group 13 Metal Complexes Containing an o-Carboranyl Chelating Ligand Systems

김소연 강상욱<sup>1</sup> 이종대

조선대 화학과 <sup>1</sup>고려대 소재화학과

The reaction of  $\text{LiCab}^{\text{D}}$  (closo-1-[(dimethylamino)- or (dimethylphosphino)methyl]-2-lithio-o-carborane) with  $\text{MX}_3$  ( $\text{M} = \text{Al, Ga, In}$ ;  $\text{X} = \text{Cl, Br}$ ) in a 1:1 ratio produced the four-coordinated metallacyclic organoaluminum, -gallium, and -indium compound  $\text{Cab}^{\text{D}}\text{MX}_2$ , in which the group 13 metal atoms were stabilized via intramolecular C,D-coordination. The X-ray structural studies of  $\text{Cab}^{\text{D}}\text{MX}_2$  ( $\text{D} = \text{NMe}_2$ ,  $\text{M} = \text{Ga}$ ,  $\text{X} = \text{Cl, Br}$ ) and  $\text{Cab}^{\text{D}}\text{MMe}_2$  ( $\text{D} = \text{PMe}_2$ ,  $\text{M} = \text{Ga, In}$ ) indicate that the aluminum atom is located in the center of a distorted tetrahedron. The reaction of  $\text{LiCab}^{\text{D}}$  with  $\text{MX}_3$  ( $\text{D} = \text{NMe}_2, \text{PMe}_2$ ;  $\text{M} = \text{Ga, In}$ ;  $\text{X} = \text{Cl}$ ) in a 2:1 ratio afforded the bis[(dimethylamino)methyl-o-carboranyl]gallium or bis[(dimethylphosphino)methyl-o-carboranyl]gallium or indium compounds. The NMR spectra revealed that intramolecular M-D coordination occurs in solution, resulting in a pentacoordinate  $(\text{Cab}^{\text{D}})_2\text{MX}$  structures.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Constrained-Geometry Group 13 Metal Complexes with $\eta^5;\eta^1$ -Coordination: Syntheses, Structures, and Theoretical Studies of Dicarbolylamino Group 13 Metal Complexes

황조현 강상욱<sup>1</sup> 이종대

조선대 화학과 <sup>1</sup>고려대 소재화학과

A series of group 13 main group complexes (with a formula  $[(\eta^5\text{-RC}_2\text{B}_9\text{H}_9)(\text{CH}_2)_n(\eta^1\text{-NR}'_2)]\text{MMe}$  ( $\text{M} = \text{Al}, \text{R} = \text{H}, \text{Me}; \text{Ga}, \text{R} = \text{H}, \text{Me}; \text{In}, \text{R} = \text{H}, \text{Me}; n = 1, 2; \text{R}' = \text{Me}, \text{Bn}$ )) with  $\pi,\sigma$ -type bonding interactions was produced by the reaction of group 13 metal alkyls ( $\text{MMe}_3$ ;  $\text{M} = \text{Al}, \text{Ga}, \text{In}$ ) with dicarbollylamine ligands (nido-8-R-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>10</sub>-7-(CH<sub>2</sub>)<sub>n</sub>NHR'<sub>2</sub> ( $\text{R} = \text{H}, \text{Me}; \text{R}' = \text{Me}, \text{Bn}$ )). The reactions of dicarbollylamino with  $\text{AlMe}_3$  in toluene initially afforded tetra-coordinated aluminum complexes with  $\sigma,\sigma$ -type bonding interactions,  $[(\eta^1\text{-RC}_2\text{B}_9\text{H}_{10})(\text{CH}_2)_n(\eta^1\text{-NR}'_2)]\text{AlMe}_2$  ( $\text{R} = \text{H}, \text{Me}; \text{R}' = \text{Me}, \text{Bn}$ ), which readily underwent further methane elimination to yield the corresponding constrained geometry complexes (CGCs) of aluminum with  $\pi,\sigma$ -bonding interactions. However, the reactions between dicarbollylamino and  $\text{MMe}_3$  ( $\text{M} = \text{Ga}, \text{In}$ ) in toluene produced gallium and indium  $\pi,\sigma$ -CGCs directly, without proceeding through  $\sigma,\sigma$ -intermediates. The structures of group 13 metal CGCs

were established by X-ray diffraction studies of dicarbollyaminoaluminum, -gallium complexes, which confirmed the characteristic  $\eta^5;\eta^1$ -coordination mode of the dicarbollylamino ligand to the group 13 metals.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization, and X-ray Crystallographic Studies of Intramolecularly Stabilized Organotin Compounds Containing the o-Carboranyl Ligand Systems

박상하 강상욱<sup>1</sup> 이종대

조선대 화학과 <sup>1</sup>고려대 소재화학과

A variety of organotin complexes, containing the dimethylamino- or methoxymethyl-o-carborane ligand ( $\text{Cab}^{\text{C,D}}$ ; D = N or O), has been prepared by the reaction of  $\text{LiCab}^{\text{C,N}}$  or  $\text{LiCab}^{\text{C,O}}$  with organotin halides. In this way, the tetraorganotin compounds ( $\text{Cab}^{\text{C,D}}$ ) $\text{SnMe}_3$ , triorganotin halide ( $\text{Cab}^{\text{C,D}}$ ) $\text{SnR}_2\text{X}$  (R = Me, X = Cl, R = Me, X = Br), and monoorganotin trichloride ( $\text{Cab}^{\text{C,D}}$ ) $\text{SnCl}_3$  have been synthesized and characterized.  $^1\text{H}$  and  $^{119}\text{Sn}$  NMR spectroscopy indicates that the tin center in the tetraorganotin ( $\text{Cab}^{\text{C,D}}$ ) $\text{SnMe}_3$  is tetracoordinate, whereas this center in mono-, di-, and triorganotin compounds is pentacoordinate as a result of intramolecular Sn $\cdots$ D coordination. The molecular structures of triorganotin complexes were determined by X-ray analysis. As a result of the Sn $\cdots$ D interaction, the tin atoms in triorganotin complexes exhibit distorted trigonal-bipyramidal configurations with the electronegative atoms (N and Cl) in apical positions.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Syntheses and Characterization of Bis(triptycene)metallafluorene Derivatives for Explosive Sensor and O-LED Application

이성기 손홍래

조선대 화학과

Metallafluorene have recently received much attention because of their unusual electronic properties. These unusual optical and electrical properties can be useful in electronic devices, such as electron transporting materials, light-emitting diodes (LEDs), and chemical sensors. It is also reported that silole-containing polymers are selective chemosensors for nitroarematec oxidants, including TNT. Detection has been achieved though fluorescence quenching of the silole by the electron-deficient analyte. The luminescence of silole is due to a  $\sigma^*$ - $\pi^*$  LUMO stabilized though conjugation of the  $\sigma^*$  orbital of the silicon chain with the  $\pi^*$  orbital of the butadiene moiety. The selectivity of the sensor is due to the helical structure of metallafluorene, which permits the intercalation of planar nitroaromatics. Here we report the synthesis of new type of photoluminescent metallafluorene. New metallafluorene have been characterized by NMR, FT-IR, UV-vis absorption spectroscopy and X-ray single crystallography. Their optical characteristics have been also investigated using photoluminescence spectroscopy.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemical Sensor Based on Porous Silicon Dual Transducers

김성룡 손홍래

조선대 화학과

Novel porous silicon (PSi) chip exhibiting dual optical properties, both Fabry-Perot fringe (optical reflectivity) and photoluminescence had been developed and used as chemical sensors. PSi samples were prepared by an electrochemical etch of p-type silicon. The PSi was illuminated with a 300 W tungsten lamp for the duration of etch. Etching was carried out as a two-electrode galvanostatic procedure at an anodic current. The surface of PSi was characterized by FT-IR instrument. The porosity of samples was about 80%. Three different types of PSi, fresh PSi (Si-H terminated), oxidized PSi (Si-OH terminated), and surface-derivatized PSi (Si-R terminated) were prepared by the thermal oxidation and hydrosilylation. Then the samples were exposed to the vapor of various organics, such as chloroform, hexane, methanol, benzene, isopropanol, and toluene. Both reflectivity and photoluminescence were simultaneously measured under the exposure of organic vapors. These surface-modified samples showed unique respond in both reflectivity and photoluminescence with various organic vapors. While polar molecules exhibit



greater quenching photoluminescence, molecules having higher vapor pressure show greater red shift for reflectivity. The possible application of PSi as sensors will be discussed.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Improved Photoluminescence of Silicon nanoparticles by FRET

조보민 손홍래

조선대 화학과

Photoluminescent silicon nanoparticles were prepared by an electrochemical etch of n-type silicon under the illumination with a 300 W tungsten filament bulb for the duration of etch. The red photoluminescence emitting at 650 nm with an excitation wavelength of 450 nm is due to the quantum confinement of silicon nanocrystallites in porous silicon (PSi). Surface-oxidized red luminescent PSi was obtained by an electrochemical treatment of fresh PSi with the current of 150 mA for 600 seconds in water and sodium chloride. Prepared PSi was sonicated and centrifuged in toluene solution to obtain photoluminescence silicon quantum dots. Dichlorotetraphenylsilole exhibiting an emission band at 530 nm was reacted with silicon quantum dot to give a silole-derivatized silicon quantum dots. Optical characteristic of silole-derivatized silicon quantum dots were investigated by UV-vis and fluorescence spectrometer. The emission efficiency of fluorescence for the silole-derivatized silicon nanoparticles was increased by about 2.5 times due to FRET from silole moiety to silicon quantum dots.

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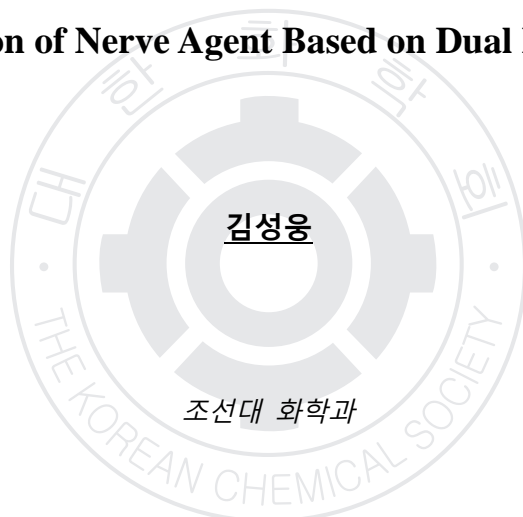
장소: 일산KINTEX

발표코드: INOR.P-270

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Detection of Nerve Agent Based on Dual PSi Chip



Novel porous Si exhibiting dual optical properties, both Fabry-Pérot 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.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fragmentation kinetics of icosahedral clusters: $\text{Ar}_{12}(\text{Ar})$ and $\text{Ar}_{12}(\text{Ar}^+)$

이종백 H. K. Shin<sup>1</sup> 김성희

전남대 화학교육과 <sup>1</sup>Dept. of Chem. University of Nevada

We study the fragmentation kinetics of icosahedral  $\text{Ar}_{12}(\text{Ar})$  and  $\text{Ar}_{12}(\text{Ar}^+)$  clusters in the temperature range of 10 ? 300 K, using a classical dynamics method for detailed forms of host-host and host-guest interaction energies. For ionic clusters, the energy includes charge-induced dipole and induced dipole-induced dipole interactions. The extent of fragmentation of charged clusters is about 20 % and weakly dependent on temperature, whereas that of neutral clusters is strongly temperature dependent. The dominant products from  $\text{Ar}_{12}(\text{Ar}^+)$  are 10-Ar and 9-Ar clusters, but all sizes are found from  $\text{Ar}_{12}(\text{Ar})$ , showing very different size distributions between the two types. The fragmentation of  $\text{Ar}_{12}(\text{Ar}^+)$  occurs on two timescales; rapid fragmentation at short-time with rate coefficients  $\sim 3 \times 10^{11} \text{ s}^{-1}$  and slow process at long time with  $\sim 2 \times 10^{10} \text{ s}^{-1}$ . In the neutral case, where rate coefficients are  $\sim 10^9 \text{ s}^{-1}$ , the time evolution of the concentration of fragmented host atoms is sigmoidal. An autocatalytic mechanism is shown to operate in the fragmentation of weakly bonded neutral clusters explaining host-atom cooperativity.

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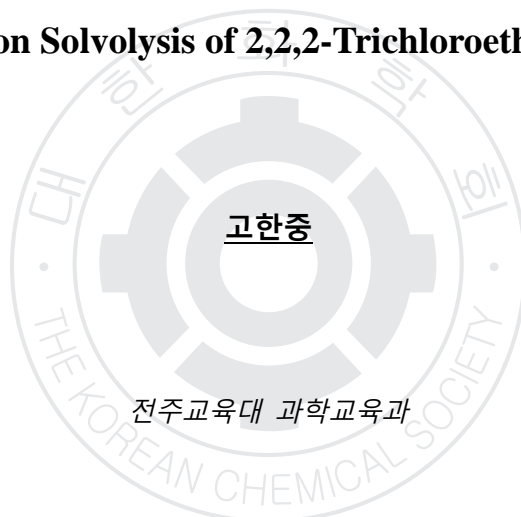
장소: 일산KINTEX

발표코드: **PHYS.P-272**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Kinetic Study on Solvolysis of 2,2,2-Trichloroethyl Chloroformate



The solvolysis rate constants of 2,2,2-trichloroethyl chloroformate in 30 different solvents are well correlated with the extended Grunwald-Winstein equation, using the N solvent nucleophilicity scale and the Y solvent ionizing scale, with sensitivity values of  $1.28 \pm 0.06$  and  $0.46 \pm 0.03$  for l and m, respectively. The activation enthalpies are 10.1 to 12.8 kcal/mol and the activation entropies are -27.8 to -36.8 cal/mol $\cdot$ K, which is consistent with the proposed bimolecular reaction mechanism. The kinetic solvent isotope effect (MeOH/MeOD) of 2.39 is also in accord with SN2 mechanism probably assisted by general-base catalysis.

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발표코드: **PHYS.P-273**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Relations between resonance structures in different limit intervals of  
Rydberg series in three-channel-systems studied by multichannel  
quantum defect theory**



이천우

아주대 화학과

Relations between fitted parameters below and above the thresholds in the systems involving 3 channels are obtained using phase-shifted version of the multichannel quantum-defect theory (MQDT). Analytical continuations of the photoionization cross sections are examined using several representations.

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발표분야: 물리화학

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## **Study of the resonance structures of the preionizing spectrum of molecular hydrogen by phase-shifted multichannel quantum defect**

**theory**

**이천우**

아주대 화학과

At least 6 interloper Rydberg series participate over most of its energy range and more interloper series participate at a narrow range around 124500 cm<sup>-1</sup> in the preionization spectrum of H<sub>2</sub> in the region immediately above its H<sub>2</sub><sup>+</sup> ionization threshold, converging toward its rotationally excited limit. Only a limited success was attained in handling this spectrum in the previous study. The intended general formulas are obtained.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

**N<sub>2</sub>에 있어서 위상변이 MQDT를 이용한  $n$  에 따른 P, Q, R branch  
의 상대적 강도 변화와 회전-진동-전자 운동 채널간의 상호작용에  
관한 연구**

**이천우**

아주대 화학과

질소분자의 리드버그 스펙트럼은 수소분자의 리드버그 스펙트럼과 더불어 가장 많이 실험적, 이론적 연구가 되어 있는 분야로, Worley 시리즈, Worley-Jenkins 시리즈, Carroll-Yoshida 시리즈가 유명하다 (Lofthus and Krupenie, 1977). 또한 여러 연구자들에 의해 MQDT 계산이 수행되었다 (Huber and Jungen, 1990; Jungen et al., 2003; Dehmer et al., 1984; Huber et al., 1994; Giusti-Suzor and Lefebvre-Brion, 1984). 질소분자의 자동이온화 (autoionization) 스펙트럼에서 많이 연구가 되어 있는 것이 리드버그 시리즈에서 주양자수가 작은 값에서 큰 값으로 변하게 되면 Hund 경우의 b 에서 d 로 바뀌게 되는데 (이는 프레임 변환 MQDT 에 의해 잘



기술된다) 이에 따라, 스펙트럼의 회전구조에서 흥미로운 법칙이 실험적으로 발견이 되었는데 (Dehmer et al., 1984), 작은  $n$ 에서는  $1\Sigma_u^+ \rightarrow 1\Sigma_g^+$  전이의 경우  $P\Sigma$  와  $R\Sigma$  가지가 관찰이 되고,  $1\Pi_u \rightarrow 1\Sigma_g^+$  전이에서는  $P\Pi$ ,  $Q\Pi$ ,  $R\Pi$  가지 모두가 관찰이 되는데 반해 중간의  $n$  값에서는  $P\Sigma$  와  $R\Sigma$  가지가 매우 약해져  $Q\Pi$ ,  $R\Pi$ ,  $P\Sigma$  만이 관찰되는데  $P\Sigma$  는 그 중 가장 약하고 가장 퍼져 있게 된다. 더 큰  $n$ 에서는 이들 가지들은 모두 하나의 피크로 합해져서 나타나게 된다 (Carroll, 1973; Dehmer et al., 1984). MQDT 는 스펙트럼의 전체 모양을 불과 몇개의 변수에 의해 아주 잘 재현하므로 이러한 리드버그 계열의  $n$  값의 변화에 따른 스펙트럼의 회전 구조의 연구에 아주 적합하다. 위상변이 MQDT 를 쓰면, 우리는 이들 회전구조에 미치는 채널의 영향을 분석할 수 있으므로 이러한 현상을 위상변이 MQDT 로 연구했다.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Stability of loop shape boron cluster studied by dynamic reaction coordinate method using DFT-calculated electronic energies

장효원

순천대 화학과

In addition to the usual harmonic vibrational mode analysis, we apply the DRC method to examine the thermal stability of certain boron cluster forming regular hexagonal loop shape. The classical trajectories at 200K, 300K, and 400K are calculated on the DFT potential energies calculated on-the-fly during the trajectory propagation. The initial kinetic energies are distributed among all harmonic normal mode as determined by Boltzmann distribution at the given temperatures with or without randomizing the velocity directions. At low temperatures, the cluster remains in the valley of the equilibrium geometry upto 0.5ps, but at 400K, we observed that a geometry transition to other geometry occurred around 3ps. The saddle point geometry and activation energy accompanied are tried to be characterized.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mechanism of prebiotic adenine synthesis from HCN by oligomerization

정선화 최종철

동국대 화학과

We have explored the potential energy surfaces (PESs) for the adenine (formally  $\text{H}_5\text{C}_5\text{N}_5$ ) synthesis by oligomerization of HCN in the gas phase. Based on quantum chemical calculations with the CBS-QB3 method, a complete reaction pathway is proposed for HCN dimerization and the sequential HCN additions to give trimer, tetramer, and pentamer, which forms adenine finally. An alternative pathway with the aid of protons is also proposed, in which  $\text{HCNH}^+$  is added to each oligomerization step instead of HCN. From the obtained PESs, the possibility of adenine synthesis under interstellar conditions will be discussed.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dimerization of HCN in the gas phase: A theoretical mechanistic study

**임민경 최종철**

동국대 화학과

Potential energy surfaces for the formation of covalently bound HCN dimers from two molecules of HCN or HNC were determined from CBS-QB3/APNO calculations. Several novel pathways, with and without the aid of proton, were found for the formation of iminoacetonitrile ( $\text{HN}=\text{CHCN}$ ), an intermediate in adenine synthesis from HCN by oligomerization. Covalent C-C or C-N bonds between the two monomers were formed after rearrangement of bimolecular complex intermediates. Energetic and kinetic analyses suggested that the thermal formation of iminoacetonitrile by the dimerization of HCN cannot occur efficiently under interstellar conditions, whereas it can through ion-molecule reactions aided by protons.

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발표분야: 물리화학

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## Observation of Vibronic Emission Spectrum of Jet-Cooled 2-Fluoro-m-Xylyl Radical Generated during Corona Discharge

윤영욱 이상국

부산대 화학과

The jet-cooled 2-fluoro-m-xylyl radical was generated and vibronically excited in a corona excited supersonic expansion from precursor 2-fluoro-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-fluoro-m-xylyl radical was recorded 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-fluoro-m-xylene.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Boron-11 solid-state NMR study of some boronic acids (I)**

**오세웅 David L Bryce<sup>1</sup>**

목포대 화학과 <sup>1</sup>Department of Chemistry, University of Ottawa, Canada

Boronic acids are used extensively in organic chemistry as chemical building blocks and intermediates and the most widely used example is the Suzuki-Miyaura coupling, which is useful synthetic route to biaryl compounds. These diverse numbers of applications of boronic acids means that an understanding of the structural and electronic properties of these compounds is imperative. In this study, some arylboronic acids are investigated using <sup>11</sup>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 <sup>11</sup>B electric field gradient and chemical shift tensors are determined. Calculations of the <sup>11</sup>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.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Encapsulation Property of Stimulus-Responsive Azobenzene Supramolecule: Hollow Nanospheres**

**이상윤 김종만<sup>1</sup> MASAHIKO HARA<sup>2</sup>**

*RIKEN Advanced Science Institute, RIKEN-HYU 협력연구센터 <sup>1</sup>한양대 응용화학생명공학부*

*<sup>2</sup>RIKEN Advanced Science Institute*

Using stimulus-responsive azobenzene supramolecular structures derived from benzentricarboxamide derivative (BTCA), we found that the BTCA supramolecules shows a formation of spheres via self-assembly upon exposure to aqueous tetrahydrofuran (THF) environment. In this presentation, we demonstrate encapsulation property of the hollow spheres formed from BTCA in aqueous THF. Employing fluorescence probes sensitive to solvents, our photoluminescence measurements of the hollow spheres indicate that the core site is in a THF-rich environment. Consequently, we verify that THF-dispersible quantum dots are encapsulated in the BTCA spheres by fluorescence microscopy. Moreover, we present that the fluorescence quenching do not occur after BTCA encapsulation of the fluorophores in aqueous THF, where rhodamine B and single-walled carbon nanotube work as a fluorophore and the fluorescence quencher, respectively.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Modeling of Covalent-Organic Polyhedra Based on Schiff Base Formation

김대진 정동현 국혜인 최기향<sup>1</sup> 최승훈

(주)인실리코텍 <sup>1</sup>고려대 화학과

Schiff base containing imine bonds has the polydentate nature which makes covalent-organic polyhedral based on Schiff base (COP-SB) excellent scaffolds for the coordination of multiple metal ions. These multimetallic complexes frequently exhibit intriguing magnetic, catalytic, or supramolecular behavior. Supramolecular behavior of COP-SB may be a positive characteristic for application to hydrogen storage because it can take up and release hydrogen reversibly with fast kinetics. In this work, we suggest new models of COP containing Schiff bases. COP-SB can be synthesized by the [6+4] condensation which means that 6 dialdehyde molecules with 4 triamine molecules make 12 imine bonds. During the reversible process of imine bond formation and break, the reaction is driven toward the most stable product, and this process is called dynamic covalent bond. For the utilization of dynamic covalent bond, exothermic process is predominant in the experimental synthesis. So, modeled COP-SBs are constructed by the combination of various dialdehyde and triamine reactants. Density functional theory (DFT) calculations



are performed for the prediction of thermodynamic stabilities of reactant and product. In this work, we investigate the synthetical probability by means of calculated reaction energy of COP-SBs. Low symmetry and introduction of hydroxyl group enhance the stability of COP-SBs.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facilitated protein-DNA binding: Theory and Monte Carlo simulation



김태준 김효준

동아대 화학과

We present the facilitated diffusion effect on protein-DNA binding. The coupling between one-dimensional and three-dimensional diffusive motions is studied by a rigorous theoretical approach. For a simplified model, we show that the approach can provide numerically exact results. We also perform the lattice-based Monte Carlo simulations to confirm the results.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhanced Monte Carlo Simulation Method for diffusion-influenced reaction

안서연 김태준 김효준

동아대 화학과

The diffusion-influenced reactions have been tackled with a variety of theoretical approaches and simulation methods. The lattice-based Monte Carlo simulation method is one of the most efficient methods. In this presentation, we show our recent methods to improve the efficiency of the simulation methods further. Since the enhanced Monte Carlo simulation methods are especially practical for long time dynamics where many interesting universal laws can be found, they will be useful for analysis of many diffusion-influenced reactions.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Hydrogen Atom Migration in Graphite

국혜인 김대진 정동현 최승훈

(주)인실리코텍

The dynamic behavior of hydrogen atoms adsorbed on graphite surfaces has raised attention since hydrogenation of graphite by spillover mechanism is thought to be a prominent hydrogen storage method. In order to explain the hydrogen spillover into graphite, the hydrogen atom migration mechanism should be investigated thoroughly. It has been theoretically predicted that hydrogen atom migration on the pristine graphene surface is unfavorable due to high kinetic energy barrier. However, hydrogen spillover phenomena have been explored in activated carbon that is containing graphite flakes, a lot of defects, amorphous phase carbon and so on. Therefore, it is needed to investigate more realistic models to find possible migration pathways. To this end, we explored pathways for hydrogen atom migration in graphite and suggest models for hydrogen atom migration. We used the 3x3x3 graphite and investigated the kinetic energy barrier for the hydrogen atom migration in the intralayer, interlayer and the outmost layer of graphite using density functional theory (DFT) method. Hydrogen atom in the outmost graphite layer is more stable than hydrogen atom in the interlayer in our result. However, the kinetic energy barrier of the

interlayer or intralayer for hydrogen atom migration is lower than that of outmost layer about 1.7 eV. It shows that if hydrogen atom is introduced in the interlayer of graphite, it is possible for hydrogen atoms to migrate long distances in the interlayer or intralayer of the graphite.



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## Impact of Surface Chemical Heterogeneity on Protein Self-Assembly in Water

정성호 함시현

숙명여대 화학과

Hydrophobicity is thought to underlie self-assembly in biological systems. However, the protein surface comprises hydrophobic and hydrophilic patches, and understanding the impact of such a chemical heterogeneity on the protein self-assembly in water is of fundamental interest. Here, we report structural and thermodynamic investigations on the dimer formation of amyloid-beta proteins in water using the unguided, fully atomistic, explicit-water molecular-dynamics simulations as well as the integral-equation theory of liquids. We demonstrate a key role of hydrophilic residues in initiating the dimerization process: a long-range water-mediated attractive force of enthalpic origin acting on the hydrophilic residues provides the major thermodynamic force that drives two proteins to approach from a large separation to a contact distance. After two proteins make atomic contacts, the nature of the water-mediated attraction changes from a long-range enthalpic interaction to a short-range entropic one. The latter acts both on the hydrophobic and hydrophilic residues. Along with the direct protein-protein interactions that lead to the

formation of inter-monomer hydrogen bonds and van der Waals contacts, the water-mediated attraction of entropic origin induces structural adjustment of constituent monomer proteins toward the formation of a compact dimer structure.



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## Characterizing Familial Alzheimer's Disease Mutations from Molecular Dynamics Simulations with Explicit Water

이가람 정성호 함시현

숙명여대 화학과

Alzheimer's disease is a neurodegenerative disorder characterized by progressive deposition of 40-42 residue amyloid-beta (Ab) proteins in brain parenchyma and cerebral blood vessels. Several pathogenic mutations of Ab proteins have been identified that exhibit enhanced neurotoxicity and aggregative ability such as Dutch (E22Q) and Italian (E22K) mutations. However, the structural and mechanistic information on those Ab mutants has been still limited. Here, we report multiple all-atom molecular dynamics simulations for the wild-type 42-residue Ab protein and its Dutch and Italian mutants. We discuss the mutation effects on the structure of Ab protein focusing in particular on features that may promote its aggregation propensity.



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## Kinetics of diffusion-influenced reactions with long-range reactivity

손창윤 김재훈 이상엽

서울대 화학부

Recently we proposed a new method of solution for the Fredholm integral equations of the second kind. The method would be useful when the direct iterative approach leads to a divergent perturbation series solution. By using the method, we obtained an accurate expression of the propagator for diffusive dynamics of a pair of particles interacting via an arbitrary central potential and hydrodynamic interaction. The propagator expression provided accurate rate expressions for the diffusion-influenced geminate and bimolecular reactions occurring at contact distance. In this work, we extend the proposed solution method to treat the reactions with long-range reactivity, like electron and energy transfer reactions, under the influence of arbitrary interaction potential and hydrodynamic interaction. It is shown that our rate expressions provide very accurate results for all tested reaction sink functions and interaction potentials

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## Relative Stability and Axial ( $A \cdots Pd^{II}$ ) Interaction of Tetracoordinate $Pd([9]aneB_2A)L_2$ Complexes

곽옥금 최호준 윤용진<sup>1</sup> 구인선 김봉곤 박종근

경상대 화학교육과 <sup>1</sup>경상대 화학과

The relative stability and the orbital interactions for the equatorial coordination bond of macrocyclic  $[9]aneB_2A$  tridentates to  $PdL_2$  and the axial (soft  $A \cdots Pd^{II}$ ) interaction in tetracoordinate endo- $Pd([9]aneB_2A)L_2$  complexes were investigated using B3P86/lanl2DZ for Pd and 6-311+G<sup>\*\*</sup> for other atoms. The relative stability of some  $Pd([9]aneB_2A)L_2$  isomers is dependent on the axial ( $A \cdots Pd^{II}$ ) interaction and the electronic properties of the soft A (or hard B) and electron-rich trans-L ligand. The unstable tetracoordinate  $Pd([9]aneB_2A)L_2$  type without axial ( $A \cdots Pd^{II}$ ) interaction easily converted to the more stable  $Pd([9]aneBAB)L_2$ . The equatorial or axial directionality for the binding A (or B) site that were coordinated to the Pd center was dependent upon the relative Pd affinity of the soft A (or hard B) donor. The pentacoordinate endo- $Pd([9]aneB_2A)L_2$  complex with the fifth axial (soft  $A \cdots Pd^{II}$ ) bond was stably optimized under the restricted condition. The equatorial and axial ( $A \cdots Pd^{II}$ ) orbital interactions for

the coordination bonds of [9]aneB<sub>2</sub>A to PdL<sub>2</sub> as well as the bridging role of the partially unfilled 3a<sub>1g</sub>(5s)-orbital for the induction effect of L have been described in detail.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Interpolated Mechanics / Molecular Mechanics (IM/MM) Simulation of Proteins**

박재우 이영민

포항공과대 화학과

Fluorescent proteins (FPs) have become widely applied key tools for biological research over the last few decades. Accordingly, their photodynamics has been one of the major targets of interest of many FP researchers. Studying FPs with theoretical chemistry means was difficult, however, due to the complication associated with the constructions of excited state potential energy surfaces (PESs). Here, we extend the interpolated PES technique for condensed phase dynamics [J. Chem. Phys. 2011, 135, 014107] toward the molecular dynamics (MD) simulations of excited state dynamics of the blue fluorescent protein (BFP) and its variants. This strategy, which uses the interpolated PES for an “important” area and the conventional force field for the remaining part, will be called interpolated mechanics - molecular mechanics (IM/MM). Using this approach, we have conducted MD simulations of excited state BFP and its mutants over 10.0  $\mu$ s of aggregate simulation time.

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## **Nanoporous TiO<sub>2</sub>/SiO<sub>2</sub> prepared by atomic layer deposition as adsorbents of methylene blue in aqueous solutions**

서현욱 김영독

성균관대 화학과

TiO<sub>2</sub> films supported by porous SiO<sub>2</sub> with high surface area were synthesized by atomic layer deposition (ALD). Porous structure of SiO<sub>2</sub> could be maintained even after deposition of TiO<sub>2</sub> using 500 ALD cycles. All the TiO<sub>2</sub>-covered SiO<sub>2</sub> samples showed comparable methylene blue (MB) adsorption abilities to that of bare ones. Moreover, MB adsorption capability of TiO<sub>2</sub>/SiO<sub>2</sub> was almost fully recovered by simple re-annealing process, whereas MB adsorption capacity of bare SiO<sub>2</sub> was not fully recovered by the same treatment. FT-IR study demonstrated that thermal decomposition of adsorbed MB molecules was much facilitated in the presence of TiO<sub>2</sub> films, hence preventing deposition of surface-bound species created on the adsorbents surface during the thermal treatment process. Photocatalytic activity of TiO<sub>2</sub>/SiO<sub>2</sub> samples was also investigated as a function of TiO<sub>2</sub> film thickness, and the result will be discussed.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Study of concentration effects on the interaction of PEO with SDS in Magnetized Water

이성현 전상일

강릉원주대 화학과

자화수(magnetized water)는 원래 물분자가 자화 되어서 자기장의 특성을 갖는다는 의미가 아니라, 자기장에 의하여 물분자 배열이 바뀌어져서 특이한 물의 특성을 보이는 상태를 의미한다. 자화수는 물 분자가 더 조밀하게 구조화되어 작은 cluster 들을 많이 형성함으로써 반응성 및 용해도가 증가됨을 보인다. 이전 실험에서 계면활성제의 CMC(critical micelle concentration)는 대조군인 증류수보다 자화수에서 낮은 농도에서 형성되는 것을 확인하였으며, 계면활성제에 고분자 물질의 첨가로 인하여 계면활성제만의 CMC 보다 낮은 농도에서 마이셀을 형성하는 CAC(critical aggregation concentration)도 대조군인 증류수보다 자화수에서 낮은 농도에서 측정됨을 확인하였다. 본 연구에서는 음이온 계면활성제인 SDS(Sodium dodecyl sulfate)에 다양한 농도의 PEO(polyethylene oxide)를 첨가함으로써 SDS의 농도에 따른 PEO의 반응을 점도, 표면장력, 전도도 측정 방법을 이용하여 살펴봄으로써 자화수가 CAC 및 C<sub>2</sub> 형성에 미치는 영향을 알아보고자 한다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-293**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Titanium nitride films produced by laser ablation in nitrogen atmosphere**

정다운 박승민 송재규 신승근

경희대 화학과

Thin TiN films were deposited at room temperature on silicon wafer substrates using the Smolley type source technique. The obtained TiN film were ablated by using a Nd-YAG laser (1064 nm). The samples before and after annealing were characterized at room temperature. The as-deposited TiN thin films were analyzed by Photoluminescence (PL) spectroscopy and X-ray diffraction and Raman spectroscopy.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-294**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Infrared predissociation spectroscopy of aniline-dimer, aniline monohydrated dimer and isolated adenine-thymine base pair**

**MD.ALAUDDIN 박승민 송재규 신승근**

경희대 화학과

Infrared (IR) photodissociation spectra of aniline-dimer ( $\text{An}_2^+$ ), aniline monohydrated dimer ( $\text{An}_2\text{W}^+$ ) and adenine-thymine ( $\text{AT}^+$ ) hetero-dimer clusters have been recorded in the region of 2700-3900  $\text{cm}^{-1}$  in order to investigate the most stable structures of aniline-dimer, aniline monohydrated dimer and adenine-thymine hetero-dimer. From the close investigation of electronic and vibrational gas phase spectra of  $\text{An}_2^+$  and  $\text{An}_2\text{W}^+$ , we found that the cis-arrangement of NH-N type structure of  $\text{An}_2^+$  is the most preferable structure. On the other hand, the vibrational spectrum of isolated  $\text{AT}^+$  base pair was assigned to cluster structures with  $9\text{H}\cdots\text{O}=\text{C}/\text{N}\cdots\text{HN}$  hydrogen bonding by comparison with the DFT calculated vibrational spectra of the most stable  $\text{AT}^+$  isomers. Furthermore, the Watson-Crick AT base pair is not the most stable isolated base pair and its vibrational spectrum is not in agreement with the observed experimental spectrum.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-295**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Stability of metal nanoparticles by laser ablation in various solvents

박영은 송재규 신승근 박승민

경희대 화학과

Laser ablation synthesis in liquid is very simple and eco-friendly technique. Copper and silver nanoparticles were prepared by liquid-phase laser ablation at 1064 nm. We studied the stability of metal nanoparticles in various solvents and analyzed by UV-Visible spectrophotometer and transmission electron microscopy(TEM). We found that aggregation mechanisms were related to the dipole moment of the surrounding molecules. In the future, it is expected to be useful in the nanoparticle engineering.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-296**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The effect of ions in solution on the stability of Au and Ag nanoparticles prepared by laser ablation in liquid**

권혜진 김국기 송재규 박승민

경희대 화학과

Gold and silver nanoparticles were synthesized by laser (Nd: YAG  $\lambda = 1064$  nm) ablation of a gold and silver target immersed in various aqueous electrolyte solutions (7 mM of LiCl, NaCl, KCl, NaBr, and NaI) as well as in deionization water. To investigate the effect of ions in aqueous electrolyte solutions on the stability of nanoparticles, the surface plasmon absorption peak (silver at 400 nm, gold at 520 nm) was measured depending on elapsed time by UV-Vis spectrophotometer. Transmission electron microscopy (TEM) and dynamic light scattering (DLS) also used to observe the size change of nanoparticles depending on elapsed time and ions in aqueous electrolyte solutions.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-297**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Study of plasma plume produced by laser ablation of noble metal in water**

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 pure noble metal in water. The optical intensity of plasma plume depends on magnetic field and ion. Liquid-phase plasma plume analyzed by intensified charge coupled device (ICCD). Also we have studied laser-light scattering for growth processes of silver nanoparticles in liquid phase laser ablation.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-298**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Time Resolved Photodissociation of Chlorobenzene at 266-290 nm

Madhusudan Roy MD.ALAUDDIN 송재규 박승민

경희대 화학과

The time-resolved photodissociation experiment is always fascinating to Mass Spectroscopiest. Here, we have tried to photodissociate  $C_6H_5Cl$  using 266-290 nm. This wavelength was obtained by doubling the wavelength generated in TDL 90 dye laser which was pumped by second harmonic output of a Nd: YAG Laser (Quantel YG 980). The parent ions were generated by fourth harmonic output of a Nd: YAG Laser (Spectra-physics GCR 150). From the experimental results, we found the decay constant increases with the increase in total internal energy of the parent ions and subsequently the decay time decreases. By comparison our experimental results with calculated one (RRKM and VTST), no significant difference have been found.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-299**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication of Si-encapsulated nanoprobe for SERS imaging of multiple protein markers expressed in live cells**

**이상열 전향아<sup>1</sup> 주재범**

한양대 생명나노공학과 <sup>1</sup>한양대 바이오테크놀로지학과

Highly sensitive optical imaging technology using metal nanoparticles has been extensively applied to cellular imaging and biomedical diagnostics. Surface-enhanced Raman scattering (SERS), using the inelastic light scattering of gold or silver nanoparticles, is emerging as a powerful alternative for specific biological targets in live cells. It allows ultra-sensitive biochemical analysis in terms of multiplex targeting using individual spectral signatures or its combinations. Using the SERS technique, it is known that the detection sensitivity is enhanced up to 10<sup>14</sup> orders of magnitude over conventional Raman spectroscopy. Consequently, the SERS technique provides a sensitivity that is comparable with fluorescence detection. Raman mapping is a newly developed and noninvasive preclinical imaging technique that offers picomolar sensitivity and multiplex detection capabilities to the field of molecular imaging. In this study, we demonstrate the applicability of Raman imaging technique for the classification of three different types of protein markers expressed on breast cancer cells. Multiplex SERS imaging of

protein markers on the surface of cancer cells has been carried out using newly developed core-shell SERS nanoprobe. All the SERS nanoprobe were successfully identified by UV/Vis, DLS, TEM, and SERS. The Raman mapping images using the SERS probe could be successfully used for the classification of three different cancer cell lines. The result shows a potential capability of the SERS imaging technique for the preclinical diagnosis of breast cancer.



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장소: 일산KINTEX

발표코드: **PHYS.P-300**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Photophysical properties of dithienothiophene(DTT) core-modified  
expanded porphyrins : Doubly fused rubyrin and doubly fused  
octaphyrin**

김서희

연세대 화학과

분자 중심에 Dithienothiophene 이 결합된 두 가지 분자 - Doubly fused rubyrin 과 Doubly fused octaphyrin-의 광물리적 특성을 알아보고자 여러 분광학 실험을 하였다. Dithienothiophene 은 휘지않으며, 전자가 많은 분자이기 때문에 확장 포피린에 결합시키면 방향성(aromaticity)가 증가할 것으로 기대를 하였다. 기본적인 흡수(absorption), 방출(emission), 들뜬상태에서의 흡수(Transient absorption), 이광자흡수(Two photon absorption) 등의 실험을 통해 Dithienothiophene 이 결합되지 않은 확장 포피린에 비해 방향성이 증가하는 것을 확인하였다. 앞으로 이 Dithienothiophene 을 통한 여러 확장 포피린의 합성과 분광학적 특성을 통해 확장범위가 큰 포피린의 적용까지 기대를 해 보게 될 것이다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-301**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## UV photolysis of substituted thiophenol : Quantum-state specific view of 2-fluorothiophenol-(d<sub>1</sub>)

유현식 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 H/D atom loss processes from gas phase 2-fluorothiophenol-(d<sub>1</sub>), following photolysis at many wavelengths within the range of vibronic bands of S<sub>1</sub> electronic state. These experimental techniques allowed to probe bound (S<sub>1</sub>,  $\pi\pi^*$ ) / repulsive (S<sub>2</sub>,  $n\sigma^*$ ) electronic states characterized by  $R_{S-H}$  of thiophenol species and determine the spatial anisotropy and translational energy distribution of the nascent H/D fragment. 2-FC<sub>6</sub>H<sub>4</sub>S<sup>?</sup> are formed in a selected subset of available vibrational levels and the detected H/D atom confirm the previous findings, regarding thiophenoxy radical formation in both ground and first excited electronic states. Especially, we observe a dependence of the relative yields of two reaction channels and recoil anisotropy of fragments upon photoexcitation energy. So, we expect that the assignments of vibrational levels in S<sub>1</sub> state provide detailed insights into the fragmentation mechanism including coupling modes of CIs related to bifurcation



dynamics and coupling between two (S1/S2) electronic states. Also, comparison with bare thiophenol and phenol will serve to highlight similarities and differences for previously reported photolysis mechanism according to substitution.



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장소: 일산KINTEX

발표코드: **PHYS.P-302**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Upconverting Nanoparticles 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. By using upconverting nanoparticles, we can convert infrared light into visible light. These materials can be a possible candidate to overcome the spectral mismatch of dye-sensitized solar cells(DSSC). Upconverting nanoparticles such as  $\beta$ -NaYF<sub>4</sub> doped with Yb, Er, Ho are the possible candidates for application since they have excellent upconverting efficiencies along with emissions around ~550nm, which can be efficiently absorbed by the N-719 dye. By making different morphologies of  $\beta$ -NaYF<sub>4</sub>(Yb,Er,Ho), we can apply it to different parts of the DSSC and enhance its efficiency by using not only visible light, but also infrared light. Keywords: upconversion, DSSC, dye-sensitized solar cell,  $\beta$ -NaYF<sub>4</sub>

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-303**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication of Cu<sub>2</sub>O/TiO<sub>2</sub> Tube by Electrodeposition for p-n Junction photoelectrode**

**김창우 서상필 Zheng jin you 강영수**

서강대 화학과

We report Cu<sub>2</sub>O/TiO<sub>2</sub> tube by electrodeposition for p-n junction photoelectrode. We prepared successfully heterostructure with visible light activity using a two-step electrochemical process of anodization and an electrodeposition method. Cu<sub>2</sub>O nanoparticles were highly dispersed inside the TiO<sub>2</sub> nanotubes with various conditions. The structure and optical properties of the TiO<sub>2</sub> nanotubes and their heterostructure have been well characterized and displayed a strong photo response in the visible region and low recombination rate of the electron-hole pairs.

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장소: 일산KINTEX

발표코드: **PHYS.P-304**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Photodynamic Behavior of Heteroleptic Ir(III) Complexes with Carbazole-Functionalized Dendrons Associated with Efficient Electron Transfer Processes**

**위경량 이종대<sup>1</sup> 강상욱**

고려대 소재화학과 <sup>1</sup>조선대 화학과

We prepared dendrimers of heteroleptic iridium(III) complexes, which have the dfppy ligand connected to carbazole-functionalized dendron. While parent complex [(dfppy)2Ir(dpq)]<sup>+</sup> (G0) shows an intense emission at 635 nm with a lifetime of 1  $\mu$ s 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 ( $\tau_p$  = 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 ( $\tau_F$  = 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. At 77 K, however, the MLCT emission lifetime for both G1 and G2 is 7  $\mu$ s that is nearly identical to that of G0 (6.8  $\mu$ s), and the carbazole fluorescence lifetime is  $11.5 \pm 0.5$  ns, which is again almost the same as that of Czn-OH (11.5 ns). 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.



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장소: 일산KINTEX

발표코드: **PHYS.P-305**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Gold Nanoparticles Silver-Nanosoldered by Laser Irradiation



손명희 장두전

서울대 화학부

Gold nanoparticles have been silver-soldered to fabricate nanowires by irradiating gold nanospheres of 25 nm in diameter and silver nanospheres of 8 nm in diameter held together on a carbon-coated copper grid with 30 ps laser pulse of 532 nm for 20 min at fluence of 3.0 mJ/cm<sup>2</sup>. Laser-induced nanowelding of silver nanoparticles as well as that of gold nanoparticles has also been carried out by varying the wavelength and fluence of irradiation laser pulses. It has been found that nanosoldering as well as nanowelding depends on laser fluence nonlinearly. Irradiation with an optimum condition of laser fluence is essential for the proper silver nanosoldering of gold nanospheres to produce gold@silver core-shell composite nanowires. The excitation of the surface plasmon resonances of base-metallic gold nanospheres rather than filler-metallic silver nanospheres paves the way for the silver nanosoldering of gold nanoparticles.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-306**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile Synthesis of Single-Crystalline $\text{ZnS} \cdot (\text{en})_{0.5}$ Hybrid Nanobelts

**김연호 장두전**

서울대 화학부

A template-free and one-pot solvothermal process has been developed for the facile synthesis of  $\text{ZnS} \cdot (\text{en})_{0.5}$  (en = ethylenediamine) hybrid nanobelts having controlled length-to-width (aspect) ratios. While typical hybrid nanobelts synthesized at 180 °C for 6 h have an average width of 130 nm, a mean thickness of 55 nm, and an average length of 16  $\mu\text{m}$ , their aspect ratios have been controlled by adjusting solvent volume ratios of hydrazine monohydrate (hm) to en. A sufficient amount of sulfide from the reduction of sulfur by hm has been found to be essential for the efficient anisotropic one-dimensional growth of highly crystalline  $\text{ZnS} \cdot (\text{en})_{0.5}$  hybrid nanobelts. The photoluminescence spectra of  $\text{ZnS} \cdot (\text{en})_{0.5}$  hybrid nanostructures exhibit three bands located at 327, 415-430, and 587-654 nm, which are assigned to band-edge emission, trap sites-related emission, and anion-vacancy emission, respectively. The mean lifetime of photoluminescence having three decay components of 30, 170, and 2700 ps decreases with the volume ratio of hm to en due to the decrease of defect sites with the increase of the aspect ratios of  $\text{ZnS} \cdot (\text{en})_{0.5}$  hybrid nanobelts. Compared with bare-ZnS nanobelts prepared by the hydrothermal treatment

of  $\text{ZnS} \cdot (\text{en})_{0.5}$  hybrid nanobelts, hybrid ones have shown enhanced optical properties that would give them potential for optoelectronic devices.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-307**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Exchange coupling and Size Control of Hard and Soft Phase NdFeB/ $\alpha$ -Fe Magnetic Nanoparticles

Abhijit Pandurang Jadhav 강영수

서강대 화학과

Permanent magnets play very important role in electronics industry. Exchange coupled product of hard phase and soft phase magnetic materials gives enhanced (BH)Max value for the nanocomposite magnetic material. This nanocomposite material can be able to supply miniature electronics parts for the energy conversion of electrical to mechanical and vice versa. Careful control of reaction parameters such as precursor concentration, reaction temperature, choice of suitable solvent and surfactant helps to control particle size in nanometer regime. Homogeneously dispersed nanoparticles of NdFeB were prepared by thermal decomposition method while soft phase magnetic material  $\alpha$ -Fe was prepared in-situ by polyol process. Exchange coupled product of hard phase and soft phase were prepared by surfactant assisted self-assembly method. This nanocomposite material can be able to retain large fraction of saturation field after removal of magnetic field and it is desirable for permanent magnet for electronic industry. Keywords: nano-interface junction, hard phase magnet, soft phase magnet, exchange coupling, energy storage.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-308**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Controlled Formation of Gold Nanorod-Nanosphere Assemblies

임종휘 윤준희 윤상운

단국대 화학과

Assembly of noble metal nanoparticles is important in both fundamental and application aspects. Close proximity of nanoparticles in assemblies leads to the creation of strongly coupled plasmon modes. The resulting strong extinction in the redshifted longer wavelength region enables applications of the assembly structures to biological imaging and photothermal therapy. In particular, anisotropic coupling of nanospheres with nanorods opens possibilities of engineering the surface plasmon coupling in an unprecedented wide range. In this presentation, we report a novel method and its principle to assemble gold nanospheres with gold nanorods. Distance and material-dependent surface plasmon coupling is explored.

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장소: 일산KINTEX

발표코드: **PHYS.P-309**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Fabrication of TiO<sub>2</sub> / SrTiO<sub>3</sub> Hybridstructure for improved  
photocatalytic activity through TiO<sub>2</sub> Tube with Enlarged Pore  
Diameter**

서상필 김창우 강영수

서강대 화학과

SrTiO<sub>3</sub> and TiO<sub>2</sub> heterostructured tubes were fabricated by hydrothermal method using anodized TiO<sub>2</sub> tubes. The pore size of as-fabricated TiO<sub>2</sub> tubes was enlarged for the TiO<sub>2</sub>/SrTiO<sub>3</sub> heterostructure formed inside and outside. Formations of their hetero-structures are proposed and their photocatalytic activity is compared with various SrTiO<sub>3</sub> morphology. Compared with TiO<sub>2</sub> anatase tubes, the enhanced photocatalytic property of TiO<sub>2</sub>/SrTiO<sub>3</sub> tubes of enlarged pore diameter could be attributed to the enhanced of charge separation by TiO<sub>2</sub> tubes / SrTiO<sub>3</sub>.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Asymmetric Core-Satellite Assembly of Gold Nanoparticles: Highly Efficient Assembly Method and Distance-Dependent Surface Plasmon Coupling**

**윤준희 임종휘 윤상운**

단국대 화학과

Assembly of noble metal nanoparticles offers an appealing means to control and enhance plasmonic properties of nanostructures. Therefore, producing homogeneous well-defined assembly structures in a colloidal state with easily modifiable interparticle distances and compositions is highly desirable not only for fundamental studies of plasmonics but also for a variety of applications in biomedicine and photocatalysis. Here we report a novel strategy to assemble gold nanoparticles (AuNPs) into asymmetric core-satellite assembly in a colloidal state with near perfect yield. Our approach is based on exclusive desorption between large and small AuNPs from amine-functionalized glass substrates in ethanol via sonication. Nanogaps between the core and the satellite in these assemblies are controlled on a molecular scale using alkanedithiol linkers, permitting a systematic study of surface plasmon coupling between

AuNPs in unprecedentedly close proximity. Large (51 nm) and small (13 nm) AuNPs are assembled on a glass substrate to form core-satellite nanoclusters and selectively desorbed into ethanol.



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## Synthesis and One-Axis Oriented Fabrication of Tungsten Trioxide Nanoplates on FTO Surface

Song guang 강영수

서강대 화학과

Two kinds of single crystalline tungsten trioxide nanoplates have been synthesized. Monolayer of these two kinds of nanoplate films have been fabricated on FTO surface by simple seed layer assisted hydrothermal method. The high temperature synthesized monoclinic  $\text{WO}_3$  layer shows one-axis oriented property after 500°C calcination while low temperature synthesized orthorhombic  $\text{WO}_3 \cdot \text{H}_2\text{O}$  layer lost its hydrate and one-axis oriented property under same calcination condition. Crystal structure and crystalline of these nanoplates have been determined by XRD, SEM and TEM. Electrochemical properties such as photocurrent and cyclic voltammetry have also been checked for the discussion of the further application of these films. Keywords: tungsten trioxide nanoplate, monolayer, one axis oriented growth, photocurrent.

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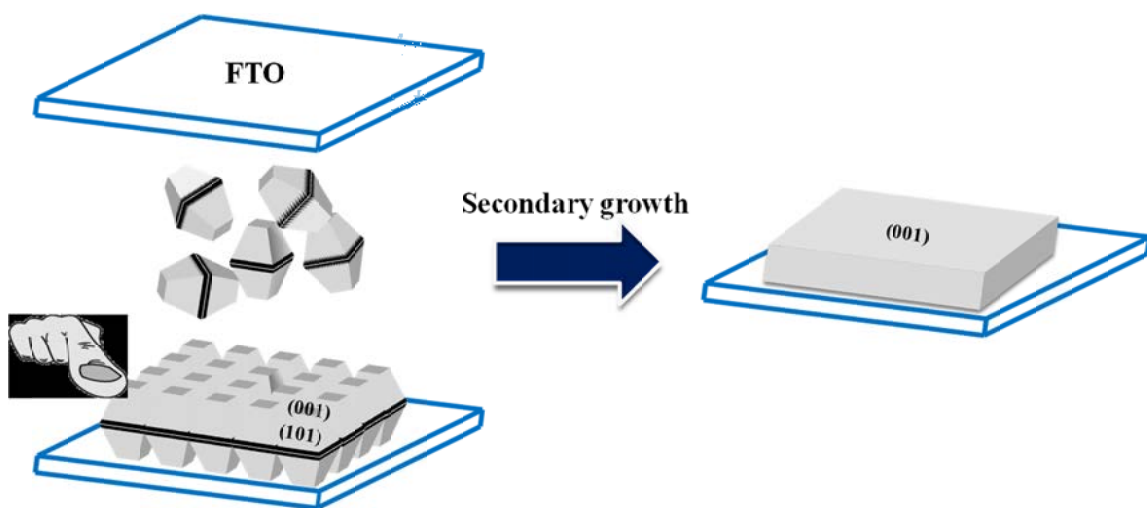
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **TiO<sub>2</sub> films with oriented anatase {001} facets and their photoelectrochemical property**

김태완 차현길 강영수

서강대 화학과

As an important metal oxide, anatase titanium dioxide has been widely investigated because of its many promising properties for catalysis and photocatalysis. The properties of anatase TiO<sub>2</sub> crystals are largely determined by external surfaces exposed. Many efforts have been made to improve the percentage of high-reactive facets like {001} facets of anatase TiO<sub>2</sub> to enhance its catalytic properties. TiO<sub>2</sub> films with oriented anatase {001} facets grown on transparent conductive fluorine-doped tin dioxide substrate were prepared via a facile rubbing method and hydrothermal route. The obtained TiO<sub>2</sub> film as a photoanode shows efficient photoelectrochemical water splitting ability(photocurrent). The presence of high-energy facets in titania improves significantly its adsorption, electronic, and photocatalytic properties, making this material attractive for various environmental and energy-related applications. Keywords : anatase TiO<sub>2</sub>, {001} facets, synthesis and assembly, properties and applications





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## **ZnO Assisted Electron-Hole Separation for Artificial Photosynthesis**

Amor Uttaam Pawar 강영수

서강대 화학과

Research in artificial photosynthesis seeks to replicate the natural process of photosynthesis that converts water and carbon dioxide into carbohydrates and oxygen using sunlight as the energy source. The visible-light driven splitting of water into hydrogen and oxygen and the production of methanol from CO<sub>2</sub> reduction are sometimes included in the definition. ZnO with a direct wide-band gap (3.37 eV) and a larger excitation binding energy (60 meV) has been increasingly studied for many years due to its excellent physical properties and applications in various fields. It is widely reported that the main properties of ZnO nanostructures strongly depends on their morphology, crystalline structure, defect and impurity contents. In this sense, the ZnO preparation route affects in a significant way to those properties. For photocatalytic applications, the improvement of the photoactivity might be achieved by influencing those properties that control either the charge carrier dynamics (carrier generation, transfer and diffusion) or the surface catalytic process, which are the quality of the structure and the surface features. In this sense, here we describe the hexagonal ZnO using solvothermal synthesis would provide the adequate

structural and surface properties for photocatalytic applications. Keywords: artificial photosynthesis, solvothermal, hexagonal ZnO.



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## Hydrodynamic Interactions on the Dynamics of Lennard-Jones Spheres in Crowded Environments

권계민 성봉준

서강대 화학과

Hydrodynamic interaction(HI) on the dynamics of binary mixtures of Lennard-Jones spheres is investigated by using computer simulations. Macromolecular crowding has been known to affect the dynamics of the particles such as diffusion because the environment is far different from the dilute solution. There have been many studies to investigate the dynamic behavior in dense environments. Such studies have usually focused on the decrease of diffusion induced by cage effects without understanding the hopping mechanism and the particle displacement probability that enable us to quantify the properties of crowding. Furthermore, little attention has been paid to the effect of HI in crowded environments. Therefore, we investigate the effect of HI on the dynamics of binary spheres by comparing Brownian Dynamics(BD) to Fast Lubrication Dynamics(FLD) simulations. We find that HI reduces the diffusion of fluid spheres by an order of magnitude in crowded environments. We also find that particle displacement with and without HI are qualitatively similar but the timescales are significantly different.

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## 다양한 그래핀 시트에서의 CO<sub>2</sub> 흡착에 관한 DFT 연구

이건준

한남대 화학

최근 탄소 동소체인 탄소나노튜브, 풀러렌, 흑연 등의 표면에 CO<sub>2</sub> 흡착에 관한 이론과 실험적인 연구가 많이 되고 있으며 그래핀에 CO<sub>2</sub> 를 흡착시키는 연구도 최근 많은 관심을 불러일으키고 있다. 본 연구에서는 각각 32, 40, 그리고 53 개로 구성된 그래핀의 크기에 따른 구조적 변화와 CO<sub>2</sub> 의 위치에 따른 흡착 경향을 순 이론적 (ab initio) 양자 역학적 방법과 범 밀도 함수 이론(density functional theory, DFT)을 이용하여 계산하였다. 그 결과를 이전에 연구된 이론 및 실험 결과와 비교하였으며, 또한 그래핀에 암모니아(NH<sub>3</sub>), 일산화탄소(CO), 일산화질소(NO) 등 다른 기체의 흡착 결과와 비교하였다. 그래핀의 크기를 증가시키는 연구에선 크기의 증가에 비례해서 구조와 에너지적인 면에서 안정해지는 것을 볼 수 있었다.

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## Facile Synthesis of Micron-Sized Spherical CuWO<sub>4</sub> and Hexagonal-Shaped Cu-WO<sub>3</sub>·0.33H<sub>2</sub>O: Characterization and Their Photocatalytic Properties

Zheng jin you 강영수

서강대 화학과

WO<sub>3</sub>, n-type semiconductor, is a candidate photocatalyst for water splitting. The hole mobility and diffuse lengths of WO<sub>3</sub> are 10 cm<sup>2</sup> V<sup>-1</sup>s<sup>-1</sup> and 0.15 μm, respectively, which are the advantages for water splitting. However, WO<sub>3</sub> photoanodes have two defects: its bandgap is 2.7 eV, just on the cusp of the visible part of the spectrum (blue-violet), and WO<sub>3</sub> is only stable under acidic conditions and dissolves to form soluble tungstates at pH > 5. CuWO<sub>4</sub> is an n-type semiconductor with indirect band gap of 2.25 eV, 0.45 eV smaller than the gap of WO<sub>3</sub>. Comparing with WO<sub>3</sub>, the CuWO<sub>4</sub> is more stable than WO<sub>3</sub> for the O<sub>2</sub>-evolution half reaction of water splitting in aqueous electrolytes at pH 7. As its smaller band gap and greater stability in neutral solution, the CuWO<sub>4</sub> would be one of the best candidates for water oxidation and CO<sub>2</sub> reduction photocatalyst. To the best of our knowledge, CuWO<sub>4</sub> with good structure was not reported. In our works, we synthesized micron-sized spherical CuWO<sub>4</sub> and hexagonal-shaped

Cu-WO<sub>3</sub>·0.33H<sub>2</sub>O by novel and facile methods. The preparation, characterization, and optical properties of CuWO<sub>4</sub> electrodes were investigated. Especially, the powder of CuWO<sub>4</sub> was used for water splitting directly. Keywords: copper tungstate, hexagonal-shaped tungsten oxide



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## Sensitization of TiO<sub>2</sub> Nanotubes Arrays with BiOI by SILAR Method

Haider Zeeshan 강영수

서강대 화학과

TiO<sub>2</sub> nanotubes arrays (TNTA) were synthesized by electrochemical anodization of Ti foil using ammonium fluoride in organic electrolyte i.e glycerol at anodization potential of 60 V for 10 h. TNTA were sensitized with visible light active, narrow band gap (1.94 eV) bismuthoxyiodide, which is a p-type semi conductor. BiOI was sensitized through sonication assisted successive ionic layer adsorption and reaction by adsorption of bismuth and iodide ions sequentially. Sonication was helpful to diffuse precursor ions to penetrate inside of the nano channels of titania nanotubes instead of surface deposit. TiCl<sub>4</sub> pretreatment of TNTA was helpful to increase the surface roughness and loading the higher amount of BiOI. Composite photocatalyst indicated higher photocurrent response than TNTA due to visible light activation as well as separation of photogenerated charge carriers. Composite photocatalyst was characterized with XRD, SEM, TEM, UV-Visible spectroscopy and photocurrent measurement. Keywords: TiO<sub>2</sub> nanotubes arrays, bismuthoxyiodide, TiCl<sub>4</sub> pretreatment, successive ionic layer adsorption and reaction.

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## **Nanocrystals of Hematite with Unconventional Shape-Truncated Hexagonal Bipyramid: A Class of Promising Functional Material**

van thanh khue 강영수

서강대 화학과

Abstract: The capping agent plays a critical function for the anisotropic crystal growth to induce polyhedral morphology of a nanocrystal. Uniform and single-crystalline  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> polyhedral nanoparticles in the hexagonal single crystal system named truncated hexagonal bipyramid for the first time was successfully 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  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> 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  $E_g$  is 2.08 eV. The magnetic property studies of truncated hexagonal bipyramid hematite particles shows that this kind of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> 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  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> morphology in whole of the synthetic process was also proposed.



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## Synthesis of Mono-dispersed Sheet-like Monoclinic BiVO<sub>4</sub> Single-Crystals

노현석 차현길 강영수

서강대 화학과

We have developed a hydrothermal process to synthesize mono-dispersed sheet-type monoclinic BiVO<sub>4</sub> single crystals and control their morphology. Monoclinic BiVO<sub>4</sub> single crystals were prepared in an aqueous solution containing bismuth nitrate and sodium vanadate at 110 °C for 10 h with Ethylenediaminetetraacetic acid. A sheet-like monoclinic BiVO<sub>4</sub> single crystal was homogeneously nucleated and precipitated in solution. Crystal growth and preferential growth faces were controlled by the concentration of EDTA and pH. Morphology and crystal structure of the obtained product was compared with XRD, SEM, and TEM.

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## Synthesis of Tetragonal $\text{LaVO}_4$ by Hydrothermal Method and Application to downconversion phosphor of DSSC

김두경 강영수

서강대 화학과

Abstract: Tetragonal  $\text{LaVO}_4$  is an apt host for rare-earth activators. The characteristic of downconversion 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 photooxidized.  $\text{LaVO}_4$  was prepared using  $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ ,  $\text{Dy}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ ,  $\text{NH}_4\text{VO}_3$ , oleic acid and ethanol by hydrothermal method. The adsorption of oleic acid on certain surfaces make nanoparticle as a plate shape which is  $40 \times 40 \times 10$  nm. Using oleic acid as a surfactant makes nanoparticles well disperse into the organic solvents. This property makes easily apply to dye-sensitized solar cell through coating method. Properties of nanoparticles have been checked by XRD, TEM and photoluminescence. Keywords: downconversion, phosphor, tetragonal  $\text{LaVO}_4$ , hydrothermal, DSSC

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## MD Simulation of Imidazolium-based Room Temperature Ionic Liquid Super Capacitors

조성식

서울대 화학부

In a capacitor, ions are attracted to a electrode which has opposite charge and electrode potential is screened. Being difficult to approach the vicinity of electrode, It is predicted that organic ion with long chain length screen less potential. Capacitors made of Imidazolium-based Room Temperature Ionic Liquid [mim][BF<sub>4</sub>] confined between two graphene sheets were studied by MD simulations. Varying the chain length of imidazolium cation, (# = 2, 4, 6) potential drop and capacitance of both electrodes were examined. To examine the effect of steric interaction of chain on screening, cation structure in vicinity of electrodes was investigated. All of these behaviors of RTIL ions in vicinity of electrode were compared with those in vicinity of neutral graphene sheets.

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## Highly Active Oxide Photoanode for Photoelectrochemical Water Oxidation

차현길 강영수

서강대 화학과

A clean and efficient way to overcome the limited supply of fossil fuels and the greenhouse effect is the production of hydrogen fuel from sunlight and water through the semiconductor/water junction of a photoelectrochemical cell, where energy collection and water electrolysis are combined into a single semiconductor electrode. We present a highly active photoanode for water oxidation, consisting of one-axis oriented hematite, which was coated insulator layer of Aluminum based metal oxide and activated for hydrogen evolution with electrodeposited Pt nanoparticles. The roles of the different surface coating components were investigated at a different potential versus the reversible hydrogen electrode.

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## PM3 and ab initio Molecular Orbital Study on the Activity of Physiology for the Capsaicinoids

권혁재 송영대<sup>1</sup> 이갑용<sup>2</sup>

대구가톨릭대 화학과 <sup>1</sup>경운대 한방자원학부 <sup>2</sup>대구가톨릭대 생명화학과

To investigate the activity of physiology for capsaicinoids, we analyzed the quantum chemical indices for the octanoyl-vanillamide, nonivamide, nordihydro-capsaicin, capsaicin, homocapsaicin, and homodihydrocapsaicin by calculation using the semiempirical PM3 and ab initio methods. It was found that the electron is transferred from HOMO energy of guanine among DNA bases to LUMO energy of capsaicinoids. It is appear that capsaicinoids compound plays an important role in the formation of complex with guanine of DNA bases.

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## One-Step Fabrication of Anatase TiO<sub>2</sub> Nanotube Arrays at Room Temperature

이대기 이완인<sup>1</sup> 장두전

서울대 화학부 <sup>1</sup>인하대 화학과

In recent years, significant interest has been attracted to prepare self-organized crystalline TiO<sub>2</sub> nanotubes without employing an additional annealing process, which may lead to cracks and aggravate sample integrity. In this work, anatase TiO<sub>2</sub> nanotube (TNT) arrays have been fabricated through electrochemical anodization of pure titanium foil in an NH<sub>4</sub>F-contained mixed electrolyte solution of ethylene glycol and glycerol with a certain ratio at room temperature. The resulting arrays have a highly ordered, vertically aligned, and one side-opened structure. By controlling the concentration of glycerol, we have obtained TNTs having various morphologies. When the electrolyte becomes more viscous, the tube length is decreased whereas the outer diameter and the wall thickness are increased (i.e., TNTs have more porous structure). The photo-oxidation ability of the crystalline nanotube has been investigated in comparison with those of the amorphous nanotube and the commercial form of TiO<sub>2</sub> (Degussa P25).

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## **The substrate effect on the reactions of ethanol over TiO<sub>2</sub>-supported Au catalysts**

**김정진 김유권<sup>1</sup>**

아주대 에너지시스템학부 응용화학<sup>1</sup> 아주대 자연과학부

Oxide-supported Au catalysts have been prepared to generate hydrogen gas from alcohol or remove environmental-toxic gases. Titanium dioxide (TiO<sub>2</sub>) catalyst was recognized as a candidate for this purpose. In the present study, we explored the effects of their shape and the surface area. TiO<sub>2</sub>-supported gold catalysts were prepared by a deposition-precipitation method with the Au loading of 0 - 1.0 wt%. From the peak variation in the x-ray diffraction (XRD) patterns at  $2\theta = 77.5^\circ$  we confirmed the presence of Au nanoparticles. In temperature programmed reduction (TPR) experiments, ethanol gas flow rate had been set to  $\sim 0.7 \mu\text{mol/sec}$  and the temperature was slowly raised at a rate of 0.2K/sec. We identified various reaction products of ethanol over Au/TiO<sub>2</sub> by the analysis of the TPR profiles. We found that with Au, acetaldehyde formation was favored over ethylene. The subsequent reaction products of acetaldehyde were also detected and found to desorb from the surface. We also found that the surface area of the support materials had a big influence on the overall activity.



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## Morphology Controlled Monoclinic BiVO<sub>4</sub> Film on the FTO

손영석 김창우 강영수

서강대 화학과

We report BiVO<sub>4</sub> film on the FTO by hydrothermal method. Using BiVO<sub>4</sub> seed layer by spin-coating, BiVO<sub>4</sub> film with various morphologies was grown on the seed layer. As a photo anode, BiVO<sub>4</sub> film with visible light activity was compared with various morphologies. The structure and optical properties of BiVO<sub>4</sub> film have been well characterized and displayed a strong photo response in the visible region. Keywords: BiVO<sub>4</sub>, Photoanode, Photocatalyst.

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## **Incorporation of silver nanoparticles and its effect on optical and electronic properties of small-molecule organic solar cells**

허일수 한지영 유연규 임상규

국민대 생명나노화학과

Organic Photovoltaic(OPV) cells have recently attracted growing attention due to their potential for the low-cost fabrication of flexible and lightweight Solar modules. In this work, the modification of optical and electronic properties of hole transporting layer(HTL) in ZnPc/C60 based small-molecule OPV cells by incorporating Silver nanoparticles into the layer was studied. Optical, morphological and electronic properties of the layer were characterized by UV-visible spectroscopy, normal and integrated mode transmittance measurement, scanning electron microscopy and Kelvin force microscopy. It was observed that the well-dispersed nanoparticles in the HTL scattered the incident light and this redirection of light paths led to the enhancement light path lengths and consequently effective light absorption in the active organic layer. This advantage was, however, offset by the reflection of a part of incident light due to the nanoparticles, and hence the enhancement of power conversion efficiency of the OPV cells was quite limited.

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## **Fabrication of arrayed polyaniline nanostructure and its applications**

**권혜민 박다솜 임상규**

국민대 생명나노화학과

Polyaniline (PANi), one of the most widely used conducting polymers, is attracting growing attention due to their potential for various applications such as chemical sensor, transparent conducting film and capacitor. The physical and electronic properties of PANi strongly depend on polymerization conditions such as reaction temperature and type of acid used. In this work, two-dimensionally (2D) arrayed PANi nanostructures on various substrates were fabricated using polystyrene (PS) nanospheres. The two different acids, hydrochloric acid and perchloric acid were used for the polymerization of anilines. The surface morphologies of PANi nanostructures were strongly dependent on the type and concentration of the acids. The 2D-arrayed hollow PANi nanostructure could also be fabricated by removal of PS nanospheres. The morphological and electronic properties of the nanostructure were characterized by scanning electron microscopy, sheet resistance and cyclic voltammetry. It is expected that the prepared PANi nanostructures can be applied to fabricating highly efficient capacitors due to its hollow nanostructure and highly corrugated surface morphology.

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## Molecular Assembly and Structure of Terphenylthiol Self-Assembled Monolayers on Au(111)

강훈구 Eisuke Ito<sup>1</sup> Masahiko Hara<sup>2</sup> 노재근

한양대 화학과 <sup>1</sup>RIKEN, Japan <sup>2</sup>TITech, Japan

Terphenylthiol (TPT) molecules have been considered as an extremely promising molecular system for device applications because they have a  $\pi$ -conjugated and rod-like molecular structure. The surface structure and adsorption conditions of TPT self-assembled monolayers (SAMs) on Au(111) were examined using scanning tunneling microscopy (STM) and X-ray photoelectron microscopy (XPS). STM imaging revealed that TPT SAMs formed in a 0.01mM ethanol solution at 60 °C have ordered domains containing well-ordered ( $\sqrt{3} \times \sqrt{3}$ ) R30° structures and bright rows. Also, the surface structures of TPT SAMs formed in a 0.01mM ethanol solution at 60 °C can be controlled by changing the immersion time. Especially, TPT SAMs formed after 2 hr show unique bright rows contained some TPT molecules, results that have never been observed for other thiol SAM systems. XPS measurements for TPT SAMs on Au(111) showed the two sulfur peaks at 161.2 and 162.2 eV, implying the formation of chemisorbed

monolayers. Our results are anticipated to be useful for understanding the formation and structure of TPT SAMs on gold surfaces.



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## **1+2' Resonance-enhanced Multiphoton Ionization Spectroscopy of 2-methylpyrazine: Methyl torsional modes in S1 state**

김재한 이지혜 홍용준<sup>1</sup> 황현석 김홍래 권찬호

강원대 화학과 <sup>1</sup>국방과학연구소 국방신기술센터/융복합기술부

Vibrational and torsion bands of 2-methylpyrazine in S1 state have been measured by 1+2' resonance-enhanced multiphoton ionization spectroscopy. The complicate spectrum somewhat in the low frequency, which is induced by methyl torsional modes has been analyzed by comparing with the vibrational frequencies and Franck-Condon factors calculated at time dependent density fuctional theory levels using cc-pVTZ basis sets.

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## **Vacuum Ultraviolet Mass-analyzed Threshold Ionization Spectroscopy of Acetone in Ground Electronic State**

**김재한 강도원 이지혜 홍용준<sup>1</sup> 황현석 김홍래 권찬호**

강원대 화학과 <sup>1</sup>국방과학연구소 국방신기술센터/융복합기술부

Mass-analyzed threshold ionization (MATI) time-of-flight mass spectrometer using coherent vacuum ultraviolet laser generated by four wave difference frequency mixing in Kr has been constructed and utilized to obtain the spectrum of acetone cation in the ground electronic state. Ionization energy of acetone to the ionic ground state has been determined to be 78290 cm<sup>-1</sup> from the MATI spectrum. Vibrational analysis in the spectrum has been accomplished with calculating the vibrational frequencies and Franck-Condon factors at the B3LYP/cc-pVTZ levels. Some low-frequency peaks have been assigned to the torsional modes by two methyl group in the acetone cation.

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## **H atoms from photodissociation of benzaldehyde at 205 nm**

**강충만 박성만 권찬호 황현석 김홍래**

강원대 화학과

Laser-induced fluorescence spectra of H and D atoms produced from photodissociation of benzaldehyde at 205 nm in the gas phase have been measured employing the two photon,  $1s \rightarrow 3s,3d$  absorption with the detection of  $3s \rightarrow 2p$  emission. From Doppler analyses in the spectra, translational energy releases are determined for both H atom dissociation channels,  $C_6H_4COD + H$  and  $C_6H_5CO + D$ . Quantum chemical calculations have been performed to construct potential energy surfaces for the ground and electronically excited states leading to the individual dissociation channels, from which the observed translational energy releases and hence the dissociation dynamics are discussed in detail.



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## Development of a Micro Time-of-Flight Mass Spectrometer Using Field Emission Ion Source

오준식 유동욱<sup>1</sup> 정광우<sup>2</sup>

원광대 생명나노화학부<sup>1</sup> 원광대 생명나노화학과<sup>2</sup> 원광대 화학과

In this work, we present the fabrication and test of a micro time-of-flight mass spectrometer ( $\mu$ -TOF MS) using carbon-nanotube (CNT)-based field emission ion source. The  $\mu$ -TOF MS is composed of two parts, i.e., a field emission ion source and a micro-ion separator. Molecules are ionized by the impact of electrons emitted from CNTs. Through the characteristic test of a field emission ion source, we confirmed that the fabricated ion source is feasible for the  $\mu$ -TOF MS. Mass can be analyzed by using the time-of-flight depending on the mass-to-charge ratio. The electron current of the field emitter was measured for various anode voltages and the ion separator was tested for air and argon.

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## Measurement of surface on substrate (GaAs, Carbone materials) fabricated by lithography with AFM (Atomic Force Microscope)

김창호 차호석<sup>1</sup>

ANT Co. 연구지원팀 <sup>1</sup>ANT Co. Technical Sales

반도체(GaAs, Si, Ge 등) 재료 및 카본 재료(SWCNT, Graphene)를 이용한 나노 소자/센서 제작이 각광받아오고 있다. 이런 재료를 이용한 나노 구조체의 제작은 SEM 을 통한 E-beam 을 이용한 방법, CVD 성장을 통한 방법 등을 통해서 만들어지고 있다. 이런 E-beam 과 CVD 성장은 그 나노센서 특성에 맞춰 장점을 살려 사용될 수 있으나 고진공 및 여러 가스 사용, 제작의 복잡성 등의 단점도 가지고 있는 것도 사실이다. 여기에서 사용한 방법은 표면의 성질 변화 및 나노구조체 가공에 있어서 AFM 을 이용하여 간단하고 손쉽게 나노표면 개질 및 표면의 물리적 특성을 변화시킬 수 있는 lithography 를 사용하였다. AFM(NT-MDT)을 이용하여 기계적인 AFM Force Lithography 을 수행하여 GaAs 혹은 카본 재료(Graphite, Graphene, CNT)위에 나노구조체 생성과 함께 AFM 이미지를 통하여 구조를 확인하였다. 이런 AFM Force Lithography 를 통하여 나노센서상의 전기적인 단락을 가할 수도 있고 나노구조를 변화시킬 수 있으므로 원하는 전기적 성질의 센서제작 및 구조체 제작에

용이하다. 또한 AFM Current Lithography 를 통하여 표면의 morphology 변화 없이 surface potential 의 성질을 변화 시켜주었고 AFM(NT-MDT Co.) many-pass technique 을 이용하여 EFM mode 와 KPM mode 를 사용하여 표면의 전기적인 변화를 측정하였다. 이렇게 함으로써 센서표면의 전하 분포 및 surface potential 을 원하는 대로 변화시킬 수 있고 전극과 전극 사이의 전하분포의 영향을 받는 분자의 정렬 및 원하는 방향성을 줄 수 있도록 조정할 수 있다. 이런 AFM Lithography 를 통한 나노구조 생성/가공과 표면의 전기적 성질 개질의 방법은 간단히 나노 센서제작 및 조작을 할 수 있는 유용한 방법이다.



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## Comparison of Adsorption Structure and Geometry Among Phenylalanine Derivatives on the Ge(100) surface: Role of Chain Length

박영찬 양세나 이한길

숙명여대 화학과

The variation of the adsorption structures and geometric configurations among phenylalanine derivatives (2-Amino-4-phenylpropanoic acid (PhenA), 2-Amino-5-phenylpropanoic acid (PhenB), and 2-Amino-6-phenylpropanoic acid (PhenC)) adsorbed on the Ge(100) surface has been investigated using density functional theory (DFT) calculations to confirm the effect of chain length bonded to  $\alpha$ -carbon of phenylalanine derivatives which must be considered the most favorable adsorption structure when it applies to the self-assembled monolayers (SAMs). We confirmed that the “O-H dissociated-N dative bonded structure” is the most favorable structure among five possible adsorption structures in their molecules. Interestingly, we found that a geometrical difference in adsorption configurations among them indicates that the phenyl ring of PhenA and PhenB is located in tilted to the Ge(100) surface with about 30 degree off angle whereas the phenyl ring of PhenC is located in tilted to the Ge(100) surface with 60

degree off angle. We therefore confirmed that PhenA and PhenB are available to use the self-assembled monolayers (SAMs) considering the geometrical configurations and the adsorption energies. We will systematically demonstrate the theoretical results which are theoretically corroborated by DFT calculations of the reaction pathways leading to the adsorption geometries.



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## **The adsorption structures and bonding configurations between cysteine and methionine adsorbed on a Ge(100) surface**

양세나 이한길

숙명여대 화학과

The difference of the adsorption structures and geometric configurations between cysteine and methionine adsorbed on a Ge(100) surface has been investigated using core-level photoemission spectroscopy (CLPES) and low-energy electron diffraction (LEED) in conjunction with density functional theory (DFT) calculations. Analysis of the S 2p, C 1s, N 1s, and O 1s core-level spectra revealed quite different adsorption behaviors as a function of cysteine and methionine coverage. We confirmed that the “O-H dissociated-N dative-S dative-bonded structure” is most favorable structure in both molecules at low (initial) coverage. On the other hand, there is another stable adsorption structure of cysteine, “O-H dissociated-N dative bonded structure”. In other words, thiol group of cysteine is removed from adsorption structure on Ge(100) surface at low coverage. On the other hand, two types of sulfur peaks with thiol formation and two nitrogen peaks with neutralized and charged characteristics were monitored at a higher coverage (0.60 ML and above), which can be described as an “O-H dissociated-S dative-

bonded structure”. Moreover, we additionally confirmed that the relative population of the two types of thiols and amines being included in cysteine and methionine in between half monolayer induces a surface reorientation in the ordering from  $2 \times 1$  to  $1 \times 1$  employing LEED.



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## High-yield Expression and NMR Structural Studies of Antimicrobial Peptides, LPcin

정지호 김용애

한국외국어대 화학과

Lactophorin (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 antibiotic 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 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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## Adsorption Structure of Threonine on the Ge(100) surface

이명진 양세나 이한길

숙명여대 화학과

We investigated the adsorption structures of Threonine on a Ge(100) surface by density functional theory (DFT) calculations. The adsorption energies calculated using DFT methods suggested that four of six adsorption structures were plausible. These structures were the “O-H dissociated-N dative bonded structure”, the “O-H dissociation bonded structure”, the “Om-H dissociated-N dative bonded structure”, and the “Om-H dissociation bonded structure” (where Om indicates the hydroxymethyl oxygen). These structures are equally likely, according to the adsorption energies alone. The calculated results were corroborated theoretically by calculating the reaction pathways leading to the two adsorption geometries. The reaction pathways indicated that the “O-H dissociated-N dative bonded structure” is the major product of threonine adsorption on Ge(100) due to comparably stable adsorption energy.

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## Synthesis and Characterization of Mn-doped CdSe@ZnSe Semiconductor Nanocrystals

표지영 김연호 장두전

서울대 화학부

In recent years, a great deal of attention has been devoted to transition metal ion-doped semiconductor nanocrystals (d-dots). In this paper, water-soluble, nearly monodisperse and highly luminescent Mn-doped CdSe@ZnSe quantum dots have been synthesized via an aqueous-based route. 3-mercaptopropionic acid as a ligand has been capped on the surface of the resulting d-dots. The d-dots exhibit an emission peak at 500-600 nm and the photoluminescence (PL) band is relatively broad and symmetric as compared to that of bare Mn:CdSe quantum dots (QDs). Also, the Mn:CdSe@ZnSe d-dots show high PL quantum yield (QY = ~50%). This indicates that the Mn dopants have been incorporated into the core CdSe QDs successfully and ZnSe outer layer also has been deposited on the core QDs. By controlling the shell thickness, we investigate the change of the PL QY resulting from the interaction between the dopants and the ligands. We have found that the optimized thickness of the outer shell enhances the PL QY of the d-dots effectively. These highly emissive and stable d-dots possess

characteristics of potential emissive materials for applications especially requiring high power and high concentration of emitters.



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## Expression, Purification, and NMR Measurement of Syndecan4-TM

송주영 최성섭 김용애

한국외국어대 화학과

Syndecans have important roles as a major family of cell surface receptors that participate in cell-cell and cell-matrix interactions. Syndecan-4 is one of the syndecan family peptides. To get better understand the mechanism and function of syndecan-4, it is crucial to investigate the three-dimensional structure of a single transmembrane spanning region of them. Unfortunately, it is hard to prepare the peptide because syndecan-4 is membrane-bound protein that transverse the lipid bilayer of the cell membrane. In fact, high yield production of transmembrane peptides has been limited by experimental adversities of insufficient yields and hydrophobicity of peptide. Here, we demonstrate experimental processes and results to optimize expression, purification, and NMR measurement condition of syndecan-4 transmembrane domain (Syd4-TM). Peptide was released from the fusion protein, and then purified by semi-preparative reversed-phase HPLC. Finally, more than 5mg of Syd4-TM peptide was obtained with high purity from 1L of M9 minimal media under optimized conditions. The analysis of the CD spectrum shows that Syd4-TM adopts a stable alpha-helical structure in micelle environments. Solution NMR

studies showed that Syd4-TM forms an asymmetric dimer in micelles. For further studies, we also study mutant syndecan-4 which has a modified peptide sequence of Syd4-TM, doesn't show dimerization but consists of monomer and Syd4-eTC which has extracellular, transmembrane and cytoplasmic domain of syndecan-4. We also report an efficient method for the recombinant expression and purification of mutant Syd4-TM and Syd4-eTC peptide. Consequently, we confirmed that mutant Syd4-TM forms a monomer and Syd4-eTC forms a dimer.



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## **Facile One-Pot Synthesis of CdSe-0.5en and CdSe-0.5en-Pt Composite Nanorods**

김형배 장두전

서울대 화학부

Metal-semiconductor hybrid nanocrystal systems have been studied with great interest over the past several years. Especially, photocatalytic processes have been focused in metal-semiconductor systems. So far CdSe-metal based hybrid-photocatalysts including CdSe-Pt, CdSe-Au, and core-shell CdSe@Pt have been demonstrated. However, CdSe-0.5en-Pt nanocomposite has not been reported yet. Herein, we have fabricated CdSe-0.5en-Pt nanocomposite for the first time and have chosen greener solvents and facile methods and have characterized CdSe-0.5en and CdSe-0.5en-Pt nanocomposite by using the various instruments, respectively. Particularly, we have demonstrated photoluminescence shift of CdSe-0.5en nanorods with various reaction times, which has not been reported yet. Although the nanorods have been treated by post-hydrothermal reaction, the external shape remains rod-like anisotropic structures but showing hollow holes due to the ethylenediamine excavation, which results have also not been reported yet. For the application CdSe-0.5en nanorods, we have fabricated Pt-decorated nanorods via microwave-

assisted synthetic methods and they have showed photocatalytic activity as previous CdSe-Pt nanorods synthesized by U. Banin group. Although photocatalytic efficiency of the hybrid-nanocomposite is poorer than that of U. Banin group's reports, it is worthy of attracting report that the inorganic-organic hybrids compounds also can do photocatalytic activity and the photocatalytic efficiency of the hybrid-nanocomposites has decreased with removal of ethylenediamine molecules inside of the hybrid-nanocomposite.





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## Conformational analysis of cis and trans isomerization in phosphorylated Serine/Threonine-Proline peptides

송재미 조민행

고려대 화학과

Pin1 leads to the hypothesis of a new signaling mechanism, catalytically regulates the conformation of its substrates after phosphorylation to control protein function. Unlike all other peptidyl prolyl cis-trans isomerase(PPIases), Pin1 binds to and isomerizes specific phosphorylated Serine/Threonine-Proline(pSer/Thr-Pro) motifs in certain proteins. Despite of these functions' Pin1, mechanism of Pin1 has not been fully understood yet. That's why we don't know defining the structural and functional differences of proteins that adopt cis and trans conformations. To study its possible effects on Ser/Thr-Pro motifs, we recently carried out pH- and temperature-dependent circular dichroism(CD) as well as <sup>1</sup>H NMR studies of the phosphorylated Ser/Thr-Pro peptides and compared them with their unphosphorylated analogs.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Theoretical Study of HC<sub>4</sub>N molecule; Molecular and Electronic Structures

정규성 윤돈희 김민정 김나리

건양대 나노바이오화학과

The electronic structures for an astrochemically important HC<sub>4</sub>N molecule and their negative ions were investigated with both an ab initio method and the density functional theory. We have considered various possible isomers with the carbene structure in order to see their structural features with unique bonding properties and relative energy relations. The results show that the isomers with three membered ring are more state than those with simple chain structures in the singlet state, whereas the triplet state shows the bent structures are more favorable than the ring structures. In the negative ions with the doublet state, the structural features are similar to the neutral molecule with triplet state. On the other hand, the electron and proton affinities calculation shows that astrochemical reactivity of these carbene species in interstellar cloud are very sensitive to their bonding nature.

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장소: 일산KINTEX

발표코드: **PHYS.P-344**

발표분야: 물리화학

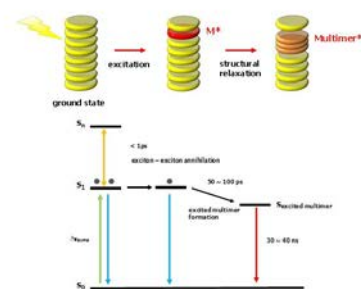
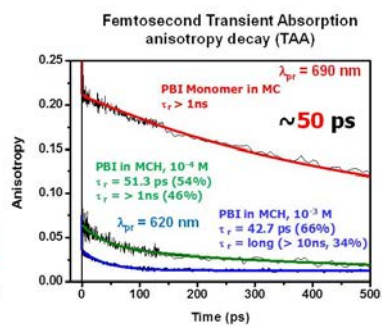
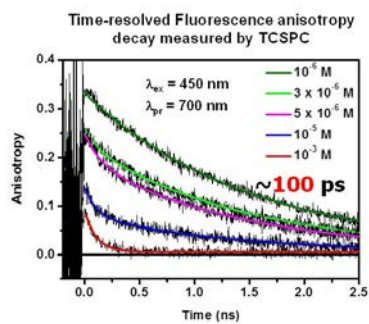
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Photophysical properties of perylene bisimide helical aggregates: the exciton dynamics and localization process**

**임종민 김동호**

연세대 화학과

In this research, we have investigated the photophysical properties of exciton dynamics in perylene bisimides (PBI) aggregates systems. Due to the pi-pi interaction and steric effect associated with the end groups, the aggregates system reveals helical arrangement of stacking structure and excimer-like fluorescence behaviors. This indicates that the low-lying excimer-like sites acting as traps in exciton communication process such as exciton migration and diffusion phenomena. By using various photophysical measurements, we have scrutinized the exciton dynamics and energy relaxation process in the aggregates structures.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparative Photophysical Properties between Bicyclo[2.2.2]octadiene (BCOD)- and Benzo-fused Free-base Triphyrins (2.1.1)

성영모

연세대 화학과

Most of investigated subporphyrinoids up to date contain boron centers. We recently have prepared two free-base subporphyrinoids, bicyclo[2.2.2]octadiene- (BCOD-) and benzo-fused triphyrins (2.1.1) (Scheme 1). Although a distinct difference in the chemical shift among inner- and outer- protons does not appear due to a strong hydrogen bonding in the macrocycle of free-base triphyrin in the  $^1\text{H}$ -NMR spectra, the nucleus independent chemical shift (NICS (0)) values of both triphyrins reveal -13.4 ppm at the center of the macrocycle rings.<sup>1,2</sup> While boron-centered subporphyrinoids have cone-shaped structure due to their steric hindrance between boron and nitrogen, these free-base triphyrins show relatively planar structure in X-ray crystal structures. In the present study, we have investigated the excited-state dynamics of two triphyrins, with a focus on the origin of deactivation processes, by performing various temperature dependent spectroscopic measurements, protonation experiments, and theoretical calculations.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Matrix-assisted variable wavelength laser desorption ionization of peptides; Influence of the matrix absorption coefficient on expansion

cooling

안성희 배용진<sup>1</sup> 김명수<sup>1</sup>

서울대 자연과학대학 화학부 <sup>1</sup>서울대 화학부

The product ion yields in the in- and post-source decays of three model peptide ions,  $[Y5X + H]^+$  ( $X = Y$  (tyrosine), K (lysine), and R (arginine)), generated by matrix-assisted laser desorption ionization (MALDI) were measured at six wavelengths, 307, 317, 327, 337, 347, and 357 nm, using  $\alpha$ -cyano-4-hydroxycinnamic acid (CHCA) and 2,5-dihydroxybenzoic acid (DHB) as the matrices. The spot size of the laser was kept the same regardless of the wavelength. The laser pulse energy used was two times the threshold value determined for each matrix at each wavelength. The temperatures of the early and late plumes generated by MALDI were estimated via kinetic analysis of the product ion yield data. For both matrices, the temperature drop ( $\Delta T$ ), i.e. the difference in the temperature between the early and late plumes, displayed negative correlation with the matrix absorption coefficient. This was in agreement with

the previous qualitative reasoning that deeper laser penetration and larger amount of material ablation arising from smaller absorption coefficient would result in larger extent of expansion cooling.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ion Yields for Some Salts in MALDI: Mechanism for the Gas-Phase Ion Formation from Pre-Formed Ions

문정희 배용진<sup>1</sup> 김명수<sup>1</sup>

한국생명공학연구원 단백질의학연구센터<sup>1</sup> 서울대 화학부

Pre-formed ion emission is the main assumption in one of the prevailing theories for peptide and protein ion formation in matrix-assisted laser desorption ionization (MALDI). Since salts are in pre-formed ion forms in the matrix-analyte mixture, they are ideal systems to study the characteristics of pre-formed ion emission. In this work, a reliable method to measure the ion yield (IY) in MALDI was developed and used for a solid salt benzyltriphenylphosphonium chloride and two room-temperature ionic liquids 1-butyl-3-methylimidazolium hexafluorophosphate and trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl)phosphinate. IY for the matrix ( $\alpha$ -cyano-4-hydroxycinnamic acid, CHCA) was also measured. Taking 1 pmol salts in 25 nmol CHCA as examples, IYs for three salts were similar,  $(4-8) \times 10^{24}$ , and those for CHCA were  $(0.8-1.2) \times 10^{27}$ . Even though IYs for the salts and CHCA remained virtually constant at low analyte concentration, they decreased as the salt concentrations increased. Two models, Model 1 and Model 2, were proposed to explain low IYs for the salts and the concentration



dependences. Both models are based on the fact that the ion-pair formation equilibrium is highly shifted toward the neutral ion pair. In Model 1, the gas-phase analyte cations were proposed to originate from the same cations in the solid that were dielectrically screened from counter anions by matrix neutrals. In Model 2, pre-formed ions were assumed to be released from the solid sample in the form of neutral ion pairs and the anions in the ion pairs were assumed to be eliminated via reactions with matrix-derived cations.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

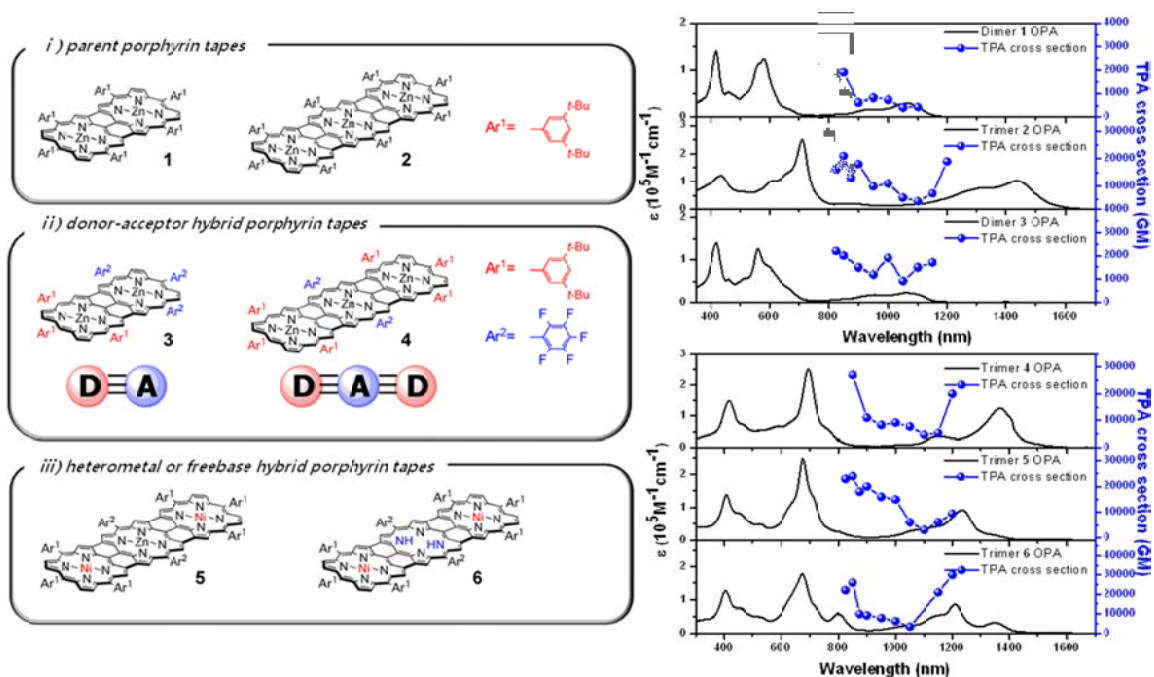
## Synthesis and Properties of Hybrid Porphyrin Tapes

이병선 김동호

연세대 화학과

Hybrid porphyrin tapes 3 and 4, consisting of a mixture of 3,5-ditert-butylphenyl-substituted donor-type Zn(II)porphyrins and pentafluorophenyl-substituted acceptor-type Zn(II)porphyrins, were prepared by a synthetic route involving cross-condensation reaction of a Ni(II)porphyrinyldipyrromethane and pentafluorophenyldipyrromethane with pentafluorobenzaldehyde followed by appropriate demetalation, remetalation, and oxidative ring-closure reaction. The Ni(II)-substituted porphyrin tapes 5 (Ni-Zn-Ni) and 6 (Ni-H<sub>2</sub>-Ni) were also prepared through similar routes. The hybrid porphyrin tapes 3 and 4 are more soluble and more stable than normal porphyrin tapes 1 and 2 consisting of only donor-type Zn(II)porphyrins. The solid-state and crystal packing structures of 3, 4, and 5 were elucidated by single-crystal X-ray diffraction analysis. Singly meso-meso linked hybrid porphyrin arrays 12 and 14 exhibit redox potentials that roughly correspond to each constituent porphyrin segments, while the redox potentials of the hybrid porphyrin tapes 3 and 4 are positively shifted as a whole. The two-photon absorption (TPA) values of 1-6 were measured by using a wavelength-scanning open aperture Z-

scan method and found to be 1900, 21 000, 2200, 27 000, 24 000, and 26 000 GM, respectively. These results illustrate an important effect of elongation of  $\pi$ -electron conjugation for the enhancement of TPA values. The hybrid porphyrin tapes show slightly larger TPA values than the parent ones.



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발표분야: 물리화학

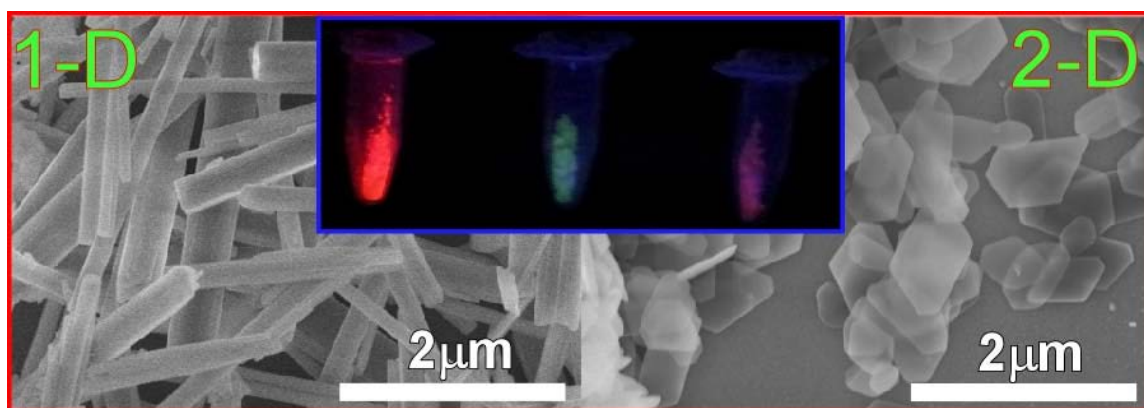
발표종류: 포스터, 발표일시: 수 18:00~21:00

## 1-D and 2-D Red-Green-Blue-White (RGBW) Emission from Lanthanide-doped Yttrium oxides

조인수 손영구

영남대 화학과

1, 2 차원 구조 (판상과 막대형)의 Y 산화물을 제조하고 그 매트릭스에 다양한 란타나이드 원소들을 도핑시켜 Red-Green-Blue-White 빛을 조절하는 시도를 하였다. 색의 파장 및 강도를 조절하는데 있어서 다음과 같은 변수들이 어떠한 영향을 미치는지 논의 해보고자 한다; 1) 매트릭스 산화물의 구조적인 변화, 2) 도핑되는 원소들의 종류, 3) 도핑물질과 매트릭스의 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. 형광체의 특성은 매트릭스 산화물에 또한 크게 의존하기 때문에 향후 매트릭스 물질개발 연구를 수행하고 Red-Green-Blue-White 발광 물질을 개발하는데 기초 및 디스플레이 산업의 응용, 경제적인 측면에서 크게 기여하고자 한다.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication of Platinum Nanobubbles Having Enhanced Catalytic Properties**

곽진아 장두전

서울대 화학부

Monodispersive silica nanospheres have been prepared via sol-gel process with tetraethylorthosilicate (TEOS) under base catalysis following the Stober method. While sizes of silica nanospheres have been controlled by amount of catalysis, platinum seeds have been simply prepared by the citrate reduction of  $\text{H}_2\text{PtCl}_6$ . Platinum seeds have been topped on silica nanospheres through the modification of the surfaces of silica nanospheres with amino groups. Platinum seeds topped on silica nanospheres have been transformed into platinum nanoshells via a seeded-growth method. After silica nanocores have been removed by hydrofluoric acid, platinum nanoshell structures with hollow interiors have been made. Hollow platinum nanostructures have been found to catalyze the degradation of rhodamine B efficiently in the presence of  $\text{KBH}_4$  compared with  $\text{SiO}_2\text{@Pt}$  core@shell nanostructures. We will present the catalytic mechanism of the nanostructures with the activation energy and the pre-exponential factor of the degradation of rhodamine B.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile Synthesis of Photocatalytic Hollow CdS Nanospheres

김연신 김형배 곽진아 장두전

서울대 화학부

A simple and facile preparation of CdS hollow nanospheres via a silica nanosphere template has been explored. The one-step Stober method has been used to produce SiO<sub>2</sub> core structures, onto which the CdS shell has been quickly and efficiently coated on the silica colloids via a microwave method. In this step, the hydrothermal method would require several hours in an autoclave while as the required irradiation time with the assistance of microwave is reduced to just 10 minutes. The as-prepared SiO<sub>2</sub>@CdS core-shell structures have then been made hollow with HF etching to redisperse the silica core. TEM and SEM images have shown our target of highly monodispersed hollow spheres with diameters of ~300 nm. The advantages of this method of fabrication 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. Although there has been previous research on CdS colloidal spheres and CdS hollow microspheres, there hasn't been sufficient research regarding highly monodispersed CdS hollow nanospheres and their efficiency as photocatalysts. Taking this into consideration, the photocatalytic activity of the resulting hollow CdS

nanospheres has been observed by examining its efficiency in the degradation of rhodamine B. These results have been compared with the photocatalytic activities of other documented CdS nanoparticles of similar size: CdS colloidal nanospheres and C@CdS composite nanospheres. As an area of research that has not been attempted before, we are currently conducting experiments controlling the size of CdS hollow shells to understand how this control affects the photocatalytic efficiency of the CdS nanoparticles.





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발표분야: 물리화학

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## **Photoluminescence behavior of iridium(III) complexes liganded with (ppz)<sub>3</sub>, (ppz)<sub>2</sub>acac series**

**김연희 김성규 안태규<sup>1</sup> 윤승수 신희원<sup>2</sup>**

성균관대 화학과 <sup>1</sup>성균관대 에너지과학과 <sup>2</sup>성균관대 신개념융복합에너지과학연구소

We present the characterization of phosphorescent facial cyclometalated Ir(III) complexes liganded with (ppz)<sub>3</sub>, (ppz)<sub>2</sub>acac series in dilute toluene. We have investigated using a steady-state luminescence spectrometer, a nanosecond time-resolved photoluminescence setup and a time-correlated single photon counting apparatus (TCSPC) at room temperature and at 77 K. The phosphorescences of the studied complexes were much greater at 77 K, while only trace amounts were barely observable at room temperature. In order to interpret the results, we carried out a cyclic voltammetry to investigate the influence of the cyclometalating ligands and ancillary ligands on highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). We believe that a non-radiative decay channel extinguishes the phosphorescence of the studied complexes at room temperature.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Deflection of Molecules by a Low power Laser

Sun Xingnan 신소은 정두수 조범석<sup>1</sup>

서울대 화학부 <sup>1</sup>Fritz Haber Institute of Max Planck Society (Germany)

The optical dipole force on the molecules which can deflects the molecular beam is proportional to the intensity gradient of the focused laser beam, and the maximum intensity  $I_0$  is inversely proportional to the focused beam waste radius. When a laser beam is more tightly focused, more efficient deflection of molecules could be achieved. We define molecular lens efficiency as maximum deflection of molecules divided by laser power. We achieved 10-fold enhancement of molecular deflection efficiency, by employing a shorter focal length mirror which could tightly focusing of the laser beam. Velocity map imaging technique was employed to detect the velocity change of  $\text{CS}_2$  molecular beam perpendicular to the laser axis around the laser focal point.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermal reactions of ethanol and 2-propanol on anatase TiO<sub>2</sub> nanosheets: the effect of N-doping

Xiaomei Yu 김유권<sup>1</sup>

아주대 <sup>1</sup>아주대 자연과학부

The thermal reactions of ethanol and 2-propanol were carried out over anatase TiO<sub>2</sub> nanosheets and the reaction products were characterized using a temperature programmed reaction technique. The reaction products of 2-propanol were found to be exclusively propene and water, while ethanol reacted to produce various reaction products such as ethylene (dehydration), water, ethyl ether (condensation), 2-butene (reductive coupling), 2-butenal (aldol condensation), and benzene. The N-doping of anatase TiO<sub>2</sub> (110) was also performed by flowing NH<sub>3</sub> gas at elevated temperature (825K). When the TiO<sub>2</sub> nanocrystals were treated with NH<sub>3</sub>, we observed that the overall reaction channels did not change except overall reaction temperatures shifted toward higher temperatures by > 50 K. We attributed the observed change of N-doping to the suppression of the surface defects such as oxygen vacancies after the N-doping.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Avidin Induced Silver Aggregation for SERS-based Bioassay

사영조 CHEN LEI 정영미

강원대 화학과

For an excellent enhancement of target molecule ( $10^6$  to  $10^{14}$  times), surface-enhanced Raman scattering (SERS) has been widely used in chemistry and biochemistry. SERS can provide larger amount of fingerprint information, and it can be enhanced comparable with fluorescence method. Applications of SERS-based bioassay can be divided into two major modes: label and label-free detection protocols. In this presentation, we proposed a method that avidin induces silver aggregation, which exhibits high SERS enhancement due to the formation of lots of hot spots. We observed SERS spectrum of atto610 which labeled on the biotin which show the interaction between biotin and avidin. Cytochrome c was detected by using this proposed silver nanoparticles aggregated with avidin, which exhibits excellent ability for label-free protein detection. Applications of SERS-based bioassay by using two detection protocols will be discussed in more detail.

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발표분야: 물리화학

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## Multispectral (CD, VCD, SAXS) studies of pH-induced denaturation of $\alpha$ -lactalbumin

유수련 Adriana Litwinczuk<sup>1</sup> Boguslawa Czarnik-Matusewicz<sup>1</sup> Rina K. Dukor<sup>2</sup> Laurence

Nafie<sup>3</sup> 정영미

강원대 화학과 <sup>1</sup>Faculty of Chemistry, University of Wroclaw <sup>2</sup>BioTools Inc. <sup>3</sup>BioTools Inc. and  
Department of Chemistry, Syracuse University

It is a key issue to understand bases of the secondary structure changes in protein that are responsible for various conformational diseases such as Alzheimer one.  $\alpha$ -lactalbumin is one of the most often used in the studies as a model protein. In this presentation, we show our results that concern studies under pH-induced conformational variations of  $\alpha$  lactalbumin that lead to formation of the molten globule state. Its properties were studied in details by UV and vibrational circular dichroism spectroscopies because the CD and VCD spectra are very sensitive to the conformational changes developed at level of the secondary structure of protein. We have applied Principal Component Analysis (PCA) and 2D Correlation Spectroscopy (2DCOS) to analyze the spectral changes of  $\alpha$  lactalbumin induced by gradual pH decrease

from 8 to 2. Small-angle X-ray scattering (SAXS) seems to be the most attractive method to measure the change in the overall dimension of a protein molecule, therefore this technique was also included in our studies. The Kratky's plots indicated on expansion of spherical shape of  $\alpha$  lactalbumin with pH changes from 8 to 2. The increased value of radius of gyration ( $R_g$ ) confirmed expanded shape of  $\alpha$  lactalbumin in the molten globule state at pH 2. Combining the results from multivariate analysis of the CD and VCD spectra with the SAXS data we obtained detailed picture of  $\alpha$  lactalbumin changes when its secondary structure evolved from the native (pH 8) to the molten globule state (pH2).



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **SERS Immunoassay by Using Patterned Silver Nanoparticles Substrate**

**이영주 CHEN LEI 정영미**

강원대 화학과

Surface-enhanced Raman scattering (SERS) has received much attention due to its considerable potential in high selective and sensitive detection of molecules of interest even in single molecular detection. SERS immunoassays based on antigen-antibody bonding have been studied for biomarkers for early cancer diagnosis. In this study, we applied microcontact printing method to prepare a patterned substrate of a sandwich type SERS immunoassay. Details of the SERS immunoassay by using patterned silver nanoparticles substrate and SERS images will be discussed.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Detection of the Thrombin by Using Label-Free SERS



신민화 정영미

강원대 화학과

As an ultrasensitive technique, surface-enhanced Raman scattering (SERS) has been proven to have great potential in high throughput protein detections. SERS spectroscopy can be used for the label-free detection of biomaterial. Label-free method has advantages which are rapid and simple. In this study, fibrinogen modified gold nanoparticles based label-free SERS probe were applied to the detection of thrombin. Addition of fibrinogen to a solution of gold nanoparticles led to ready conjugation through electrostatic and hydrophobic interactions. Introduction of thrombin into the gold nanoparticles solutions in the presence of fibrinogen generates reaction of blood coagulation. The products were investigated by means of UV-vis, SEM, and TEM. In this presentation, detection of thrombin by using label-free SERS will be discussed in details.



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## Molecular Dynamics simulation for lattice thermal conductivity in



지효석 심지훈

포항공과대 화학과

$\text{In}_4\text{Se}_{3-x}$  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  $\text{In}_4\text{Se}_3$ . In this study, we develop interatomic potentials and perform equilibrium molecular dynamics (MD) simulation to investigate lattice thermal conductivity of  $\text{In}_4\text{Se}_{3-x}$ . For  $\text{In}_4\text{Se}_3$  ( $x = 0$ ), obtained thermal conductivity is larger than experimental result ( $\text{In}_4\text{Se}_{3-x}$ ,  $x = 0.22$ ) in b-c plane while a-b plane thermal conductivity is well matched. And for  $\text{In}_4\text{Se}_{2.75}$  ( $x = 0.25$ ), the thermal conductivity on b-c plane is in a good agreement with experimental result. We confirm that the Se-defect only affect c-directional thermal conductivity by phonon dispersion and structural point of view. Decomposition result also shows that the Se-defect

supresses the long-range phonon in the c-direction much. So we conclude the Se-defect has an important role in describing low thermal conductivity of  $\text{In}_4\text{Se}_{3-x}$  compound.



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## **Two-Dimensional Correlation Analysis for Detecting Positional Fluctuations of Spectral Changes Related to Molecular Interactions**

**박준후 정영미**

강원대 화학과

Two-dimensional correlation spectra clearly show the very characteristic cluster pattern for both band position shifts and two overlapped bands. The presence or lack of the asynchronous 2D butterfly pattern is the most effective diagnostic tool for band shift detection. To demonstrate the origin of the peak position shift of OH stretching band, the concentration-dependent IR spectra of ethylene glycol in a mixed solvent of  $\text{CHCl}_3/\text{THF}$  of and the IR spectra of 10-40 wt% ethylene glycol in a mixed solvent of  $\text{CHCl}_3/\text{THF}$  with varying solvent compositions were analyzed. In this presentation, the positional fluctuations of spectral change related to molecular interactions will be discussed.

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## Free Radical Initiated Peptide Sequencing mass spectrometry

이지혜 문봉진 오한빈

서강대 화학과

A comparative study was performed to investigate hydrogen abstraction reaction and the ensuing radical migration in TEMPO-based FRIPS (Free radical initiated sequencing) method. For this purpose, FRIPS mass spectra were obtained in both positive and negative ion modes. It was found that the FRIPS dissociation behaviors were quite different from each other. MS/MS of the negatively charged peptides showed extensive backbone fragmentations, while MS/MS of the positively charged peptides underwent the homolytic cleavage in the bond between the toluyl carbon and oxygen of the TEMPO group. In other words, peptide backbone sequencing was possible in a single-step reaction for the application of negative ion FRIPS. To investigate the cause of this difference, the survival yields of MS/MS and MS<sup>3</sup> processes in the positive and negative ion mode were obtained as a function of normalized collision energy. The obtained survival yield curves revealed that in the positive ion mode the initial radical generation step is energetically catalyzed requiring much low threshold, while in the negative ion mode, the energy

threshold of MS/MS step was substantially high even higher than the  $MS^3$  step. Currently, the theoretical study to reveal the underlying intrinsic cause of this phenomenon is underway.



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## BCA Reagent-based Protein Quantitative Evaluate with Raman Spectroscopy

CHEN LEI 이영주 정영미 ZHAO BING<sup>1</sup>

강원대 화학과 <sup>1</sup>State Key Laboratory of Supramolecular Structure and Materials, Jilin University

Reagent-based protein assay techniques that are used routinely by nearly every laboratory involved in protein research have been developed. Unknown concentration of proteins can be determined from a standard curve consisting of known concentrations of a purified reference protein in reagent-based protein assay. Most reagents, which were used for colorimetric protein assay, are possessed of the high Raman scattering cross section. In this study, the SERRS and RR of BCA/Cu<sup>+</sup> complex were employed to establish a sensitive method for quantitative evaluation of proteins in the solution. Details of SERRS and RR spectra of BCA/Cu<sup>+</sup> complex will be discussed.

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**Solution NMR Structure and Backbone Dynamics of the Cold Shock Proteins (CSPs) and Its Complex with Single-Stranded nucleic acids from psychrotrophic bacterium, *Listeria monocytogenes***

이주호 정기웅 김양미

건국대 생명공학과

Cold shock proteins (CSPs) from psychrotrophic food-born pathogen, *Listeria monocytogenes* (*Lm*-Csp) are nucleic acid binding proteins. They function as chaperones in response to cold shock. We investigated the importance of structural and dynamic features of *Lm*-Csp to understand the mechanism of cold adaptation. According to CD experiments, the melting temperature of *Lm*-Csp was 318 K, lower than that of mesophilic CSPs. Based on 847 NMR constraints, the structure of *Lm*-Csp was calculated. *Lm*-Csp consists of five  $\beta$  strands and a long loop region, resulting in more flexible structure compared to that of mesophilic CSPs. Fluorescence quenching experiment showed that heptathymidine (dT<sub>7</sub>) strongly bind to the *Lm*-Csp ( $K_d=1.6\times 10^{-7}$ M). Chemical shift perturbation and spin relaxation study showed that large chemical shift changes were observed for E12, G14, and G54 (>0.5 ppm) upon dT<sub>7</sub> binding and high  $R_2$  values were observed for backbone N-H sites of W8, F15, F27 and R56 (>10 s<sup>-1</sup>). From Model-free

analysis, the slow motion of residues F15, F27 and R56 disappeared upon dT<sub>7</sub> binding, implying that these residues are the dT<sub>7</sub> binding site. Thus, relaxation study provides the evidences showing that conformational dynamics contribute to the nucleic acid-binding epitope and nucleic acid recognition.





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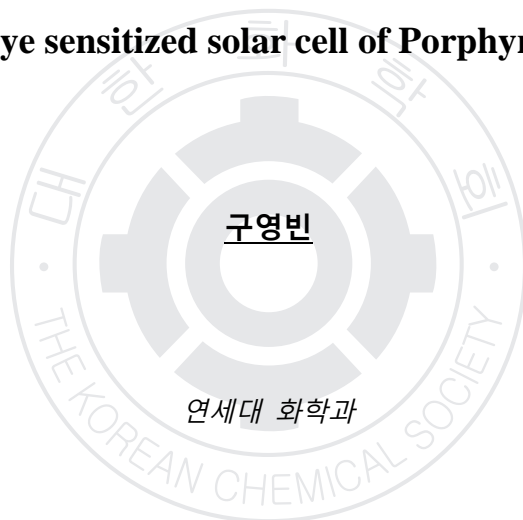
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## Dye sensitized solar cell of Porphyrin



포피린은 광화학적 안정성이 크고 합성이 점점 용이해지고 있으며 가시광선 영역의 빛을 흡수하는 능력이 뛰어나므로 염료감응 태양전지의 염료로써 상당히 촉망 받는 분자임. 이러한 포피린 분자들을 염료감응 태양전지에 적용하여 보다 높은 효율의 태양전지를 만들기 위한 실험을 실시하고자 함. 팔라듐 촉매를 통하여 포피린의 두 베타위치에 cyanoacetic acid 을 치환시킨 dye 로 태양전지를 만들어 효율을 측정함.

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## **Growth Kinetics and Thermal Stability of Octadecanethiol Self-Assembled Monolayers on GaAs**

**서한민 강훈구 Eisuke Ito<sup>1</sup> Masahiko Hara<sup>2</sup> 노재근**

한양대 화학과 <sup>1</sup>RIKEN, Japan <sup>2</sup>TITech, Japan

Growth process and formation of octadecanethiol(ODT) self-assembled monolayers on n-type GaAs has been systematically studied by contact angle (CA), X-ray photoelectron spectroscopy (XPS), and thermal desorption spectroscopy (TDS) measurements. It was found that the formation of ODT SAMs was significantly influenced by concentration and immersion time. The CA values for ODT SAMs formed in 1, 0.1, and 0.01 mM solution were measured to 70.6, 64.8, and 53.8 ° at 1 min immersion time. In addition, it was revealed that the CA values were strongly affected by immersion time. The optimum CA value of ODT SAMs on GaAs is 113 ~ 116 °. XPS measurements for ODT SAMs on GaAs showed the sulfur peaks at 162 eV, which implies the formation of chemisorbed ODT SAMs on GaAs. In TDS data, desorption peaks corresponding CH<sub>3</sub>(CH<sub>2</sub>)<sub>17</sub>S<sup>+</sup> species from ODT SAMs on Au(111) and GaAs surfaces were observed at 170 and 240 °C, respectively, which means that ODT SAMs on GaAs have a

higher thermal stability compared to those on Au(111). We will be discussed that Surface coverage was dependent thermal deposition behavior for ODT.



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## Formation and Structure of Dialkyl Monosulfide Self-Assembled Monolayers on Au(111)

이동진 강훈구 Eisuke Ito<sup>1</sup> Masahiko Hara<sup>2</sup> 노재근

한양대 화학과 <sup>1</sup>RIKEN, Japan, <sup>2</sup>TITech, Japan

Dialkyl monosulfides self-assembled monolayers (SAMs) are more robust to oxidation, and their chemical structures with various alkyl chains can be modified readily by a simple synthetic method compared to alkanethiol SAMs. In this study, dialkyl monosulfide SAMs were prepared by spontaneous adsorption of ethyl octyl sulfide (EOS), dioctyl sulfide (DOS), dodecyl octyl sulfide (DDOS) on Au(111) using both solution and ambient-pressure vapor deposition methods. The surface structure, adsorption condition, and thermal stability of the SAMs on Au(111) were characterized by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and cyclic voltammogram (CV). STM imaging showed that dialkyl monosulfides SAMs have completely different surface structures compared to alkanethiol SAMs. On the other hand, XPS measurements showed that sulfur peaks for EOS, DOS and DDOS SAMs are nearly identical with those for alkanethiol SAMs. CV measurements revealed that DOS SAMs with symmetric alkyl chains have single reductive desorption peak at, whereas EOS SAMs with

unsymmetric alkyl chains have two desorption peaks at, We found that reductive desorption behaviors of dialkyl sulfide SAMs strongly depend on the composition and strength of van der Waals interaction of SAMs.



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## Formation and Structural Order of Ethanethiol and Trifluoroethanethiol Self-Assembled Monolayers on Au(111)

임동원 강훈구 Eisuke Ito<sup>1</sup> Masahiko Hara<sup>2</sup> 노재근

한양대 화학과 <sup>1</sup>RIKEN, Japan <sup>2</sup>TITech, Japan

Fluorinated alkanethiol self-assembled monolayers (SAMs) represent one of most studied subjects of functionalized SAMs because of their potential to produce extremely low energy and highly hydrophobic surface coatings. In this study, the fluorinated alkanethiol SAMs containing short alkyl-chain were formed by the spontaneous adsorption of trifluoroethanethiol (TFET) on Au(111), which was compared to ethanethiol (ET) SAMs. The surface structures, adsorption characteristics, and electronic property of the SAMs on Au(111) were characterized by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and Kelvin probe. The STM observation showed that the ET SAMs formed at 70 °C for 2 hr have more uniform surface structure and ordered domains compared with that formed at room temperature for 24 hr. Generally, it was known that the fluorinated alkanethiol SAMs containing the longer alkyl-chain had the totally different surface structure compared to non-fluorinated alkanethiol SAMs. However, in short alkyl-chain systems, the surface structure of fluorinated alkanethiol, TFET

SAMs containing short alkyl-chain length was almost similar with that of non-fluorinated alkanethiol, ET SAMs. XPS measurements for TFET and ET SAMs show that sulfur atoms are chemically bond to the gold surface.



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## **Studies of thermal stability and catalytic activity of Pd-Graphene nanocomposites in Sonogashira and Heck reactions**

**홍영국 안병준 박준범**

전북대 화학교육과

Modifications of graphenes have been studied to develop a multi-functional supporting platform for catalytic applications. In this research, Pd-Graphene nanocomposites were synthesized using a wet preparation method and their morphological and chemical structures were characterized by FT-IR, XRD, TEM, STEM, and XPS. The catalytic performance of the nanocomposites were investigated in Sonogashira and Heck reactions using a microwave reactor. The correlations between the morphology of Pd NPs and catalytic performance were investigated by monitoring the Pd nanoparticle size and catalytic activity versus calcinating temperature in H<sub>2</sub> gas. The Pd-Graphene nanocomposites showed much higher thermal stability and catalytic performance in various chemical reactions, comparing with conventional zeolite based Pd catalysts. In addition, the catalytic recyclability was found to be excellent.



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## Comparative study for Growth Process of Self-Assembled Monolayers by Octanedithiol and Acetyl-Protected Octanedithiols on Au(111)

구경빈 강훈구 신승훈 Eisuke Ito<sup>1</sup> Masahiko Hara<sup>2</sup> 노재근

한양대 화학과 <sup>1</sup>RIKEN, Japan <sup>2</sup>TITech, Japan

Self-assembled monolayers (SAMs) of alkanedithiols on gold have attracted much attention due to the possibility of using them as linkers between two metals for molecular electronic applications. Alkanedithiol SAMs on gold were studied by using scanning tunneling microscopy (STM), thermal desorption spectroscopy, X-ray photoelectron Spectroscopy and contact angle (CA) measurements. We used thioacetic acid S-(8-mercaptooctyl)ester (TMOE) molecule containing a active SH group and an acetyl-protected SH group as the two end groups to compare the formation of SAMs by 1,8-octanedithiol (ODT) and S-(8-acetylsulfanyl-octyl)ester (TASOE) molecules. To study initial growth of alkanedithiol SAMs, the gold substrates were immersed in 1  $\mu$ M ethanol solution of ODT, TMOE, and TASOE for 30 s, 3 and 5 min, and 1 hr, respectively. STM imaging revealed that TMOE SAMs have “lying-down phase” like ODT SAMs at an initial state. However, as the immersion time increases, “lying-down phase” was changed to “up-right phase” in TMOE SAMs.

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## Synthesis of ZnO thin film using spin coater

박병천 경동현 김종규

단국대 화학과

ZnO thin film has the way of applications such as dye sensitized solar cell, photo diode device, gas sensor and etc. Method of basic pre-treatment is of coating on substrate before devices are made. But equipment which can coat the materials relatively is expensive compared to thermal decomposition, beam sputtering. The ZnO was synthesized to coat on Indium Tin Oxide(ITO) glass using spin coating. ZnO sol was dropped on ITO glass by using Micropipette. Crystalline structure and components of ZnO on ITO glass was identified in a simple through X-ray diffraction(XRD). Surface topography and cross section of a selected area were obtained by operating field emission scanning electron microscopy (FE-SEM).

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## Synthesis of transition metal doped ZnO using hydrothermal method

진훈열 윤혜수 김종규

단국대 화학과

ZnO generally has interest of applications such as solar cell, semiconductor, Antibacterial property etc. Transition metal doped ZnO specially was more properties than a ordinary ZnO. The transition metal doped ZnO was synthesized via simply hydrothermal reaction at relativity low temperature. The obtained powder which information of crystal structure was checked by using x-ray diffraction(XRD). Morphology of the powder was changed to nanorod which was confirmed by operating scanning electron microscopy(SEM). Atomic structure was uniquely identified using Energy dispersive X-ray spectroscopy (EDAX).

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## **Photoluminescence property of (BaSr)Si<sub>2</sub>O<sub>2</sub>N<sub>2</sub>:Eu<sup>2+</sup> yellow phosphors**

문인모 정우철 김창해 이기환<sup>1</sup>

한국화학연구원 박막재료연구팀<sup>1</sup> 공주대 화학과

Eu<sup>2+</sup>-doped (BaSr)Si<sub>2</sub>O<sub>2</sub>N<sub>2</sub> yellow phosphors were prepared by a conventional solid-state reaction. The phosphors were characterized by field-emission scanning microscopy with CL and EDS(FESEM-CL,EDS), X-ray photoelectron spectroscopy(XPS), X-ray powder diffraction(XRD) and fluorescence spectroscopy. FESEM-CL,EDS showed that the morphology consists of rod and cluster. From the cluster morphology luminescence image was observed. The XPS spectra were investigated to determine the chemical and binding state of the surface. The Eu3d<sub>5/2</sub> core level in the XPS spectra showed at ~1136eV. The fluorescence spectroscopy showed that the emission peak at  $\lambda=550\text{nm}$  is due to the 5d electron states of Eu<sup>2+</sup> ions which is affected by their composites .

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## A Computational Study on the Simulation of Electronic Absorption Spectra

Mannix Balanay Enopia Camille Marie 이상희 김동희

군산대 화학과

Theoretical calculation that accurately predicts excited state energies is significant since the ability of the dye to absorb a wide range of spectrum is determined through the absorption spectra. Optimized geometry structures of three dyes 1P-PPS, 1P-PSP, and 1P-PSS, which were first established by Chang et al. were carried over for TD-DFT calculations using three different known common methods; TD-B3LYP, TD-CAM-B3LYP, and TD-LC- $\omega$ PBE with three different damping parameters;  $= 0.15, 0.175, \text{ and } 0.20 \text{ bohr}^{-1}$ . The accuracy of the different simulated absorption spectra was examined by comparing the maximum values with the experimental data. 1P-PSS, which is the relatively most planar among the dye structures calculated based under TD-LC- $\omega$ PBE/6-31+G(d)//mPWPW9150/6-31G(d) in a solvent effect with damping parameter equal to  $0.175 \text{ bohr}^{-1}$ , gave results with highest accuracy. The accuracy of results is heightened with spatial overlap values within the range  $0.22 \leq \Lambda_{HL} \leq 0.36$ . The region of light-absorbed by the dye is very important for the optimization of the efficiency of the dye-sensitized solar cells. It is

ideal if the maximum absorption of the dye is within visible to near-IR region for this is the range where sunlight falls. The light-absorbing ability of dye is a good screening measure for a prospect sensitizer.



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## Theoretical and Experimental Approach on the Photovoltaic Performances of $\beta$ -substituted Porphyrin Analogues

Mannix Balanay 이미정 이상희 김동희

군산대 화학과

Spectroscopic and theoretical techniques were used to examine the effects of adsorption solvents and electrolyte additives on the photovoltaic performance of dye sensitized solar cells of two  $\beta$ -substituted zinc porphyrin analogues (ZCA-1 and KS-4), where KS-4 has an added methyl group at the phenyl ring attached to the meso-position of the porphyrin macrocycle. These results showed that the different solvents used in the sensitization process affects how the dyes are aggregated and how much of the dyes are adsorbed on the semiconductor surface. The highest efficiency of 4.2 % (30 min soaking time) and 4.0 % (1 hour soaking time) was achieved for ZCA-1 and KS-4 analogues, respectively. The hypsochromic shift observed in the UV/Vis spectra of the analogues when THF was used as a solvent was due to the partial deprotonation of the hydrogen at the carboxylic moiety of the analogues induced by the interaction of the THF molecule. Theoretical calculations at the B3LYP/6-31G(d) level of theory indicated that when THF was used as an adsorption solvent, it tends to form six- or five-coordinate

complexes causing the dyes to be largely separated when attached to the semiconductor thus lowering the amount of dye. The dye molecular plane of KS-4 was  $13^\circ$  closer to the  $\text{TiO}_2$  surface than ZCA-1 due to steric hindrance introduced by the methyl group. This increases the surface area occupied by the KS-4 dye, as indicated by the smaller amount of dye adsorbed on the  $\text{TiO}_2$  surface. The addition of 4-tert-butylpyridine or the replacement of lithium ions with guanidinium thiocyanate decreased the solar cell efficiency by 12 and 37 %, respectively, which was attributed to a decrease in the electron injection processes.





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## **Photocatalytic Reduction of Carbon Dioxide with Water to Methanol by Ag<sup>+</sup>-N-TiO<sub>2</sub>/HPA**

**박기성 이계호 윤민중**

충남대 화학과

Plant photosynthesis is one of the most efficient energy generation systems on the earth. Thus mimicking the plant photosynthesis, Photo-reduction of CO<sub>2</sub> is a sustainable energy technology not only for environmental protection but also for alternative fuels. In this work, model of two-color visible light-sensitive photocatalysts were fabricated by incorporating the Ag<sup>+</sup>-N-TiO<sub>2</sub> nanochains with HPA (Heteropoly Phosphotungstic acid), and they were used as photocatalysts to reduce CO<sub>2</sub> in water under the irradiation of solar simulation (Xe lamp with A.M. 1.5 filter, 100 mW/cm<sup>2</sup>). It was found that methanol (high efficiency; 113 μmol/g?hr) was produced via the electron transfer route mimicking the Z-Scheme of the plant photosynthetic system.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization and In Vitro Studies of Ultrasmall Holmium Oxide Nanoparticles for Magnetic Resonance Imaging (MRI) Contrast Agent

김초롱 박자영 Kattel Krishna Xu Wenlong Badrul Alam Bony<sup>1</sup> 허우철 tirusew tegafaw

Md. Wasi Ahmad 이강호

경북대 화학과 <sup>1</sup>경북대 Chemistry

We synthesized D-glucuronic acid coated ultrasmall  $\text{Ho}_2\text{O}_3$  nanoparticles and characterized with XRD, HVEM, FT-IR, TGA, SQUID magnetometer and MRI instrument. The average particle diameter is estimated to be ~2.4 nm. The nanoparticle was found to be paramagnetic which showed decent transverse relaxivity ( $r_2$ ) and  $R_2$  map images clearly showed the dose-dependent contrast enhancement. Thus, D-glucuronic acid coated  $\text{Ho}_2\text{O}_3$  nanoparticles may provide the desired contrast agent for molecular imaging at high magnetic fields.

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## dynamic heterogeneity study of interactive kinetic constrained model via dynamic ensemble

노찬우

서울대 화학과

We study the interactive kinetically constrained model(KCM) of a glass-forming liquid via dynamic ensemble. The interactive kinetically constrained model is the kinetic constrained model that has the short ranged attractions between the spin lattice. by simple KCM study, it was already demonstrated that dynamical phase transition between active (fluid) and inactive (glass) phase occurs. We report that short-ranged attraction between the spin lattice enhance the dynamical phase transition.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Ultrasmall and Uniform Size $Gd_2O_3$ and $Dy_2O_3$ Nanoparticles for MR Agent Contrast

허우철 박자영 Kattel Krishna Badrul Alam Bony<sup>1</sup> Xu Wenlong tirusew tegafaw 김초룡

Md. Wasi Ahmad 이강호

경북대 화학과 <sup>1</sup>경북대 Chemistry

We report a facile synthesis of  $Gd_2O_3$  and  $Dy_2O_3$  nanoparticles in the presence of stabilizing surfactant, oleylamine and oleyl alcohol. They were coated with different ligands such as D-glucuronic acid, Glutaric acid, Poly(ethylene glycol) bis(carboxymethyl) ether and Polyethylenimine. We characterized them with MPXRD, HRTEM, FT-IR, TGA and MRI instrument. In case of MRI contrast agent, particle size affects contrast enhancement due to different magnetization(?) of nanoparticles.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of BSA-coated $Gd_2O_3$ nanoparticles and their characterization

**Md. Wasi Ahmad** 박자영 Kattel Krishna Badrul Alam Bony<sup>1</sup> Xu Wenlong tirusew

tegafaw 허우철 김초롱 이강호

경북대 화학과 <sup>1</sup>경북대 Chemistry

In the present investigation, at first, the surface of ultra small  $Gd_2O_3$  nanoparticles were treated with diacid, which introduces organic functional groups on the surface of  $Gd_2O_3$  nanoparticles. Secondly, solution of diacid coated  $Gd_2O_3$  nanoparticles were mixed with BSA at pH 6, gave BSA-coated nanoparticles through amide bond. The BSA coating increased water solubility of nanoparticles. Characterizations of BSA-coated nanoparticles were carried out by FT-IR, TEM, PL, XRD and TGA. The ultimate goal of our research is in biomedical applications of the BSA-coated nanoparticles especially for MRI contrast agent as well as optical imaging.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Synthesis and Characterization of Fluorescent Brightener 28 Coated Iron/Iron oxide-core/shell and Iron Oxide Nanoparticles for $T_2$ MRI Contrast Agent**

tirusew tegafaw 박자영 Kattel Krishna Xu Wenlong Badrul Alam Bony<sup>1</sup> 허우철 김초롱

Md. Wasi Ahmad 이강호

경북대 화학과 <sup>1</sup>경북대 Chemistry

Superparamagnetic iron oxide nanoparticles are widely used as nanoprobes for magnetic resonance imaging (MRI). Water-soluble iron oxide nanoparticles with average diameters that ranges from 20-30 nm were synthesized by coating with Fluorescent Brightener 28 and characterized with XRD, TEM, FT-IR, PL, TGA, confocal laser scanning microscope, SQUID Magnetometer and MRI instrument. The nanoparticles can be used as cancer cell labeling and separation.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Synthesis, Characterization and Stability of Gadolinium Oxide Nanoparticles for Magnetic Resonance Imaging (MRI) Contrast Agent**

**박자영** Kattel Krishna Xu Wenlong Badrul Alam Bony<sup>1</sup> 허우철 김초롱 tirusew tegafaw

**Md. Wasi Ahmad 이강호**

경북대 화학과 <sup>1</sup>경북대 Chemistry

Note that the Gd(III) ion itself has been known to be the best metal ion in the periodic table which can be used as a  $T_1$  MRI contrast agent. In the preparation and storage of gadolinium oxide nanoparticles in colloidal form, the stability of the colloid is of utmost importance. We report a novel strategy for the synthesis of the citrate-functionalized gadolinium nanoparticles with the high colloid stability. We characterized them with XRD, TEM, FT-IR, DLS, TGA, and MRI instrument. We observed the average particle diameter from 2 to 4 nm. In-vitro tests of the sample solution indicated clear dose-dependent contrast enhancements in both  $T_1$  and  $T_2$  map images, showing that the nanoparticles may be used as both  $T_1$  and  $T_2$  MRI contrast agents.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A copper-activated gadolinium oxide nanoparticles for MRI with enhanced relaxivity**

**Badrul Alam Bony** 박사<sup>1</sup> Kattel Krishna<sup>1</sup> Xu Wenlong<sup>1</sup> 허우철<sup>1</sup> tirusew tegafaw<sup>1</sup> 김초  
룡<sup>1</sup> Md. Wasi Ahmad<sup>1</sup> 이강호<sup>1</sup>

경북대 Chemistry<sup>1</sup> 경북대 화학과

We present a new copper-activated magnetic resonance imaging (MRI) contrast agent that possesses Gd<sub>2</sub>O<sub>3</sub> and Cu<sup>2+</sup>. Gd<sub>2</sub>O<sub>3</sub> is coated with biocompatible and hydrophilic D-glucuronic acid. The nanoparticles were characterized by XRD, HRTEM and MRI instrument. Paramagnetic Gd<sup>3+</sup>, in the absence of copper ions, exhibits a relaxivity value of  $r_1 = 19.01 \text{ mM}^{-1}\text{s}^{-1}$  and  $r_2 = 19.18 \text{ mM}^{-1}\text{s}^{-1}$ ; addition of Cu<sup>2+</sup> triggers a enhancement in relaxivity to  $r_1 = 28.46 \text{ mM}^{-1}\text{s}^{-1}$  and  $r_2 = 30.55 \text{ mM}^{-1}\text{s}^{-1}$ .



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Characterization, In Virto and In Vivo MR Studies of Dysprosium Hydroxide Nanorods as a New Potential $T_2$ MRI Contrast Agent

Kattel Krishna 박자영 Badrul Alam Bony<sup>1</sup> Xu Wenlong 허우철 tirusew tegafaw 김초롱

Md. Wasi Ahmad 이강호

경북대 화학과 <sup>1</sup>경북대 Chemistry

We reported paramagnetic dysprosium hydroxide nanorods for  $T_2$  MRI contrast agents. A large  $r_2$  and a negligible  $r_1$  is an ideal condition for  $T_2$  MR imaging. The dysprosium hydroxide nanomaterials fairly satisfy this because they are found to possess a decent  $r_2$  but a negligible  $r_1$  arising from L + S state 4f-electrons in Dy(III) ion ( $^6H_{15/2}$ ). Their  $r_2$  will also further increase with increasing applied field because of unsaturated magnetization at room temperature. Therefore, MR imaging and various physical properties of the synthesized D-glucuronic acid coated dysprosium hydroxide nanorods (20×300 nm) are investigated. These include hydro-dynamic diameters, magnetic properties, MR relaxivities, cytotoxicities, and 3 tesla in vivo  $T_2$  MR images. The Dy(OH)<sub>3</sub> nanostructures showed  $r_2$  of 181.57 s<sup>-1</sup>mM<sup>-1</sup> with

negligible  $r_1$  in 1.5 tesla MR field at room temperature, no in vitro cytotoxicity up to 100  $\mu$ M Dy, and clear negative contrast enhancements in 3 tesla in vivo  $T_2$  MR images of a mouse liver and kidney, which will be even more improved at higher MR fields. Therefore, D-glucuronic acid coated dysprosium hydroxide nanorods with renal excretion can be a potential candidate as a sensitive  $T_2$  MRI contrast agent at MR field greater than 3 tesla.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Synthesis, Characterization and MRI-FI Study of Dye Coated Single-Phase Mixed GdEuO<sub>3</sub> Nanoparticles**

**Xu Wenlong Kattel Krishna 박자영 허우철 Badrul Alam Bony<sup>1</sup> tirusew tegafaw 김초룡**

**Md. Wasi Ahmad 이강호**

경북대 화학과 <sup>1</sup>경북대 Chemistry

We report a facile synthesis of ultra-small dye coated Eu<sup>3+</sup> doped gadolinium 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 (d<sub>avg</sub>) is estimated to be ~1.74 nm. The GdEuO<sub>3</sub> nanoparticles were found to be paramagnetic and emitted strong red fluorescence. The nanoparticles exhibited no appreciable cytotoxicity up to 0.1 mM concentration and in vivo MR experiment showed the positive contrast-enhancement on mouse liver and kidneys after the injection of nanocolloid. Hence, it can be used as a dual imaging probe such as MR-optical imaging agent.

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**Single-molecule studies of optical properties and dynamics of single  
protein molecules in trehalose glass by wide-field fluorescence  
microscopy**

**박민규 조한국 정병서**

인천대 화학과

The single molecule detection (SMD) technique based on epi-fluorescence microscopy is used to investigate the optical properties and dynamics of single tetramethylrhodamine (TMR) molecules and bovine serum albumin (BSA) protein molecules conjugated with TMR in trehalose glass of two different compositions (1% and 5%). Trehalose, a nonreducing disaccharide of glucose, provides an interesting medium for biological applications due to its ability to stabilize proteins. Fluorescence images of single TMR or BSA-TMR molecules were recorded as a function of time, and the temporal fluorescence emission characteristics, in particular, the fluorescence-intensity histogram and bleaching pattern of single molecules were analyzed to gain insight into dynamic behaviors of protein molecules and surrounding nanoenvironments in trehalose. The results were compared with those observed from single TMR and rhodamine 6G molecules in poly(vinyl alcohol), hydrophilic polymer film.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Spectroscopic investigation of adsorption and acidic behavior of ellagic acid on silver nanoparticles by Raman spectroscopy**

**이승장 조한국 정병서**

인천대 화학과

FT-Raman and surface-enhanced Raman scattering (SERS) spectroscopy was applied for the vibrational characterization of the highly fluorescent natural dye, ellagic acid at the solid state and adsorbed on a colloidal silver surface. Normal mode assignments of the observed bands were aided by density functional theory calculations employing the B3LYP functional. The SERS spectra were also measured at different pHs and excitation wavelengths to gain information on the adsorption and pH-dependent behavior of ellagic acid on the metal surface. The interaction of adsorbates with the metal surface leading to different adsorbate conformations and/or molecular structures were discussed based on the changes in the observed SERS spectra.

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## Quantum mechanical dynamics of CH<sub>2</sub>N<sub>2</sub>

박영춘 안희선<sup>1</sup> 최희철 백경구<sup>1</sup> 이윤섭

KAIST 화학과 <sup>1</sup>강릉원주대 화학과

In this poster, we present two dimensional quantum mechanical dynamics of CH<sub>2</sub>N<sub>2</sub> which is known to have Fano resonance in S<sub>1</sub> state dissociation. In experiment, the resonance is affected mainly by two symmetric and asymmetric C-N vibrations. Following the experimental results, two restricted dimensions describing C-N vibration is set. The potential energy surfaces (PESs) of the S<sub>0</sub>, S<sub>1</sub> states are obtained from CASSCF(10,12)/6-311++G(d,p) and fitted analytically. The spectrum obtained from the dynamics is compared with the experiment.

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## **Live-cell imaging with upconverting nanoparticles: the long-term intracellular pathway of nanoparticles**

**배윤미 박용일<sup>1</sup> 남상환<sup>2</sup> 김정현<sup>1</sup> 이경희<sup>2</sup> 김형민<sup>2</sup> 최준식 현택환<sup>1</sup> 이강택<sup>2</sup> 서영덕<sup>2</sup>**

충남대 생화학과 <sup>1</sup>서울대 화학생물공학부 <sup>2</sup>한국화학연구원 나노바이오융합연구센터

Recently, lanthanide-doped upconverting nanoparticles (UCNPs), which can absorb NIR photons and emit in the short-wavelength photons in the visible spectral range, have received much attention as promising nano-probes in cell biology and clinical application owing their highly advantageous optical properties. Here, we investigated the huge benefits of using UCNPs for live cell imaging and the spatiotemporal evolution of UCNPs within single HeLa cells. Based on the snapshot images taken over 24 hours, the UCNPs were supposed to be internalized through endocytosis, actively transported to and accumulate at a perinuclear region, and eventually discarded from the cells through exocytosis. Each step in such pathway was confirmed by additional controls including various biochemical inhibition studies. Our work provides a picture of how nanoparticles behave within single cells.

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## Simulation study of two dimensional ring polymer melts

**박창현 성봉준**

서강대 화학과

Understanding the static and dynamic properties of ring polymer melts has been an challenging issue in polymer science. Ring polymers show uncommon properties because of their topological constraint. Unlike the linear polymer, ring polymer has no free chain ends. There have been experimental studies and simulation studies to study how those constraint affects the properties of ring polymers. But most of simulation studies were limited only on cubic lattice and experimental studies had an considerable error because of linear polymer contamination. To study those ring polymer more preciesly we perform two dimensional discontinuous molecular dynamics simulations to figure out what parameter mainly controls the conformation and dynamics of system. The polymers are consists of tangent hard disc chains. We prepared several conditions (different density, different polymer length) to find out the effect of polymer size and density. We found radius of gyration( $R_g$ ) of ring polymer in 2D melts scales as  $N^{0.74}$  when Area fraction(AF)=0.1,  $N^{0.56}$  at AF=0.3 and  $N^{0.52}$  at AF=0.5 unlike linear polymer scales as  $N^{0.56}$  regardless of



area fraction, and diffusion coefficient scales as  $N^{-0.74}$  in low density and  $N^{-1.22}$  in high density. Simulation study of two dimensional ring polymer melts



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermochromic Properties of Star-Shaped Oligothiophenes with Conformational Change and Planarization Process

정희재

연세대 화학과

To define a relationship between degree of planarization and its intersystem crossing rate. Thus, we first measured the steady-state spectroscopy and TCSPC to get each molecules fluorescence lifetime and figured out Trimer and Hexamer have a different rigidity due to their degree of steric congestion. Also, we had done temperature dependent measurements to control the conformational changes of each molecule. Trimer and Hexamer both go through a geometric change from the non-relaxed non-planar to the relatively relaxed planar excited state S1, and each of ultrafast intersystem crossing rates (kisc) is different. Especially, Trimer intersystem crossing rates are largely changed due to its structural flexibility. At excited state, in case of Trimer effective planarization process is observed, which results in extended conjugation length.

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## **Photochemical Analysis of Single-walled carbon nanotube Functionalized with Porphyrin**

**YanCui**

성균관대 에너지과학과

Single-walled carbon nanotubes (SWCNTs) with covalently linked porphyrin antennae have been synthesized and characterized as potential supramolecular donor-acceptor complexes. The resulting products were determined from NMR, spectroscopic (XPS, UV-vis-NIR, FTIR and Raman), and microscopic (SEM and TEM) methods. An extensive photophysical investigation by steady-state fluorescence emission spectrum of porphyrin-SWCNT shows that CNT act as efficient electron acceptors

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## Effect of oxygen plasma treatment power on water proof coated surface

민은선 민문홍<sup>1</sup> 남상일

경북대 화학과 <sup>1</sup>한국염색기술연구소 융합제품가공연구팀

The effect of oxygen plasma treatment power on surface properties of water proof material coated fiber were investigated. Surface chemical composition, surface roughness and surface morphologies of fiber were analyzed by X-ray photoelectron spectroscopy(XPS), atomic force microscopy(AFM) and scanning electron microscopy(SEM), respectively. We could fabricate a switchable surface O<sub>2</sub> plasma treatment. And, we observed that O<sub>2</sub> plasma treatment could give partly hydrophilic site at the hydrophobic surface. 30s plasma exposure time was find to be optimum for switches. The coated polymer on the surface of the fiber responds to thermal variations with switching between hydrophilic and hydrophobic properties.

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## Mass Spectrometry를 통한 Angiotensin II와 Cu 금속이온간의 결합 자리에서 Arginine과 Aspartic acid의 R-group 영향 확인

임승훈 배장호 강예송 김호태

금오공과대 응용화학과

우리의 몸에는 혈압강하시 혈압을 상승시켜주는 Angiotensin II가 있다. 금속이온들이 Angiotensin II와 결합하게 되면 혈압상승효과에 영향을 주는 것으로 알려져있다. 이 금속들 중 Angiotensin II+Cu 에 대해 질량분석기를 통해 결합자리를 알아보았을 때 일반적으로 1~4 자리의 Oxygen 에 결합한다고 추정되었다. 이것은 Angiotensin II+Cu 의 양자역학적 계산결과에서 1,2 번 자리의 아미노산의 R-group 이 수소결합을 하기 때문이라고 생각되어진다. 본 실험은 이 Aspartic acid-1 과 Arginine-2 를 Glycine-1 과 Glycine-2 로 바꿔준 뒤에도 Cu 가 1-4 번자리의 Oxygen 결합자리를 선택하는 가능성을 MS/MS 와 MS/MS/MS 를 통해 실험하였다.

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## **GlyGlyGlyHis/GlyHisGly와 Copper ion( $\text{II}$ )( $\text{Cu}^{2+}$ ) Complex의 형성**

### **과 구조에 대한 연구**

**강예송 배장호 임승훈 김호태**

금오공과대 응용화학과

금속 이온과 펩타이드의 결합에서 금속 이온의 Specific binding site 는 생체 sensor 개발에 도움을 줄 수 있다. Cu 이온을 전달하는 혈청 알부민에서 N-terminal 은 3 개의 아미노산 AspAlaHis 로 이루어져 있는데, Asp1 과 Ala2 를 Side group 이 없는 Gly1Gly2 로 치환한 GGH 는 Cu 이온과의 결합에서 좋은 모델 Peptide 로 연구되었다. AspAlaHis 과 GlyGlyHis 이 Cu 이온과 결합할 때 N-terminal 과 Peptide bond 의 N, 그리고 His 의 Imidazole ring 의 N 이 결합에 참여한다고 알려져 있다. 본 실험에서는 His 의 R-group 인 Imidazole ring 의 역할을 Cu 이온과의 결합에서 알아보려고 한다. 그리하여, GGH 의 모델 펩타이드 대신으로, GGGH 와 GHG 를 사용하여 실험하였다. 이 실험을 위해서 GGGH, GHG 그리고 Cu 이온의

농도를 각각  $2 \times 10^{-4} \text{ M}$  로 하고 부피 비 1:1 로 혼합하여 ESI-MS, MS/MS, MS/MS/MS 를 수행하였다.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparison on three types of ionization sources for time-of-flight mass spectrometry of liquid explosives

홍용준 고은미 조수경

국방과학연구소 국방신기술센터/융복합기술부

Some different kinds of liquid explosives are analyzed by means of three types of ionization sources through the linear time-of-flight mass spectrometer made by Jordan Co. Inc. The first ionization source is the thermionic electron emission from hot cathode filament, which is the most common electron source for Electron Ionization(EI). The second is the pulsed laser beam with the UV wavelength for photoionization(PI) source. The last one is the cold electron source which is generated from a channel electron multiplier(CEM) and a micro-channel plate electron multiplier(MCP) illuminated by UV photons from LED. It is also examined as a pulsed electron source. When compared with the mass spectra of explosive materials taken by three different ionization source, the pulsed cold electron beam appears to provide better spectra than the other sources. The hot electron source is not sensitive on the ionization energy of a molecule and the PI method using the laser has a good resolution due to the very short pulsed



operation. Our preliminary application results show that the pulsed cold electron source is of great use in the practice of EI for a TOF mass spectrometer.



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## Borate 완충용액에서 생성되는 아연의 부동화 피막의 전기적 특

성

김진아 이동건 김연규

한국외국어대 화학과

Borate 완충용액에서 Zn의 부식과 부식에 의하여 생긴 부동화 피막은 ZnO로 구성되어 있으며, 나아가 산화 피막은 대수함수 속도법칙에 따라 성장하며, n-형 반도체의 전기적 특성임을 조사하였다. 일정한 전극전위 구간마다 다양한 특징들을 볼 수 있으며, Mott-Schottky 식에 적용하여 두 종류의 주개가 존재하는 현상을 발견하였다.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Near-field Optical Microscopy of Nanostructures with an Up-Conversion Nanoparticle as a Point Light Source

김주영 김지환

고려대 화학과

We demonstrate the use of up-conversion nanoparticles (UCNPs) as local point light source for nanometric optical imaging of nanostructures. The UCNPs are made of core@shell Yb<sup>3+</sup>/Er<sup>3+</sup>@NaYF<sub>4</sub> and the UCNPs produce strong fluorescence at 540 nm and 660 nm when excited with a cw-laser light at 980 nm without any photo-bleaching or blinking, which is 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 poly-L-lysine linkers, and the transmitted emission at  $\lambda_{\text{max}} = 540$  and 660 nm are collected through Au-Fisher patterns. We find that the transmission images show features that are below the excitation (980 nm) or emission wavelengths (540 and 660 nm), which demonstrate that the UCNPs indeed serve as a near-field (incoherent) point light source. We also discuss the possibility of the UCNP-tip for the high-resolution imaging of individual molecules based on the energy transfer between the UCNPs and individual fluorescent molecules.

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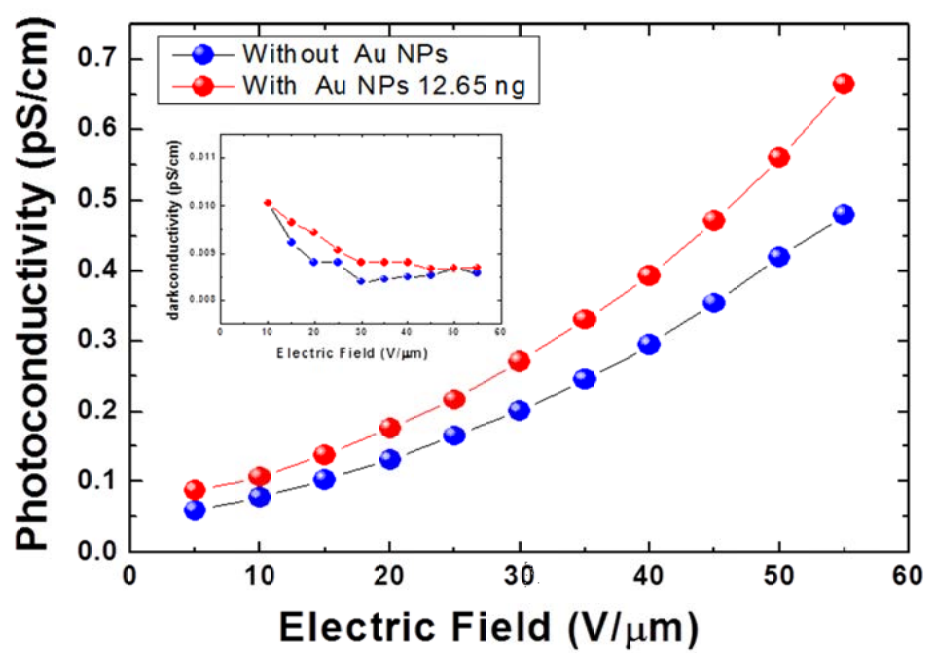
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The Influence of Gold Nanoparticles on the Photorefractive Polymeric Composites**

지석환 허윤중 문인규<sup>1</sup> 김낙중

한양대 화학과 <sup>1</sup>서강대 인공광합성 연구센터/나노물질연구소

Several studies have been reported on manipulation of the photorefractive properties by using small concentrations of various dopants. In this work, we investigate the photorefractive properties of polymeric photorefractive composite doped with gold-nanoparticles (Au NPs) to enhance photoconductivity and refractive index modulation.



$\lambda=632.8\text{nm}$  ( $I=13\text{mW/cm}^2$ )

Thickness ( $d=50\mu\text{m}$ )



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## DFT를 이용한 $C_{20}H_{17}(OH)_3$ cluster의 5개 기하이성질체에 대한 원

### 자 및 전자성질연구

이설 이기학<sup>1</sup>

원광대 생명나노화학부 <sup>1</sup>원광대 화학과

$C_{20}H_{17}(OH)_3$  는 15 개의 이성질체를 가지고 있다. 이에 관한 구조를 최적화하여 구조적 에너지와 각 이성질체의 상대적인 에너지를 비교하였고, HOMO,LUMO 를 이용한 energy gap 을 분석하여 규칙성을 연구하였다. 각각의 이성질체의 strain energy 를 분석함으로 Reference 가 되는  $C_{20}H_{20}$  에 어떤 영향을 주는지 확인하였다. 프로그램은 Gaussian 03W 를 사용하였고, basis set 은 6-31g(d,p)를 이용하였다.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of cation charge distribution on the heterogeneous dynamics of ionic liquid systems

김소리 정연준

서울대 화학부

We study the effect of cation structure, especially charge distribution, on the dynamic heterogeneity. We use symmetric charge model and asymmetric charge model to represent different ionic liquid systems. We use four-point density correlation functions to investigate the dynamic heterogeneity of ionic liquid systems. The most important physical quantities in our work are the dynamic susceptibility and the dynamic structure factor. From the dynamic susceptibility, we can obtain life time of dynamic heterogeneity. Further, the dynamic structure factor reveals the length scale of dynamic heterogeneity. The scaling laws between physical quantities like relaxation time, heterogeneity life time, and correlation length show different behavior for the symmetric charge model and asymmetric charge model.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comprehensive Studies on the pKa of Substituted Phenol : A Theoretical Study

한인숙 김창곤 김찬경 이해황

인하대 화학과

To investigate the origin of substituent effects on the acidity of phenol, a series of substituted phenol 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, BONDY 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 gas-phase have also been fully optimized and characterized by frequency calculations. All the calculations were performed with the Gaussian-03 program.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Kinetics and Mechanism of the Pyridinolysis of Diethyl Isothiocyanophosphate in Acetonitrile

Adhikary Keshab Kumar Hasi Rani<sup>1</sup> 이해황 김찬경

인하대 화학과 <sup>1</sup>인하대 물리화학과

The kinetics and mechanism of the pyridinolysis ( $\text{XC}_5\text{H}_4\text{N}$ ) of diethyl isothiocyanophosphate are investigated in acetonitrile at  $55.0^\circ\text{C}$ . The Hammett and Bronsted plots for substituent X variations in the nucleophiles exhibit the two discrete slopes with a break region between  $\text{X} = 3\text{-Ac}$  and  $4\text{-Ac}$ . These are interpreted to indicate a mechanistic change at the break region from a concerted to a stepwise mechanism with rate-limiting expulsion of the isothiocyanate leaving group from a trigonal bipyramidal pentacoordinated intermediate. The relatively large  $\beta_{\text{X}}$  values with more basic and less basic pyridines imply much greater fraction of frontside nucleophilic attack TSf than that of backside attack TSb.

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## Electron and Hole Mobilities in PbSe Nanocrystal Arrays

최완 심은지

연세대 화학과

We investigated size-dependency of electron and hole mobilities in PbSe nanocrystal arrays. Size of semiconductor nanocrystals is closely related to electronic properties. Experimentally, as the size of its individual crystal becomes larger, the carrier mobility has been known to increase. However, a recent study showed that the electron mobility decreases as the size becomes larger when the nanocrystal diameter is over 6 nm. In this work, PbSe nanocrystal arrays are modeled with a five-state system-bath Hamiltonian. Time-evolution of the density matrix is evaluated using the on-the-fly filtered propagator functional path integral method, which is used to extract charge transfer rate. Then, electron and hole mobilities are evaluated from the charge transfer rates. Computed electron and hole mobilities showed excellent agreement with the experiment[Nano Lett. 2010, 10, 1960]. We found that the non-monotonic trend of the electron mobility was due to conflicting effect of the electronic coupling and the charging energy.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Kinetics and Mechanism of the Anilinolysis of Diethyl Isothiocyanophosphate in Acetonitrile

Hasi Rani Adhikary Keshab Kumar<sup>1</sup> 김찬경<sup>1</sup> 이해황<sup>1</sup>

인하대 물리화학과 <sup>1</sup>인하대 화학과

To extend the kinetic studies on the phosphoryl transfer reactions involving a leaving group of isothiocyanate, the nucleophilic substitution reactions of diethyl isothiocyanophosphate with substituted anilines ( $\text{XC}_6\text{H}_4\text{NH}_2$ ) and deuterated anilines ( $\text{XC}_6\text{H}_4\text{ND}_2$ ) are investigated kinetically in acetonitrile (MeCN) at  $55.0 \pm 0.1$  °C. The Hammett and Bronsted plots for substituent X variations in the nucleophiles exhibit the two discrete slopes with a break region between X = H and 4-F. The obtained DKIEs ( $k_{\text{H}}/k_{\text{D}}$ ) are secondary inverse ( $k_{\text{H}}/k_{\text{D}} = 0.74\text{--}0.87$ ) with the strongly basic anilines while secondary and primary normal ( $k_{\text{H}}/k_{\text{D}} = 0.71\text{--}1.58$ ) with the weakly basic anilines. A concerted  $\text{S}_{\text{N}}2$  mechanism (or a stepwise mechanism with a rate-limiting bond formation step) involving a backside attack is proposed for the weakly basic anilines, and a stepwise mechanism with a rate-limiting leaving group departure from the TBP-5C intermediate involving both backside TSb and frontside attack involving a hydrogen-bonded, four-center-type TSf is proposed for the strongly basic anilines.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Theoretical Investigation on Asymmetric Cyanation of Activated Olefins with Ethyl Cyanoformate Catalyzed by Titanium Catalyst

su zhishan 이해황<sup>1</sup> 김찬경<sup>1</sup>

인하대 물리화학<sup>1</sup> 인하대 화학과

The mechanism and the origin of selectivity of asymmetric cyanation of activated olefins with ethyl cyanoformate catalyzed by a Ti(IV)-complex catalyst have been investigated by DFT and ONIOM methods. The calculations indicate that the reaction proceeds through a dual activation mechanism, in which TiIV acts as Lewis acid to activate the olefin substrates while the tertiary amine in cinchona alkaloid works as a Lewis base to promote the activation and isomerization of HCN. The overall reaction involves two stages: (i) the formation of C-C bond; (ii) the transfer of H atom and the regeneration of catalyst. The first step is predicted to be the rate-determining step and selectivity-controlling step with an energy barrier of 7.9 kcal mol<sup>-1</sup>. The large steric hindrance from 3,3'-biphenol, combining with the quinoline fragment of cinchona alkaloid and the orientation of hydrogen bonding of iPrOH, play a key role in controlling the stereoselectivity, which is in good agreement with experimental observations.

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## Flexible Reduced Graphene-Oxide Sheet for Position-Sensitive Photodetector

형은수 윤수진 문인규<sup>1</sup> 김낙중

한양대 화학과 <sup>1</sup>서강대 인공광합성 연구센터/나노물질연구소

Reduced graphene-oxide is considered to be a promising material for optoelectronic devices due to exceptional electrical and photonic properties; 2-D spread structure and mechanical flexibility. More interestingly, reduced graphene-oxide also has the ability to absorb photons over a wide spectrum from visible to near infrared, which is significant for making optoelectronic devices. Here in this work, we prepared a reduced graphene-oxide paper through vapor-phase reduction for graphene with HI/acetic acid. We also fabricated a photodetector using the gold electrodes which were attached to both sides of reduced graphene-oxide 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 clearly show that macroscale thick films of reduced graphene-oxide can serve as a position photosensing at the range of visible through rear infrared.

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## Control of Nanosheet Morphology

현정인 한민우 심은지

연세대 화학과

Modification of nanosheet is an intriguing and exciting subject since there are a lot of ways to control shape, size, and functions of nanosheets. And many scientists have synthesized nanosheets which consist of biomolecules, inorganic materials, or polymers. Therefore, the nanosheet has great potential for various useful devices such as catalysis, drug delivery, and electronics. In this work, coarse-grained tethered monolayers are modeled in solution and their transformation from flat membranes to secondary structures is investigated using dissipative particle dynamics simulations. We show that morphology of its secondary structure strongly depends on the nanosheet bonding scheme as well as the properties of surface coils. Relationship between various morphology and properties of the nanosheet is discussed.

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## **Coherent coupling of perylenediimide linear and trefoil trimer probed by single molecule spectroscopy**

유혜진 김동호

연세대 화학과

We have investigated two perylenediimide (PDI) trimer molecules which have linear and trefoil structures to observe the relationship between the structures and molecular interaction. To discriminate heterogeneities of each molecular structure depending on the nanoenvironments as well as two (linear/trefoil) different molecular structure, spectral shift and change of emission distribution of PDI trimer molecules have been addressed by single molecule spectroscopy which allows to probe excited state dynamics in real time.

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## **Dynamics of Ligand Binding to Apomyoglobin Measured by Fluorescence Lifetime Correlation Spectroscopy**

**박성철 임만호**

부산대 화학과

The dynamics of the binding reaction of nile red (NR) to horse apomyoglobin (apoMb) has been investigated by fluorescence correlation spectroscopy (FCS). FCS is useful in measuring chemical reaction rates and diffusion coefficients of molecules in equilibrium in the range of  $10^{-7}$  s  $\sim$  10 ms. When the 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 can be determined directly. To take pseudo-first-order conditions, it is necessary to separate the autocorrelation function (ACF) of individual components of bound and free ligand. Since NR strongly fluoresces when it is within the hydrophobic heme pocket of the protein but is weakly fluorescent in solution. This weakly fluorescent contribution may be significant. The FLCS method, a fusion of time-correlated single photon counting (TCSPC) 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. Specifically, the on rate is  $30 \text{ M}^{-1} \text{ s}^{-1}$



and the off rate is  $730\text{s}^{-1}$  at pH7 and  $20^{\circ}\text{C}$ . The on rate appears to be activation controlled reaction, when we compared with 8-anilino-1-naphthalene sulfate (ANS).



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## GalaxyGemini: A homology-based protein oligomeric state prediction algorithm

이하설 석차욱

서울대 화학부

Many proteins perform their functions as homo-oligomers, called 'homomers'. Predicting homomer structures from the amino acid sequences is of prime importance for understanding many biological processes. We have developed a method that predicts protein homo-oligomer structures based on sequence homology. Homologues are detected using HHsearch and rescored using a combined score of HHsearch score, secondary structure score, aligned-column match score, template coverage score, and interface sequence alignment score. Different strategies are used depending on whether consensus is found among the oligomeric states of top-ranking homologues. If there exists a cluster of homologues of the same oligomeric states that gives a cluster score greater than a cut-off value, the best-scoring homologue in the cluster is selected as the oligomer structure template. If not, the top homologue after rescoring is selected. The weight parameters of the rescoring function were trained on a set of 218 PDB entries from Ref. [1]. The current method, named GalaxyGemini, is tested on the CASP9 oligomer set. [1]

Ponstingl H., Kabir T. and Thornton J., Automatic inference of protein quaternary structure from crystals.  
J. Appl. Cryst. 36 (2003) 1116-1122.



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## The Br formation dynamics of 2-bromopropene near 234nm

김현국 김태규

부산대 화학과

The photodissociation dynamics of 2-bromopropene near 234 nm have been investigated using velocity map imaging technique coupled with a state-selective [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme. There has two chromophores, one is  $\sigma^* \leftarrow n$  another one is  $\pi^* \leftarrow \pi$ . The nascent Br atoms stem from the primary C-Br bond dissociation leading to the formation of C<sub>3</sub>H<sub>5</sub> and Br(2P<sub>j</sub>; j= 1/2, 3/2). Trimodal energy distribution (single Boltzmann and two Gaussian functions) of Br(2P<sub>j</sub>) have been observed. The experimental result also showed that Br formation is dominant with the relative quantum yield 0.92 in 234nm. The measured total translational energy distributions, recoil anisotropic parameters, and the relative quantum yields were used to explore the inside of surface interaction among the potential energy surfaces in detail.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## DFT를 이용한 $C_{20}H_{18}(CH_3)_2$ clusterdml 5개 기하이성질체에 대한

### 원자 및 전자성질연구

이설 이기학<sup>1</sup>

원광대 생명나노화학부 <sup>1</sup>원광대 화학과

$C_{20}H_{18}(CH_3)_2$  는 기하이성질체를 5 개를 가진다. 이 이성체를 혼성 범밀도함수법을 이용하여 최적화한 후 각 구조적 성질과 상대적인 에너지를 비교함으로써 안정도를 확인하며, HOMO, LUMO 를 이용한 energy gap 을 비교하여 이성체의 규칙성을 연구하였다. 또한 각 이성질체의 진동수를 계산하여 이 들의 결합에 관한 연구를 하였다. 프로그램은 Gaussian 03W 를 이용하였고, Basis set 은 6-31g(d,p)를 사용하였다.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **$H_n@C_{20}$ 과 $H_n@C_{20}H_{20}$ 에 대한 구조특성 연구( $n=1\sim3$ )**

**조인수 이기학**

원광대 화학과

$H_n@C_{20}$  과  $H_n@C_{20}H_{20}$  에 대하여 분자구조, 그리고 에너지 등을 계산하였다.( $n=1\sim3$ ) 위의 모든 분자들에 대하여 SCF 방법으로 에너지를 계산하였고, B3LYP/6-31(d,p)의 이론 수준에서 최적화 하여, 각 화합물의 가장 안정한 분자구조를 확인하고 결합에너지를 계산하였다. 모든 계산은 Gaussian 03 을 이용하였다.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Quantitative Detection of Biomolecule by Using Scanning Electron Microscopy Point Counting

박형주

한국전자통신연구원 BT융합연구부

We reported that quantitative detection of prostatic specific antigen (PSA), cancer marker, could be carried out by calculating the number of Au nanoparticle probes, gold nanoparticles conjugated with PSA-pAb, attached on the chip surface. The probes were bound by using antigen-antibody interaction, and the number density was characterized by scanning electron microscopy point counting (SEMPC). As the PSA concentration increased, the density of the Au nanoparticle probes attached on chip surface also increased. We observed the correlation between PSA concentration and number density of Au nanoparticle probe through the analysis of SEM images.

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발표코드: **PHYS.P-415**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**포획된 이원자분자가 C<sub>20</sub>H<sub>n</sub> (n=0,20) Cage 원자구조에 미치는 영  
향에 관한 DFT연구**

**전성기 이기학<sup>1</sup>**

원광대 생명나노화학부 <sup>1</sup>원광대 화학과

Gaussian 03W 를 이용하여 CO@C<sub>20</sub>H<sub>n</sub>(n=0,20)를 single point 로 계산 후 가장 낮은 에너지를 최적화시켜 각 구조들을 비교 연구하였다.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Driving and Monitoring Photochemical Reaction using Gap-Plasmons

**최한규 김지환**

고려대 화학과

We report that the strongly enhanced field formed at nanoparticle-thin film junction can locally induce the chemical reaction and the surface-enhanced Raman scattering (SERS) from the junction allows one to monitor the product molecules at individual molecule level. The individual silver nanoparticle (AgNP)- 4-nitrobenzenethiol (NBT) monolayer - gold thin-film (AuTF) junctions are illuminated by a laser light (wavelength of 632.8 nm) to induce photo-reduction, and to monitor the SERS during the course of the reaction. We observe that the center frequency of  $\nu_s(\text{NO})$  peak ( $1350\text{ cm}^{-1}$ ) in the SERS spectra red-shifts by  $10\text{ cm}^{-1}$  prior to the decay in intensity. This red-shift indicates that the decay kinetics is in fact the nitrobenzene anion radicals ( $\text{R-NO}_2^-$ ) formed by the metal to NBT electron transfer reaction, rather than the neutral NBTs. Before the  $\nu_s(\text{NO})$  peak of the reactant NBTs shows an exponential decay, the peak shows the red shift ( $10\text{ cm}^{-1}$ ). We may think this shift pattern shows an electron transfer from the metallic surface. In addition, while the  $\nu_s(\text{NO})$  peak shows the pseudo 1st-order decay kinetics of many ( $\sim 200$ )

molecules at a NP-TF junction, the bands (9b, 3, and 19b) of the product show discrete rise in intensities, which we interpret as the individual product molecules, possibly 4,4'-dimercaptoazobenzenes.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Single-molecule reaction dynamics of 10-23 deoxyribozyme: Substrate sequence dependence

정지원 강주연 박소영 김성근

서울대 화학부

By using total internal reflection fluorescence spectroscopy, we investigated the substrate sequence dependence of the enzymatic reaction of RNA-cleaving 10-23 deoxyribozyme at the single-molecule level. Real-time detection of the 10-23 deoxyribozyme folding with a single-step temporal resolution allowed us to determine the substrate sequence-dependent reaction rate and kinetic parameters such as the activation energy and the Arrhenius A-factor for individual reaction steps.

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발표코드: **PHYS.P-418**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Photoinduced Plasmon Switching Controlled by Isomerization of Azobenzene-containing Alkylthiols Sandwiched with a single Au Nanoparticle/Au thin film junction**

**김진욱 김지환**

고려대 화학과

We demonstrated the irreversible shift of plasmon resonance of Au nanoparticle (NP)/azobenzene-containing alkylthiol inserted into self-assembled monolayer(Azobenzene)/Au thin film (TF). Dark-field microscope combined with a spectrometer allowed us to observe that a single Au NP/Azobenzene/Au TF junction shows reversible shift of coupled resonance with UV (365 nm) and visible (460 nm) excitations due to photoinduced isomerization of Azobenzene molecules. Our study shows the possibility that the plasmon resonances can be actively manipulated by controlling the gap distance of NP/TF junction on sub-nanometric changes.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Molecular Dynamics Study of the adsorption of Freon R12 in ZSM5 zeolite**

**Li Jun 김찬경 김창곤 이해황**

인하대 화학과

The increased awareness of the environmental hazards of Freon molecules has led to the development of new separation medias. Zeolites are widely used in industry as ion-exchanger, sorbents and catalysts, and it is recognized as interesting alternatives to other separation media at Freon cleaning process. A simple model is used for predicting the adsorption behaviours of Freon molecule R12 in zeolite ZSM5, the zeolite framework is modelled base on the well-known T model and molecular dynamics simulations are performed with the cation-framework model of Jaramillo and Auerbach. With the help of quantum calculations, the interaction among on R12 molecules is also investigated, so a serial of MD simulation are performed to study the adsorption behaviour of R12 in ZSM5 zeolite. These simulations show that the non-framework cations play an important role in the interaction with guest R12 molecules and the migration of guest molecule inside zeolite can significant affects the host-guest interaction.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Approximate Functionals on Hartree-Fock Density: Finding Global Minimum of Radical Complexes

김민철 심은지 Kieron Burke<sup>1</sup>

연세대 화학과 <sup>1</sup>Department of Chemistry, University of California, Irvine

We present a potential energy surface (PES) study of OH radical complexes. Density functional theory (DFT) using approximate functionals is known to give inaccurate results in predicting the global minimum for OH radical complexes. To overcome this we use a recently proposed HF-DFT scheme in which DFT energy is evaluated on Hartree-Fock (HF) densities using approximate functionals. In this presentation, we scan PES of OH $\cdots$ Cl<sup>-</sup> and OH $\cdots$ (H<sub>2</sub>O) complexes with DFT using approximate Kohn-Sham densities and HF densities. Energies for each geometrical point are evaluated with the PBE, BLYP, and B3LYP functionals. For each approximate functional, DFT energies are estimated upon HF densities. We also compare DFT PES with highly accurate CCSD(T) PES. The global minimum predicted with traditional DFT methods are apparently different from CCSD(T) results, locating the minima on delocalized electron configurations like two-body three-electron hemi-bonding conformations. On the

other hand, HF-DFT minima are exactly in match with CCSD(T) results with more localized hydrogen bonding conformations. All calculations were performed with the Turbomole 6.2 program package.



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## **GALAXY-Cassiopeia: Protein Chain-building by using Template-based Restraint and Physicochemical Energy**

허림 석차옥

서울대 화학부

Protein tertiary structure provides essential atomic-level information for biological and medicinal studies. For the last few decades, there have been numerous studies for predicting protein tertiary structure using computational techniques; especially prediction methods using homologue structures as templates have been successful in providing more accurate model structures. In this kind of template-based modeling, one of the key steps is building protein models using the structural information extracted from templates. MODELLER, a widely used protein chain-building program, has dealt with this problem successfully. MODELLER employs restraint energy terms obtained from templates and basic physics-based energy terms for maintaining correct stereochemistry. In this study, we developed a new chain-building method, GalaxyCassiopeia, which considers additional physicochemical interaction energy such as atomic interaction free energy described by statistical potential and effective solvation free energy based on



physical chemistry. In this way, more physically realistic structures could be generated both in local and global aspects when tested on the CASP9 targets.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## QSPR studies on the prediction of sublimation enthalpies using 3D MSEP Model

김찬경 김창곤 Li Jun 이해황 조수경<sup>1</sup>

인하대 화학과 <sup>1</sup>국방과학연구소 4-2부

Sublimation enthalpy is a property of practical significance in determining the stability of crystal structures and is the sum of fusion and vaporization enthalpies. Since it represents the contribution of intermolecular interactions to the energy content of materials, it should also be taken into account to estimate the performance of energetic materials or hazards of chemical substances. In this work, we tried to derive some QSPR equations for 1300 organic molecules. All the structures were fully optimized at the B3LYP/6-31G(d) level of theory and 3D molecular descriptors were generated from the electrostatic potential calculated on the van der Waals molecular surface of molecules, called MSEP model. The derived results are compared with the models developed from fragment contributions and genetic algorithm and further application is suggested based on the results.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Sub-diffraction-limit imaging of closely targeted fluorophores within a stretched DNA by STED nanoscopy**

김형준 김남두 김영규 김성근

서울대 화학부

In testing the prospect of using STED (stimulated emission depletion) nanoscopy in structural studies of biological systems by spatially-resolved probing of the on and off state of individual fluorophores, we demonstrated the feasibility of discriminating two single fluorophores targeted specifically in a stretched DNA. An oligonucleotide synthesized and labeled with a single fluorophore was cross-linked covalently to a specific sequence of  $\lambda$ DNA labeled separately. Upon applying the dynamic molecular combing method, the  $\lambda$ DNA was stretched on a glass cover slip, resulting in fluorophores at a distance that can be resolved by STED nanoscopy.

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발표코드: **PHYS.P-424**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A metadynamics study of a minimalist model for single molecule spectroscopy in condensed phases**

오인록 정연준

서울대 화학부

In single molecule spectroscopy, measurements are made to probe fluctuations that arise due to either spatial or dynamic (or both) heterogeneity of the interaction between a probe molecule and its local environments. Even though the molecules are identical, their spectral properties are typically different as a consequence of the fluctuation. In order to simulate these phenomenon, we developed a minimalist model of single molecule spectroscopy based on a lattice system with probe molecule embedded in an Ising-model like environment. We assume that the probe molecule interacts with the Ising spins via a dipole-dipole potential, and calculate free energy curves and lineshapes of the system. To investigate fluctuation behavior of the system we exploit the metadynamics sampling method. In particular, using the method, we calculate the free energy curve of magnetization of the lattice and that of the transition energy of the probe molecule. Furthermore, we compare efficiencies of three different sampling methods used; unbiased, umbrella, and metadynamics sampling methods. Finally, we explore the lineshape behavior of

the probe molecule as the system undergoes a phase transition from a sub-critical and to a super-critical temperature. We show that the transition energy of a probe molecule is broadly distributed due to the heterogeneous, local environments.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## REMPI and UV-UV double resonance spectroscopy of Synephrine and Its Water Cluster

김민호 이소영<sup>1</sup> 강정석 강혁

아주대 화학과 <sup>1</sup>아주대 자연과학부/화학전공

Synephrine is one of the drugs for weight loss. Synephrine binds to the Beta 3 cell receptors to increase the rate of fat release from fat cells. Small amount of synephrine also act as a noradrenergic neurotransmitter which has an antidepressant-like effect. The “Key and Lock” theory explains the binding mechanism between a neurotransmitter and a target receptor. To act as a “key”, the neurotransmitter should have a specific conformation that matches the binding pocket of the receptor. It has been revealed that some neurotransmitters like L-DOPA have only one conformer in the gas-phase. Even for those that have multiple conformers, it is expected that the many conformations merge to only one conformer *in vivo*. It was experimentally found that synephrine has at least 6 conformers in the gas-phase. We have calculated the relative stability of many conformers of synephrine and its water cluster to study the effect of solvation on the stabilization of its conformation. We found six stable conformers of isolated synephrine at MP2/cc-pVDZ level of theory. The 0-0 band of the most stable one is expected around

36,600  $\text{cm}^{-1}$  by CC2/cc-pVDZ, which is comparable to the experimentally found 0-0 band at 35,700  $\text{cm}^{-1}$ . When a water molecule is attached to synephrine, only two stable conformers remain. We have obtained REMPI spectra and UV-UV double resonance spectra of synephrine and its water cluster.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **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. In this study we investigated solvent-assisted conformational isomerization (SACI) of AAP. SACI is a phenomenon that the population of less stable conformers of a flexible molecule is transferred to that of more stable ones when small amount of solvent is added to the supersonic expansion of the molecule. One obstacle in investigating SACI of AAP by REMPI is that the spectrum of AAP is masked by broad absorption and dissociative ionization of AAP-water clusters when AAP is co-expanded with water. We employed laser-induced fluorescence (LIF) in order to investigate the electronic spectra of jet-cooled AAP and AAP-water cluster, and compared the results with those obtained by REMPI.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study of acetaminophen and 1:1 acetaminophen-water cluster by two-color resonance-enhanced multiphoton ionization spectroscopy

이소영 강혁

아주대 화학과

A small drug acetaminophen(AAP), which is used as a fever reducer and pain reliever, has two conformers defined by the orientation of the OH functional group. In our previous studies, we demonstrated that the cis/trans ratio of AAP was changed when we used carrier gas that is mixed 1% of water and helium because the less stable conformer is transferred to the more stable one by water. This phenomenon is called solvent-assisted conformational isomerization(SACI) in our group. Resonance-enhanced multiphoton ionization (REMPI) spectra of AAP expanded with pure helium and with helium and 1 % of ammonia have broad background when we used commercial sample without pre-treatment process. On the other hand, another REMPI spectrum of AAP expanded with pure helium has no broad background when we removed water from AAP by pumping the sample overnight. If water is included in AAP, AAP(H<sub>2</sub>O)<sub>n</sub> 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<sup>+</sup> is detected on the monomer AAP mass channel and therefore the REMPI spectrum of AAP is broadened. We employed two-color REMPI spectroscopy in order to put less excess energy to the ionized clusters and therefore to suppress the dissociative ionization of AAP-water clusters.



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## Non-blinking, photostable luminescence upconversion from (Zn<sub>x</sub>Ag<sub>y</sub>In<sub>z</sub>)S<sub>2</sub> nanocrystals

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서울대 화학부 <sup>1</sup>서울대 자연과학부/생물물리 및 화학생물학과 <sup>2</sup>한국화학연구원 나노기술융합  
연구단 <sup>3</sup>연세대 화학과 <sup>4</sup>한국화학연구원 형광물질연구팀

The composite nanocrystal (Zn<sub>x</sub>Ag<sub>y</sub>In<sub>z</sub>)S<sub>2</sub> (to be called tZAIS hereafter) comes in various elemental compositions, many of which are highly fluorescent from blue to red. The emission wavelength of tZAIS is tunable by varying its chemical composition, unlike typical quantum dots (QDs) that require size control. We found that tZAIS nanocrystals have unique advantages over QDs as they have no photoblinking or cytotoxicity while maintaining comparable emission intensity. We found that tZAIS also induces upconversion of photon, yielding emission at a shorter wavelength when photoexcited at a longer wavelength. We obtained confocal images of a cell that was stained by tZAIS and excited with near infrared light.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Direct observation of dynamics between restriction enzyme and methylated DNA**

박소영 김성근

서울대 화학부

The interaction between methylated DNA and protein has been extensively studied, but its dynamical aspect is still poorly understood. We investigated the temporal dynamics of interaction between a restriction enzyme and methylated DNA by total internal reflection fluorescence microscopy, which was used to track the binding and dissociating process of the restriction enzyme from DNA at the single-molecule level to understand the effects of DNA methylation.

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장소: 일산KINTEX

발표코드: PHYS.P-430

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Determination of double-stranded DNA persistence length using pyrene excimer emission

임순규 양일승<sup>1</sup> 이종우<sup>2</sup> 김영규<sup>1</sup> 김성근<sup>1</sup>

서울대 자연과학부/생물물리 및 화학생물학과 <sup>1</sup>서울대 화학부 <sup>2</sup>서울대 생물물리 및 화학생물  
학과

The mechanical flexibility of DNA is one of the most essential characteristics of DNA. Cellular processes such as genetic regulation and binding of drugs and proteins to DNA depend on the elastic properties of DNA molecules. Among the biosensors that are used to monitor the recognition and interaction of DNA, pyrene is a promising species due to its outstanding photophysical properties such as high quantum yield, long fluorescence lifetime, and the capability of forming an excited state dimer with a large Stokes' shift (excimer). We investigated the possibility of determining the persistence length of pyrene-tagged, double-stranded DNA by measuring the emission from pyrene excimer formed upon sufficient bending of DNA.

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발표코드: **PHYS.P-431**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Improved Tip-Enhanced Raman Scattering with a Nanoparticle Probe

이은별 김지환<sup>1</sup>

고려대 <sup>1</sup>고려대 화학과

We carried out the tip-enhanced Raman scattering (TERS) with a tip that is functionalized with a nanoparticle. The NP tip is fabricated by a direct mechanical pickup of a NP from a flat substrate, and the TERS signal from the NP tip - organic monolayer - Au thin film (thickness of 20 nm) is recorded. We find that such a NP-tip interacting with a thin film routinely yields signal enhancement larger than  $\sim 10^4$ , which is sufficient not only for local (with detection area of  $\sim 200 \text{ nm}^2$ ) Raman spectroscopy, but also the nanometric imaging of organic monolayers within a reasonable acquisition time ( $\sim 20$  minutes / image).

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발표코드: **PHYS.P-432**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Radical migration in TEMPO-based FRIPS (Free radical-induced peptide sequencing)**

송민수 문봉진 오한빈

서강대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-433**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Knowledge-based two-dimensional torsion-angle augmenting potential functions for protein structure modeling

김태래 신석민 이진혁<sup>1</sup>

서울대 화학부 <sup>1</sup>한국생명공학연구원 생명정보센터

Augmenting 2-D energy functions for  $\Phi$ - $\chi_1$ ,  $\psi$ - $\chi_1$ ,  $\Phi$ - $\psi$ , and  $\chi_1$ - $\chi_2$  have been devised using high-resolution X-ray diffraction protein structures deposited in Protein Data Bank, by reverse mapping of torsion angle populations onto energy landscape using Boltzmann distribution. Each grid point is connected by 2-D spline interpolation to make potential energy landscape. The validity of the augmenting potential is checked, and its effect on protein structure modeling is illustrated.



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발표코드: **PHYS.P-434**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Cobalt Selenide Nanowires synthesized by an atmospheric pressure chemical vapor deposition (APCVD) using Au catalysts**

**김진일 방수경 김태규**

부산대 화학과

In this work, cobalt selenide (CoSe) nanowires were synthesized by an atmospheric pressure chemical vapor deposition (APCVD) on Au thin film coated Si(100) substrate. Au thin film derives an Au-catalyzed vapor-liquid-solid (VLS) growth of CoSe nanowires as catalyst. We used Cobalt chloride (CoCl<sub>2</sub>) beads and Selenium (Se) powder as precursors. Graphites have been used for the purpose of control of the vaporization rate of Selenium (Se) during the experiment. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) measurements revealed that the CoSe nanowires were 60-100 nm in diameter and 10-20  $\mu$ m in length. The energy dispersive x-ray spectroscopy (EDS) data indicate that the growth of CoSe nanowires shows homogeneous character. Additionally, X-ray diffraction (XRD) method, superconducting quantum interference device (SQUID) magnetometer, zero-field-cooled (ZFC) and field-cooled (FC) magnetization measurements were used to investigate the structure and the magnetic properties of synthesized CoSe nanowires.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-435**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Reconstructing diffractive optical elements for the production of synthetic spectra**

김태성 김성규

성균관대 화학과

Diffractive elements are the optical elements from which a desired spectrum can be extracted. Their structure is designed using a recursive Fourier transform of the spectral amplitude in a phase retrieval problem. Such diffractive elements can replace a reference cell in a correlation spectrometer, which can detect a small signal from a specific sample buried in a big background signal. In this presentation, we introduce an algorithm of the phase retrieval problem, and show results for diffractive optical elements which are capable of synthesizing the infrared spectrum of HF between  $3600\text{ cm}^{-1}$  and  $4300\text{ cm}^{-1}$ , and that of  $\text{SF}_6$  between  $900\text{ cm}^{-1}$  and  $1000\text{ cm}^{-1}$ .

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cobalt-phosphate와 Cobalt-hydroxyapatite의 촉매활성 비교 및 특

성연구

조성화 권기영

경상대 화학과

최근에 cobalt-phosphate 는 다양한 산화촉매 및 전기화학적 촉매로서 활발한 연구가 진행되고 있다. 우리는 다양한 형태의 cobalt-phosphate 를 수열반응으로 합성하였다. 또한 cobalt 를 Ion-exchange 반응을 통해서 다양한 방법으로 hydroxyapatite(HAP) 표면에 도입하였다. 이러한 촉매를 XRD, TEM, SEM 을 통하여 분석하였다. 그리고 합성된 촉매를 sodium-borohydride 를 이용한 수소 발생실험의 촉매로 사용해 보고, 이들의 촉매 활성을 비교하였다.

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발표코드: **PHYS.P-437**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Molecular dynamics estimates of the Friction Coefficient



신현경 이억균

KAIST 화학과

The friction coefficient is an essential property to explore the dynamics of the Brownian particle suspended in a fluid.  $\gamma$ , the friction coefficient defined by Kirkwood(1946), cannot be obtained from the finite size molecular dynamics but can be approached by the memory kernel  $\gamma^\dagger$  obtained from molecular dynamics simulation within the framework of the generalized Langevin equation approach. Most of previous theoretical results have been obtained from the system composed of the Brownian particle  $M$  whose mass is much greater than total mass of the solvent  $Nm$ . Our simulation system composed of sufficiently large number of solvent particle to satisfy the thermodynamic limit. We analyze and compare the behavior of the friction coefficient obtained by different methods as changing system parameters, such as temperature, relative size between the Brownian particle and the solvent particle, number of solvent particle, and the number density.

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발표코드: **PHYS.P-438**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Intercalation of $\alpha$ -zirconium phosphate using alkylamine and catalytic application

김소희 권기영

경상대 화학과

The synthesis of various catalyst substrate based on phosphate salt and the heterogeneous catalyst at this supported on substrate with many kinds of transition metals having catalytic activity has been developed. We synthesized  $\alpha$ -zirconium phosphate( $\text{Zr}(\text{HPO}_4)_2 \cdot 2\text{H}_2\text{O}$ ) by simple process using zirconyl chloride and phosphoric acid. We analyzed a change of crystallinity according to concentration variation of phosphoric acid through XRD data and identified morphology through FE-SEM images. Particularly, each of synthesised products were performed intercalation with many species of alkylamine. It confirmed change of crystal structure with XRD and TEM. Further more we expected to study for applicability as potential catalyst.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-439**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Grand Canonical Monte Carlo Study of the Confined Water between a Nanoscale Tip and a Surface**

김효정 장준경<sup>1</sup>

부산대 나노융합기술학과 <sup>1</sup>부산대 나노소재공학과

By applying grand canonical Monte Carlo (GCMC) technique, we studied the confined water between an atomic force microscopy (AFM) tip and a surface. By varying humidity and the tip-surface distance, we examined the equilibrium structure of the meniscus by focusing on the width and stability of the meniscus. The capillary force due to the meniscus dominates over the van der Waals force from the surface, and the force showed a damped oscillation with increasing the tip-surface distance. Depending on the relative humidity (RH), the pull-off force tends to increase, then starts to decrease after specific RH.

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장소: 일산KINTEX

발표코드: PHYS.P-440

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Femtosecond transient absorption study of Au rod-TiO<sub>2</sub>  
nanocomposite: Shell-thickness dependence of charge transfer  
dynamics**

**황선진 임주현 양일승 이정은 설수환<sup>1</sup> 이진규 김성근**

서울대 화학부 <sup>1</sup>삼성종합기술원 분석

In an effort to expand the optical window for photocatalysis, Au nanoparticles have been used as a sensitizer in a composite material with photocatalytic semiconductors since the absorption wavelength of Au can be tuned by controlling the size of Au nanoparticle. Although the charge transfer dynamics from semiconductor to metal is well known, the charge transfer from metal to semiconductor is not as clearly understood. To better understand this phenomenon, we investigated Au rod-TiO<sub>2</sub> nanocomposite of core-shell type with a range of shell thickness. Using transient absorption spectroscopy, we studied the forward electron transfer from TiO<sub>2</sub> to Au rod as well as the reverse electron transfer from Au rod to TiO<sub>2</sub> as we varied the TiO<sub>2</sub> shell thickness. The photocatalytic property of Au rod-TiO<sub>2</sub> nanocomposite was monitored using photocatalytic degradation of an organic dye.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: PHYS.P-441

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Photochemiluminescence: Photochemical generation of a new, highly fluorescent compound from non-fluorescent resveratrol**

이정은 양일승 설수환<sup>1</sup> 박승범 김성근

서울대 화학부 <sup>1</sup>삼성종합기술원 분석

A novel phenomenon that may be termed as photochemiluminescence, due to the intense luminescence emission from a photochemical reaction product of an originally non-emitting compound, is reported. We also elucidated the chemical identity of this compound, which has remained elusive to date. We found that UV irradiation of trans-resveratrol leads to its photochemical transformation to its ketonic photoproduct, which has never been registered in the CAS. This new compound may prove to be an ideal fluorophore in biological imaging because of its high fluorescence quantum yield, large Stokes' shift, and large two-photon absorption cross section.



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발표코드: **PHYS.P-442**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescence bio-imaging with a fluorescent photoproduct of resveratrol

양일승 이종우<sup>1</sup> 황선진 이정은 이준<sup>2</sup> 김영삼<sup>3</sup> 김성근

서울대 화학부 <sup>1</sup>서울대 생물물리 및 화학생물학과 <sup>2</sup>동국대 화학과 <sup>3</sup>동국대 약학대학 약학과

Resveratrol is a natural compound known for its antioxidant, antitumor, and anti-infectious functions. Although it is a non-fluorescent compound itself, we found that it is readily converted to a fluorescent species upon UV irradiation. The photoproduct is likely to be an ideal candidate for fluorescence bio-imaging due to its high quantum yield and large Stokes' shift. To fully test its suitability as a bio-imaging agent, we examined its cytotoxicity and achieved fluorescence cellular imaging with a range of diverse imaging techniques.

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발표코드: **PHYS.P-443**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Multilayer Graphene Characterization by Vis- and IR- ANSOM

김덕수 김지환<sup>1</sup>

고려대 기초과학연구소 <sup>1</sup>고려대 화학과

We have investigated infrared and visible apertureless near-field scanning optical microscopy (Vis- and IR- ANSOM) in the linearly polarized lights from He-Ne lasers (633 nm and 3.391 $\mu$ m) and IR-OPO (3  $\mu$ m ~ 3.6  $\mu$ m). As a light source, a tunable wavelength change continuous wave infrared optical parametric oscillator (cw-IR OPO) with an output power of up to 10 mW in the 3  $\mu$ m ~ 3.6  $\mu$ m ranges have been set up. The graphenes of single and a few layers are deposited on SiO<sub>2</sub>(285 nm) / Si substrate by mechanical exfoliation. The typical dimensions of the graphene randomly deposited by this method are ~100  $\mu$ m. We carried out sensitively graphene layers optical contrast mapping of near-field around variable graphene layers using IR-ANSOM and Vis-ANSOM. We attained high resolution optical contrast maps of different graphene layers below the diffraction limit of classical microscopy.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 태양전지용 후면 알루미늄 페이스트 비드 분석

차민혁 김상호

공주대 화학과

본 연구에서는 태양전지용 후면 알루미늄 페이스트 소성 시 과소성되어 발생하는 비드에 대하여 생성 원인과 현상을 분석하였다. 최초 벨트 퍼니스에서 벨트 속도를 느리게 하여 소성시켰을 때, 발견하였으며 실험을 진행해본 결과 알루미늄 비드 형성에는 과소성이 중요한 원인임을 알게 되었다. 비드가 발생하였을 때, 일반 웨이퍼 업계에서는 불량으로 처리하며, 전지 효율에 미흡하지만 나쁜 영향을 끼치기 때문에 비드 생성원인을 알고 제거하는 것이 필요하다. 비드가 생성되는 원인은 실리콘과 알루미늄 사이의 집합체에 의해 솟아오른 것으로, 본래 실리콘과 알루미늄의 집합체가 실리콘 웨이퍼상에서 BSF 층을 형성하는데, 과소성되는 조건에서는 이 집합체가 알루미늄 페이스트 표면으로 솟아오르는 것을 확인할 수 있었다. 비드를 억제하기 위해서는 벨트 스피드를 적정 수준으로 유지하여 과소성을 방지하고, 페이스트 제조상 들어가는 Glass Frit의 성분 중 녹는점이 상대적으로 높은 물질들을 사용하여 Glass Frit의 Tg 온도를 높여서 온도에 대한 저항력을 갖게 하는

것이 관건이다. 이 연구는 태양전지 업계에서 셀의 효율의 영향을 미치는 후면 손실이 최초 발견되어 원인을 분석하고자 진행하였으며, 본 연구를 통해 태양전지 후면전극의 손실을 줄여, 셀 효율을 높이는 데 도움을 줄 것이다.



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발표코드: **PHYS.P-445**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Effect of Silica Particles on the Electric Percolating Behavior of the Epoxy/Silver Nanowire Composite**

조현우 성봉준

서강대 화학과

The effects of silica particles on the electric percolating behavior of the silver nanowires in the epoxy composites are elucidated using the experiments, Monte Carlo (MC) simulations and percolation theory. Many studies on nano composites, such as polymer/CNT composites or polymer/silver nano-particle composites, have been carried out to lower the volume fraction of the conducting materials at the electric percolation threshold. In this work, we elucidate that the electrical properties of the nano composites, mixtures of conductive nanoparticles and polymers, can be improved significantly by mixing the additive particles with the nano composites. When the silica particles are added to the epoxy/silver nanowire composites, the electric resistivity decreases by about eight orders of magnitude. According to the TEM images and the simulation results, the silver nanowires aggregate at low concentration of the silver nanowire due to their strong attractive interaction. However, when the silica particles are introduced the

silver nanowires are dispersed well, which makes the electric percolation network of the silver nanowires form easily.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Time-resolved reaction of $\text{CN} + \text{CHCl}_3$ in the condensed phase

이태곤 박재흥 임만호

부산대 화학과

In condensed phase, photodissociated fragment undergoes reaction with solvent. CN radical from ICN can abstract H or Cl, substitute in  $\text{CHCl}_3$ . ClCN and HCN is investigated in previous studies. HCN has three vibrational modes, and we measured C-H (3265 / 3160  $\text{cm}^{-1}$ ) and C-N (2093 / 2067 / 2042  $\text{cm}^{-1}$ ) stretching modes. In equilibrium spectrum of HCN, amplitude of C-H stretching band is 15 times bigger than C-N stretching. But in our data, C-N / C-H amplitude ratio is smaller than 2, so we quoted linear / bridge complex. Vibrational modes of HCN and complex make us to establish more detailed kinetic model of HCN.  $\text{CHCl}_2\text{CN}$  and  $\text{CCl}_3\text{CN}$  for substitution reaction, their extinction coefficient of C-N stretching mode is 1.3  $\text{M}^{-1}\text{cm}^{-1}$  and 10  $\text{M}^{-1}\text{cm}^{-1}$ . This value is too low, so we couldn't measured substitution reactions.

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발표코드: **PHYS.P-447**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Molecular dynamics simulation study of thermodynamic properties of C<sub>60</sub> in acetonitrile, pyridine and their mixtures**

이지혜 권찬호 김홍래 황현석

강원대 화학과

Molecular dynamics (MD) simulations are performed to study static and dynamic properties of C<sub>60</sub> molecules in pure pyridine, pure acetonitrile and their mixtures at an atomistic level. Diffusion coefficients of C<sub>60</sub> molecules in the solvents are calculated and the comparison with experimental results shows a good agreement. The radial distribution functions (RDFs) and order parameters of solvent molecules around a C<sub>60</sub> molecule are obtained to understand solvation structure as a function of the distance from the center of mass for C<sub>60</sub>. Potential of mean force (PMF) calculations as a function of the distance between two C<sub>60</sub> molecules in pure solvents and mixtures are carried out using the umbrella sampling method with MD simulations. On a basis of the PMF profiles, the solubility of C<sub>60</sub> in the solvents are discussed.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Computational analysis of vibronic spectra in small molecules using Franck-Condon factor and nuclear overlap integral calculations

이지혜 김재한 조수경<sup>1</sup> 권찬호 김홍래 황현석

강원대 화학과 <sup>1</sup>국방과학연구소 4-2부

$S_1 \leftarrow S_0$  spectra of 2-methylpyrazine and  $D_0 \leftarrow S_0$  spectra of acetone are obtained from Franck-Condon (FC) factor and nuclear overlap integral calculations through vibrational analysis. Vibrational analysis has been performed by calculating the vibrational frequencies in the electronic ground state ( $S_0$ ) of 2-methylpyrazine and acetone, the first electronic excited state ( $S_1$ ) of 2-methylpyrazine, and the cation ground state ( $D_0$ ) of acetone. Vibrational frequencies and potential energy surface (PES) were calculated at the (TD)B3LYP/cc-pVTZ for 2-methylpyrazine, and the B3LYP/cc-pVTZ levels for acetone. The one dimensional PES for 2-methylpyrazine was obtained as a function of the torsional angle of the methyl group in the  $S_1$  state, while the two dimensional PES for acetone was obtained as a function of the torsional angles of the two methyl groups in the  $D_0$ . The effects of frequency shifts, displacements, and Duschinsky rotations on the spectra are discussed. Several issues in comparison with experimental results are also addressed.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dynamics of Br formation from the primary and secondary C-Br bond dissociation of oxalyl bromide near 234 and 265 nm

Paul Dababrata 김현국 이경석<sup>1</sup> 김태규

부산대 화학과 <sup>1</sup>한국표준과학연구원 분석화학표준센터

The photodissociation dynamics of Oxalyl bromide have been investigated near 234 and 265 nm using a velocity map ion imaging technique coupled with a state selective [2+1] resonance-enhanced multiphoton ionization [REMPI] scheme. The nascent Br ( $2P_j$ ,  $j = 1/2, 3/2$ ) atoms stem from the primary C-Br bond fission of parent molecule as well as secondary dissociation of C<sub>2</sub>O<sub>2</sub>Br radicals which are energized from the ultrafast primary C-Br bond rupture at both pump energy. To obtain the detail dynamics, the translational energy distribution and recoil anisotropy of Br( $2P_{3/2}$ ) and Br\*( $2P_{1/2}$ ) atom formation process are extracted from the two dimensional ion images. A single Gaussian-shaped translational energy distributions have been observed for the Br\*( $2p_{1/2}$ ) formation channel at both wavelengths. The average translational energies of this distribution are 74.65 and 49.78 KJ/mol at 234 and 265 nm, respectively. On the other hand, single Boltzmann and two Gaussian functions at 265 nm and single Boltzmann and three Gaussian function at 234 nm give the best fit for the translational energy distribution

profile of Br formation. An additional Gaussian-shaped translational energy distribution is attributed from the secondary C-Br bond cleavage of the C<sub>2</sub>O<sub>2</sub>Br radical, which is energetically sufficient at higher energy (234 nm). The average translational energy of this component is 35.28 KJ/mol. The recoil anisotropy parameter,  $\beta$ , value of high velocity components are determined to be 0.79(0.73) and 1.11 (1.38) for Br and Br\*, respectively, at 234(265) nm. The assigned translational energy distributions of each component have also been confirmed by the measured individual recoil anisotropy parameters. The relative quantum yields of each component are also measured.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The Role of Confined Water in Ionic Liquid Electrolytes for Dye Sensitized Solar Cells**

**전지원 김형준<sup>1</sup> William A. Goddard<sup>2</sup>**

*KAIST EEWS <sup>1</sup>KAIST EEWS 대학원 <sup>2</sup>California institute of Technology*

Ionic liquids (ILs) provide an attractive medium for various chemical and redox reactions, where they are generally regarded as hydrophobic. However, Seddon et al. discovered that 4-10 wt% water absorbs into ILs that contain bulky anions, And Cammarata et al. found that the molecular state of water in ILs is dramatically different from that of bulk liquid water or that of water vapor. To determine the microstructure of water incorporated into ILs and the impact on properties, we carried out first principles-based molecular dynamics simulations. We find water in three distinct phases depending on water content, and that the transport properties depend on the nature of the water phases. These results suggest that the optimal water content is  $\sim 10\%$  mole fraction of water molecules ( $\sim 1.1\text{ wt\%}$ ) for applications such as non-volatile electrolytes for dye sensitized solar cells (DSSC). This suggests a strategy for improving the performance of IL DSSC by replacing water with additives that would play the same role as water (since too much water can deteriorate performance at the anode-dye interface).

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발표코드: **PHYS.P-451**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Molecular dynamics simulation study of ion and glucose transport through cyclic peptide nanotubes in lipid bilayers**

서용일 송연호 황현석

강원대 화학과

Cyclic peptide nanotubes (CPN), a class of synthetic ion channels, have an empty interior space that allows ions and small molecules to permeate. In this study the structure of two types of CPN,  $8 \times \text{cyclo} [-(\text{Trp-D-Leu})_4\text{-Gln-D-Leu-}]$  and  $8 \times \text{cyclo} [-(\text{Trp-D-Leu})_4]$  embedded in DMPC lipid bilayers is examined using molecular dynamics (MD) simulations. The transport mechanism of a single  $\beta$ -D-glucose and  $\text{Na}^4$  through the CPN's is also investigated with potential of mean force (PMF) calculations that are obtained by combining MD simulations and the umbrella sampling (US) method. The 20 ns MD simulation study reveals that the structure of CPN's in lipid bilayers is not static but very dynamics, sometimes displaying the dislocation of the end cyclic peptide rings from the remaining rings. The PMF calculations for a single  $\beta$ -D-glucose and  $\text{Na}^+$  show the free energy well in the middle of the CPN, indicating that the CPN has selectivity to cations and hydrophilic small biomolecules such as glucose.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Theoretical studies on the reactions of $O(^3P)$ with $SiH_4$ and $PH_3$

**김범진 장성우<sup>1</sup> 박찬량<sup>1</sup>**

국민대 생명나노화학과 <sup>1</sup>국민대 화학과

In previous studies, the energetics of the OH product from the reaction of  $O(^3P)$  with  $SiH_4$  and  $PH_3$  were fully characterized up to the energetic limit using laser-induced fluorescence(LIF). To support the suggested mechanisms for the OH production, ab initio calculations were conducted at the MP2/6-311++G(2df, 2pd) level. All the reaction intermediates and products which control the dynamics of the initial stage of the title reaction were calculated, and the correlation diagrams were constructed for both reactions. To accommodate the rotationally inverted OH population distributions, the possibilities of intersystem crossings (ISC) from the triplet to singlet surfaces at various configurations were discussed.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **DFT calculations on thermal degradation mechanisms of PET, PTT and PBT**

**장성우 김범진<sup>1</sup> 박찬량**

국민대 화학과 <sup>1</sup>국민대 생명나노화학과

The thermal degradation products of Poly(ethylene terephthalate) (PET) have been reported to be very different from those of Poly(trimethylene terephthalate) (PTT) and Poly(butylene terephthalate) (PBT) in that PET produces the anhydride-containing oligomers while PTT and PBT the vinyl-ester terminated oligomers as determined in previous MALDI experiments. To elucidate the reaction pathways and favorable products for the thermal degradation of the three polymers, DFT calculations were conducted for the reactants, products, and transition states using B3LYP method with 6-31G(d,p) basis set over wide temperature range. Possible unimolecular and biomolecular reaction pathways were searched to explain the experimentally determined reaction products, and the potential energy diagrams were constructed for the thermal degradation of PET, PTT, and PBT.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Probing thermal unfoldng and refolding of azide-bound hemoprotein

안성현 엄인태 이한주

한국기초과학지원연구원

A native structure of protein sensitively alters if its environments such as acidity, ionic strength, and temperature, change. By increasing temperature over the melting point, proteins undergo phase transition from the folded state to the unfolded. Herein, we carried out absorption and circular dichroism measurements in both vibrational and electronic frequency ranges to investigate temperature-dependent unfolding and refolding processes of azide-bound myoglobin. In particular, we show that the ligand (azide ion) bound to heme sensitively probes the local structural changes in heme-pocket.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Photochemical Synthesis of Metal-Nanodiamond Photocatalysts for Solar H<sub>2</sub> Generation in Water

장동명 명윤 임형순<sup>1</sup> 조용재 박정희 이민영<sup>2</sup> 차은희<sup>3</sup>

고려대 소재화학과 <sup>1</sup>고려대 미세소자공학협동/마이크로소자공학 <sup>2</sup>이화여대 화학나노과학부 <sup>3</sup>  
호서대 화학

Nanodiamonds (NDs) exhibit excellent photocatalytic activity towards the one-step synthesis of Au, Ag, Pt and Cu nanocrystals (NCs) in aqueous solution. The deposition of Au NC on the ND increases most effectively the generation rate of H<sub>2</sub> gas from water. It suggests that the Au NCs enhances the photon absorption due to their localized surface plasmons, and separates effectively the electron-hole pairs of photoexcited NDs. The Au-ND hybrid on the reduced graphene oxide sheets consistently showed higher photocurrent than the ND alone upon visible light irradiation.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ubiquitous process of p53 studied by single-molecule spectroscopy

**황지희 강주연<sup>1</sup> 김영삼<sup>2</sup> 김영규<sup>1</sup> 김성근<sup>1</sup>**

서울대 생물물리 및 화학생물학 <sup>1</sup>서울대 화학부 <sup>2</sup>동국대 약학대학 약학과

P53 oncogenic protein plays a key role in suppressing human cancer formation and its level is controlled by ubiquitination. In order to study the ubiquitous mechanism, we employed a set of single point mutant proteins that have arginine instead of specific lysine expected to be involved in actual ubiquitin ligation. We used alternating laser excitation fluorescence to analyze the end products of the ligation process at the single-molecule level.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fast temperature probing method using monomer/dimer equilibrium of dye molecules

박원익 이한주<sup>1</sup>

충남대 분석과학기술대학원 <sup>1</sup>한국기초과학지원연구원 서울센터

Protein folding is a highly complicated process that makes disordered polypeptides to have their own three dimensional structures and biological functionalities. In order to investigate thermodynamic kinetics during protein folding, we are employing a laser induced temperature jump (T-jump) technique that can initiate the unfolding process of the biopolymer by instantaneous heating of the bath. By combining the T-jump technique with our femtosecond circular dichroism (CD) spectroscopy, we can monitor fast structural dynamics of the biomolecules involved in their folding/unfolding process. IR absorption change of O-H stretching overtone of water is often monitored to calibrate the exact amount of the heat injected by laser pulse. However, such a measurement could be relatively inaccurate because the optical density change ( $\Delta OD$ ) depends on the sample pathlength. Here, we suggest an alternative temperature probing method using temperature dependent monomer/dimer equilibrium of dye molecules in water. Experimental details and advantages of the method will be presented.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Composition tuned polytypic ZnO/Zn<sub>x</sub>Cd<sub>1-x</sub>Se core/shell nanowire arrays

명윤 김한성 장동명 최진웅 박정희

고려대 소재화학과

ZnO/Zn<sub>x</sub>Cd<sub>1-x</sub>Se core/shell NW arrays were synthesized on ITO substrates with complete composition tuning by the Chemical Vapor Transport method. The shell layers have an average thickness of 30 nm. At  $x = 0$  and 1, the single-crystalline WZ CdSe and ZB ZnSe shells are grown on the ZnO NW array. As the composition is tuned, three distinctive WZ-ZB polytypic structures appear: (1) a WZ-ZB double shell structure at  $x = 0.2-0.3$ , (2) a WZ-ZB superlattice structure at  $x = 0.5$ , and (3) a ZB twinned superlattice structure at  $x = 0.7-0.8$ . The outer region contains the higher Cd content than the inner region. In the Zn<sub>0.3</sub>Cd<sub>0.7</sub>Se, the WZ and ZB domains exist separately as the inner and outer shells, respectively, forming a double shell structures. Their [0001]WZ and [111]ZB (or [100]ZB) directions are aligned along the [0001] growth direction of the WZ ZnO NW core. As  $x$  increases to 0.5, the ZB domain becomes the dominant one, and the ZB?WZ superlattice structure is produced. The Zn<sub>0.7</sub>Cd<sub>0.3</sub>Se consisted of short-period (2?10 nm) twinned superlattice structures, in which the ZB twinned segments have alternative

orientations along the axial  $[111]$  direction. We tentatively explain that the atomic disorder of the alloy induces the evolution of these polytypic structures.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The aggregation study of cyano-stilbene derivative at the air-water interface by Langmuir-Blodgett technique**

최소영 손대원

한양대 화학과

In the past years, great interest has been paid on aggregation behavior of conjugated organic materials particularly related to their applications in optoelectronic devices such as luminescence switch, sensor, and OLED. Cyano distyrylbenzene derivative is one example of organic fluorescent molecules and is appeared as 'unit aggregate' to form the extended array in films. Two dimensional properties and aggregation behaviors of organic fluorescent molecule, cyano distyrylbenzene derivative(DBDCS) at the air-water interface have been investigated using surface pressure measurement by Langmuir-Blodgett technique, Atomic Force Microscopy, Scanning Tunneling Microscopy, Photoluminescence Spectroscopy, and X-ray reflectivity. DBDCS molecule under different light conditions showed a different aggregation behavior as surface pressure increases due to cis-trans isomerization. DBDCS molecules made large domains like a sheet structure at low surface pressure under UV condition. As surface pressure increases in the dark condition, molecules maintain their arrangement by  $\pi$ - $\pi$  stacking and intermolecular

interaction. However, we can observe the disordered structure under UV light due to cis-trans isomerization.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Interaction of water soluble polymer, Polyethylene glycol (PEG), with water solvents: new sampling technique for large-scale polymer structure sampling**

**신혜영 김형준 William A. Goddard<sup>1</sup>**

*KAIST EEWS대학원 <sup>1</sup>California institute of Technology*

The polymer-water interaction has been a matter of concern in many studies not only because of its scientific interest but also of its importance in industrial applications. Polyethylene glycol (PEG) is one of the most interesting water-soluble polymers due to the similarity of its special characteristics in water to those found in proteins such as peptides in water as well as commercial and technological applications such as pharmaceutical drugs and secondary batteries. Hence the PEG-water interaction has been extensively studied by various experimental techniques such as dynamic light scattering (DLS), gel permeation chromatography (GPC) and Small-angle neutron scattering (SANS). However many characteristics of PEG in water are either only qualitatively understood or still controversial. For example, the aggregation behavior of PEG in water has been an issue in many studies but its origin has been still elusive. On the other hand, there is an attempt to use PEG as a draw solute for forward osmosis



desalination due to the advantages of non-toxicity and easy-removal. In this study, one of our objectives is the establishment of an atomistic level of simulation method to sample the large scale PEG (~20 kDa, 455 monomers) in solution phase. We first develop a first-principle based force field to describe the quantum mechanical (QM) interaction between water and PEG. Then, we develop an efficient computational procedure to sample various PEG structures in water box using molecular dynamics simulations for systematic analysis on the thermodynamics and structure of PEG interacting with water molecules. We expect that this study will provide the detailed insights for the PEG-water interaction, which is essential for designing the effective draw solute based on polymers.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Rebinding dynamics of nitric oxide to myoglobin(III) in room temperature solution

박재홍 이태곤 임만호

부산대 화학과

Femtosecond vibrational spectroscopy was used to probe photoexcitation dynamics of NO bound ferric myoglobin (MbIIINO) in D<sub>2</sub>O solution at 294 K after excitation with a 575 nm pulse. The stretching mode of NO in Mb(III)NO consists of a major band at 1921 cm<sup>-1</sup> (97.7%) and a minor one at 1902 cm<sup>-1</sup> (2.3%), suggesting that Mb(III)NO in room temperature solution has two conformational substates with one dominating conformation. Absorption features assigned to protein undergoing thermal relaxation without ligand dissociation add up to 14% of the total bleach implying that photolysis quantum yield of MbIIINO with a Q-band excitation is smaller than 0.86. The photodissociated NO undergoes fast geminate recombination with subnanosecond time scale and the rebinding kinetics depends on the conformation of the protein. Geminate rebinding of NO to Mb with major conformation shows highly nonexponential kinetics that was described by the stretched exponential function,  $0.77 \exp(-(t/330 \text{ ps})^{0.58 + 0.09})$ . The NO rebinding to Mb with minor conformation is slower than that with the major

conformation and exponential, which is  $\exp(-t/1.8 \text{ ns})$ . Time-resolved vibrational spectra with high sensitivity reveal a rich photophysical and photochemical processes of photoexcited MbIIINO.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Controlled Synthesis of Hydroxyapatite Supported Ruthenium as Heterogeneous Catalysts for Alcohol Oxidation**

김영용 권기영

경상대 화학과

Using two different methods, Hydroxyapatite ( HAP ) has been synthesized under aqueous solution both ambient and high pressure. In addition, incorporation of Ruthenium on HAP surface ( RuHAP ) is done by four different ways. Four different catalysts ( RuHAP ) show significant difference in catalytic activities. The properties of the catalysts are characterized using X-ray powder diffraction, Transmission and Scanning electron microscopy, Inductively Coupled Plasma mass spectroscopy.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ultrafast Energy Transfer in Artificial Photosynthetic Complexes near Plasmonic Metal Nanoparticles

이재범 이인구<sup>1</sup> 방윤수<sup>1</sup>

광주과학기술원 광공학응용물리<sup>1</sup> 광주과학기술원 광공학응용물리학과

Femtosecond transient absorption measurements in visible wavelengths have been used to investigate excited-state dynamics and energy transfer in cyanobacterial Photosystem 1 (PS1) dispersed in aqueous solution of plasmonic silver nanoparticles. PS1 is one of the most robust and efficient light-harvesting complexes in nature and consist of more than 110 co-factors including ~100 chlorophylls, ~20 carotenoids, 2 phylloquinone and 3 iron-sulfur clusters. PS1 clearly show different excited-state dynamics depending on excitation wavelength near silver nanoparticles which have absorption band centered at 430 nm. In order to find optimal nanoparticles in constructing artificial photosynthetic complexes, we synthesize various silver nanoparticles and nano-surfaces by chemical reduction. Ag nanoparticles of diameter in the wide range of 5~100 nm and of absorption maximum in the 380~460 nm range are synthesized in the form of colloidal particles and island films. Recent developments in nanoparticle synthesis and metal enhanced fluorescence measurement using rhodamine dyes will be presented. The

current study will be extended to measurements of transient absorption and induced emissions from the excited states of chromophores and energy transfers or relaxations within simple artificial photosynthetic complexes made of chromophores and metal nanoparticles will be investigated.



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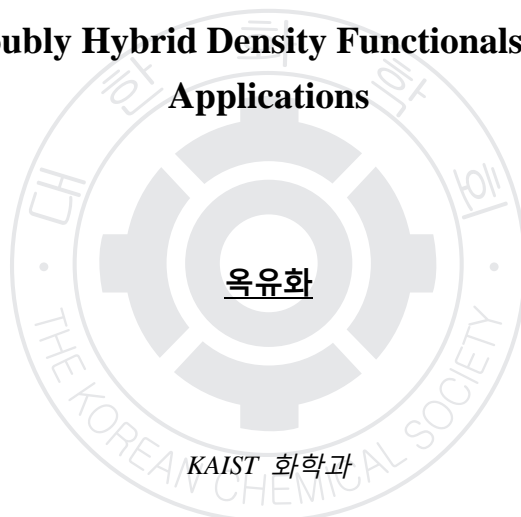
장소: 일산KINTEX

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Accessing Doubly Hybrid Density Functionals for Biological Applications



DFT calculation is common method to determine force field parameter. But previos DFT methods like B3LYP show large error compare to CCSD(T) results. So these force fields are not accurate enough to describe non-covalent interactions in biological system. We performed benchmark calculation about three representative non-covalent interactions set:S66 set, DNA pair and small peptide set. We tested not only GGA or hybrid DFT method but also doubly hybrid DFT method to define appropriate method describing biological system.

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장소: 일산KINTEX

발표코드: **PHYS.P-465**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Predicting protein loops in inaccurate model structures

이규리 석차욱

서울대 화학부

Protein loops are often involved in biological functions by contributing to binding sites or active sites. Therefore, high-accuracy loop structure prediction is crucial for understanding and regulating protein functions. A common way to evaluate the performance of protein loop modeling methods is to reconstruct the loop in the native structure after removing the loop region only. However, one frequently has to model loops in exact structural environment of low-resolution experimental structures or template-based models. We have developed a new loop modeling method that is less sensitive to inaccurate environment than existing methods but still retains high performance in native loop reconstruction, by employing a hybrid energy that combines physics-based and knowledge-based energy terms. In a native loop reconstruction test, median RMSD of 0.7 and 1.0 Å was obtained for 8- and 12-residue loops, respectively. A test on proteins with artificially perturbed side chain conformations that represent low-resolution crystal structures resulted in median RMSD of 1.1 and 1.8 Å for 8- and 12-residues loops, respectively. When compared to the best-performing previous method applied to the same set, the improvement is 1.1 and 0.5



Å. We have also introduced more realistic environmental inaccuracy including protein backbones by actual comparative modeling and obtained highly acceptable results. The overall performance is very encouraging considering that no optimization of the inaccurate environment was attempted, implying that the present loop modeling method can be applied to more realistic problems with much more efficiency than before.



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## Proteasome Protein degradation systems in droplet

이슬기찬 김성근<sup>1</sup>

서울대 생물물리 및 화학생물학과<sup>1</sup> 서울대 화학부

The protein degradation is very important in living cell. Immune system is based on the protein degradations. When protein degradation system does not work well, bacteria and virus survive in our cell. But this system excessively activated normal state, proteins could not function. We studies proteasome which functions protein degradation and is related immune system. Proteasome function will help the new medicine study. We use the microfluidics method which developed recently. The one of the microfluidics method; droplet generation system is very useful which guarantees isolated chemical environment. It is possible that Single Droplet contains the single molecule. We can detect the protein degradation through fluorescent intensity. Proteasome inhibitor or activator is usable the balance the life cycle.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Hydrophilic polymer coating on the poly(dimethylsiloxane) surface

이원재 손대원

한양대 화학과

Poly(dimethylsiloxane) (PDMS) microfluidic device is naturally hydrophobic and hard to produce oil phase polymer particle. Surface modification of PDMS was performed by photo-irradiation (UV and O<sub>2</sub> Plasma) method. We tried to make long-term stability of hydrophilic polymer coated PDMS microfluidic device and tried to produce oil droplets. 2-hydroxyethylmethacrylate (2-HEMA) solution was injected into modified PDMS microfluidic device and the coated PDMS surface was treated by oxygen plasma. PDMS surface has many formed with C-O bonding with 2-HEMA which was confirmed by ATR-FTIR spectroscopy. Contact angle was 6° and coating thickness was 19.76 μm. Stability was continuing for 2 weeks (2-HEMA+O<sub>2</sub> plasma coating: 6°→46°/O<sub>2</sub> plasma: 5°→84°). We performed production Undecanol droplet experiment into the hydrophilic microfluidic device. Undecanol droplet was produced and droplet size was 14.91 μm.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Raman Spectroscopy Study of Carbothermal Reactions in Double-Layer Graphene

박민균 류순민

경희대 응용화학과

그래핀(Graphene)의 가장자리(edge)는 결정구조의 배향성에 따라 지그재그(zigzag)와 안락의자(armchair) 형태로 구분되는데, 나노미터 크기의 그래핀의 전자적 성질은 이러한 가장자리의 구조에 의해 크게 영향을 받는다고 알려져 있다. 산화실리콘( $\text{SiO}_2$ )과 단일층 그래핀 가장자리 사이에서 일어나는 carbothermal reaction 은 선택적으로 지그재그 형태의 가장자리를 생성한다고 알려져 있다. 본 연구에서는 라만 분광법과 원자 현미경(atomic force microscopy)을 이용하여 기계적 박리법으로 만들어진 이중층 그래핀에서 일어나는 carbothermal reaction 을 연구하였다. 고온 산화 방법으로 이중층 그래핀에 지름 50 nm 이하의 원형 식각공(etch pit)을 만들고 Ar 기체 속에서 700 도 열처리를 진행한 후, 원형 식각공이 육각형으로 확장된 것을 관찰하였다. 이것은 이중층 그래핀에서도 산화실리콘 기판에 의한 carbothermal reaction 이 일어난다는 사실을 보여준다. 그러나 이중층 그래핀의 반응속도는 단일층보다 훨씬 느린 것이 확인되었는데, 이는 이중층 그래핀의 탄소 원자와 산화제로

작용하는 산화실리콘 간의 평균 거리가 단일층보다 더 크다는 사실로 설명할 수 있다. 또한 반응기 내의 비활성 기체의 유무가 **carbothermal reaction** 에 미치는 영향을 조사하였다.



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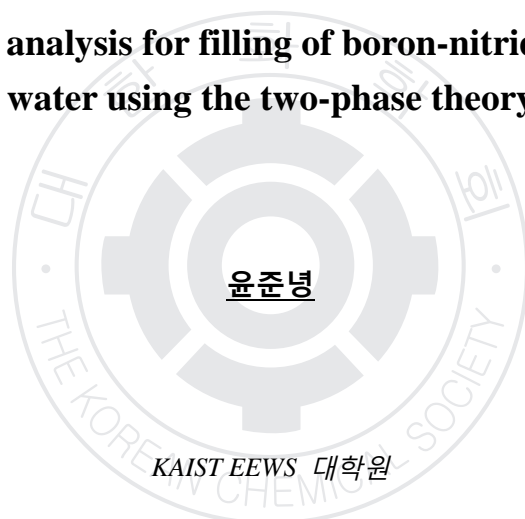
장소: 일산KINTEX

발표코드: **PHYS.P-469**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Thermodynamic analysis for filling of boron-nitride nanotubes with water using the two-phase theory**



Recent researches using molecular dynamics(MD) simulations have shown that a finite-length (5,5) boron nitride nanotube (BNNT) in contact with an water reservoir has superior water permeation property compared to a (5,5) carbon nanotube of similar diameter and length, and comparable to the (6,6) carbon nanotube which has a larger diameter. In this study, we analyzed the spontaneous filling thermodynamically using free energy, entropy, and enthalpy extracted from molecular dynamic (MD) simulation and two-phase theory (2PT) of water confined in various sizes of BNNTs (0.69nm to 1.77nm). We could show that water inside the BNNTs are always more stable than in the bulk state, but dominant factor for its stableness changes dramatically with BNNT diameter. For small size of BNNTs (0.7-1.0 nm), an entropy is the dominant factors for the stableness of water. In case of middle size (1.1-1.2nm), an enthalpy is dominant factor with its ice-like confined structure inside the BNNTS. Finally, bulk-like

liquid phase for larger BNNTs is stabilized by translational entropy. This study offers a fundamental basis for understanding water transport through BNNTs.



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**The Charge transfer of solvated metal ions using various population analysis methods (ChelpG, Mulliken, Merz Kollman, NPA, Hirshfeld, AIM, MGC)**

**Nizam Uddin 최철호<sup>1</sup>**

경북대 일반대학원 화학과 <sup>1</sup>경북대 화학과

There is no good charge transfer definition which we can rely on. The charge transfer of solvated metal ion has been analyzed using a broad variety of basis sets, three different quantum mechanical methods (Hartree-Fock, Becke3LYP, MP2) and various population analysis methods (ChelpG, Mulliken, Merz Kollman, NPA, Hirshfeld, AIM, MGC). Among these methods we found National Population Analysis (NPA) and MGC gives us more reliable results. We got charge transfer depends on coordination number. With the increasing coordination number of metal ion we found charge transfer also increases. Calculation have been carried out on alkali metal (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>) alkaline earth metal (Mg<sup>2+</sup>, Ca<sup>2+</sup>) cation water clusters containing up to six water molecules



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## **Dissociation Ion Pair (DIP) of NaCl: A combined study of ab initio and quantum mechanical molecular dynamic simulations**

**Manik Kumer Ghosh 최철호**

경북대 화학과

The ion association (or dissociation) process in solution is a crucial factor in the energetics and reaction pathways of a wide variety of systems and have important role in chemical reactions, solvation of ionic crystals into water, functionality of biological systems, solubility of biomolecules in salt buffers, marine chemistry and even functionality of aerosols in atmosphere. The dissociation of NaCl in solution were studied by both ab initio and QM/EFP MD (Quantum Mechanics/Effective Fragment Potential Molecular Dynamics). Quantum mechanical cluster calculations can provide accurate static structures of microsolvated ions, while molecular dynamics describe the dynamic aspects of solvation. In order to fill the gap between the two limiting approaches and to establish an unified view of ion association/dissociation, we introduce the concept of “Interionic Hydration Structures(HIS)”. In this study, we provided in detail the ion association/dissociation dynamics as well as a microscopic analysis of how the solvation structure changes during the process and we proposed the existance of dissociating ion

pair(DIP) during the dissociation process in addition with well-established contact ion pair (CIP) and solvent separated ion pair (SSIP).



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A theoretical study of adsorption of Formic acid on ice surface and proton Transfer from Formic Acid to Ice Surface**

**Shoaib Mahbubul alam 최철호<sup>1</sup>**

경북대 일반대학원 화학과<sup>1</sup> 경북대 화학과

The adsorption of organic molecules such as methanol, ethanol, formic acid and acetic acid on ice surface have been studied with the help of our QM/EFP scheme.<sup>1</sup> The calculation is carried out by the MP2 level of theory using 6-311++G(d,p) basis set. It was found that the ice surface structures as well as organic molecules adsorptions are strongly affected by long-range electrostatics, surface heterogeneity and hydrogen disorders of bulk ice, which demonstrate the importance of proper ice surface modeling. We have also studied the proton transfer reaction of Formic acid to ice surface. Since we found that insertion is the key of proton transfer, so we named this particular reaction as insertion activated proton transfer.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ligand binding dynamics of CO to denatured Cytochrome c in GdnHCl

김주영 박재흥 임만호

부산대 화학과

Rebinding dynamics of CO to denatured cytochrome c (uCytcCO) in 6 M Guanidine HCl (GdnHCl) and native-like cytochrome c (nCytcCO) in 1.8 M GdnHCl in D<sub>2</sub>O solution at 283 K after photodissociation, were studied using femtosecond vibrational spectroscopy. Single band near 1910 cm<sup>-1</sup> and 1920 cm<sup>-1</sup> is stretching mode of uCytcCO and nCytcCO. Geminate rebinding (GR) of CO to Cytc in 1.8 M GdnHCl (nCytc) is similar to that to chemically modified cytochrome c (cCytc) and is more efficient than that to Cytc in 6 M GdnHCl (uCytc). Less than 20% of them rebind to uCytc in 1 ns, Whereas more than 80% of the dissociated CO molecules geminately rebind to nCytc within 1 ns. The spectra of the dissociated CO from uCytc revealed a fast-growing band in the ps time scale that were assigned to CO in D<sub>2</sub>O solvent at 2090 cm<sup>-1</sup>. uCytcCO is fully unfolded in 6 M GdnHCl, so we could obtain a CO spectrum in solvent more than that in nCytcCO sample. We suggest that structure of unfolded cytochrome c is randomly arranged

and cannot trap photolyzed CO efficiently. The heme of uCyt<sub>c</sub>, active site, is not directly exposed to solvent, though.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Size Effects on the Dynamic Heterogeneity in Multicomponent Hard Sphere Systems

김정민 성봉준

서강대 화학과

Bulk metallic glasses exhibit the exceptional stability under the crystallization with low critical cooling rate. It is well known that there are slowing down of dynamics and the dynamic heterogeneity (DH) when approaching the glass transition point. Recently, the study of multicomponent glass-forming (MCGF) Pd<sub>43</sub>Cu<sub>27</sub>Ni<sub>10</sub>P<sub>20</sub> melt upon supercooling (2) shows that there is a strong component decoupling in diffusion between the fast elements and the large component Pd. Interestingly, the Stokes-Einstein (SE) relation holds for Pd, suggesting the formation of slow subsystem of Pd which is a crucial factor to form glass systems. To elucidate the size effects on the DH in multicomponent systems, we model hard sphere systems after the MCGF Pd<sub>43</sub>Cu<sub>27</sub>Ni<sub>10</sub>P<sub>20</sub> melt with van der Waals radii and atomistic radii. At the crucial density  $\phi_c=0.59$ , there is a strong violation of SE relation, i.e.,  $D\eta=\text{constant}$ , where  $D$  is the diffusion coefficient and  $\eta$  is viscosity (3,4). Also, the non-Gaussian parameter (NGP) and the self-part of van Hove function indicate the dynamic heterogeneity with slow particles rattling in the cage formed by their

nearest neighbors and fast particles hopping to another sites. Notably, component decoupling of  $t^*$  occurs at  $\phi_c$  where  $t^*$  is the time with the maximum value of non-Gaussian parameter for each components. Since  $\eta$  is collective property, we use the relaxation time  $\tau_\alpha$  with  $F_s(k, \tau_\alpha) = 1/e$  to decide whether the single component follows the SE relation or not (3). Finally, we get the waiting time  $t_w$  for each components to compare with  $\tau_\alpha$ . At the density  $\phi \geq \phi_c$ ,  $t_w \geq \tau_\alpha$ , indicating hoplike motions.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Raman Spectroscopy Study of CVD-Grown Graphene Supported on Ultra-Flat Boron Nitride**

**안광현 고택영 류순민**

경희대 응용화학과

2 차원 물질인 그래핀(graphene)의 물성은 그래핀을 지지하는 기판과의 상호작용에 영향을 받는 것으로 알려져 있다. 본 연구에서는 기계적 박리법을 이용하여 만든 결정성 h-BN(hexagonal boron nitride) 기판이 일반적으로 사용되는 비정질 산화실리콘과 어떤 차이를 보이는지 라만 분광법을 이용하여 연구하였다. 편평도가 높은 h-BN 위에서의 그래핀은 편평도가 낮고 charge defect 가 있다고 알려진 산화실리콘 위에서보다 G band의 진동수가 더 낮게 관측되었다. 이러한 변화는 기판에 의해 유발된 전하밀도의 감소와 기계적 변형(strain)으로 설명할 수 있다. 그래핀/h-BN 에서 관찰된 2D band의 비정상적인 진동수 증가는 h-BN 과 그래핀 사이에서 일어나는 van der Waals 상호작용에 의한 그래핀의 전자구조 변형을 암시한다.



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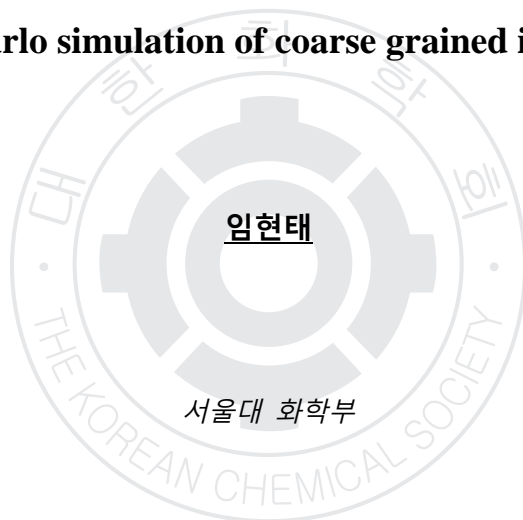
장소: 일산KINTEX

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Monte-Carlo simulation of coarse grained ionic liquid



Dynamic heterogeneity of undercooled system is unusual phenomena, which not observed in normal liquid system. We study dynamical properties of room-temperature ionic liquids (RTILs), especially relaxation function, structural relaxation, and dynamic susceptibility. In this work, we adopt lattice-gas monte carlo simulation based on coarse-grained asymmetric charge model (ASM). And we also study how electrostatic interaction and steric interruption affect glassy behavior int RTILs.

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**치환기 X에 따른  $C_{20}H_{20}$  과  $C_{20}X_{20}$  케이지 내부 부피 변화 비교**  
**(X=F, Cl, and Br)**

이기학 황용규<sup>1</sup>

원광대 화학과 <sup>1</sup>원광대 반도체.디스플레이학부

혼성 범밀도 함수법 B3LYP/6-31G(d,p)을 사용하여,  $C_{20}H_{20}$  에 대해서 H 를 F, Cl 또는 Br 로 치환 할때 일어나는 케이지 내부 부피 변화에 대하여 연구하였다.

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## On the band-gap dependence of efficient density matrix computation from Hamiltonian

김재훈

KAIST EEWS대학원

Density matrix purification is an efficient way of avoiding the expansive cubic scaling diagonalization in self-consistent field calculations. Although there are many recursive method to evaluate density matrix, purification and its derivatives do not usually use the distribution information of eigenvalue of Hamiltonian, and semi-optimal scheme was found in the universal algorithm for density matrix computation. In this study, we suggest an algorithm using band-gap information of a system of interest, to accelerate purification.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhanced Chemical Stability of Graphene Supported on Mica Substrates

고택영 이주연 류순민

경희대 응용화학과

최근 여러 화학 반응에 대해서 산화 실리콘기판에 고착된 단일층(single layer) 그래핀이 복층(multilayer) 그래핀보다 10 배 이상의 높은 반응성을 보인다는 사실이 알려졌다. 본 연구에서는 기판 표면의 편평도와 기판-그래핀간의 상호작용이 그래핀의 반응성에 미치는 영향을 이해하기 위해서, AFM(atomic force microscopy)과 라만 분광법을 이용하여 그래핀의 기체상 고온 산화반응과 Ar 플라즈마에 의한 상온 식각반응을 연구하였다. 기계적 박리법을 통해 비정질 산화실리콘과 결정성 마이카(mica) 기판 위에 고착된 그래핀 시료를 비교하였다. 편평도가 낮은 산화실리콘 위에서는 그래핀의 두께가 작을수록 산화반응 속도가 크고 삼중층 이상의 경우 흑연과 비슷한 반응성을 보인다고 알려져 있다. 그러나 편평도가 높은 마이카 위에서는 이중층 그래핀 또한 흑연과 반응성의 차이가 없음이 관찰되었다. 특히 마이카 위의 단일층 그래핀에서는 복층 그래핀과는 달리 기판-그래핀간의 강한 상호작용 때문에 산화에 의한 식각이 거의 일어나지 않아 화학적 안정성이

증대되었음을 알 수 있었다. 플라즈마 반응 또한 산화실리콘보다는 마이카 기판 위에서 현저히 느리게 진행되어 산화반응과 유사한 경향을 보였다. 본 연구는 기판의 표면구조와 상호 작용을 통해 그래핀의 화학적 특성을 조절할 수 있다는 가능성을 보여 준다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: PHYS.P-480

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Synthesis of *N*-benzoylbenzamide And Luminescence Properties of Ln(III) Complex with Homoleptic BBA ligand or mixed BBA and phen (BBA = *N*-benzoylbenzamide and phen =1,10-phenanthroline)**

김민아 강준길

충남대 화학과

First, we synthesized *N*-benzoylbenzamide(BBA) by reacting benzamide with benzoyl chloride under microwave irradiation, and then lanthanide complexes with homoleptic BBA ligand or mixed BBA and phen ligands. The chemical formulas of the synthesized compounds were confirmed by IR, NMR, UV, EA and ICP. It was found that the efficient sensitized-luminescence of Ln(III) complexes were resulted from the energy transfer from BBA to Ln(III) for Tb(III) complexes. The process of the sensitized luminescence was proposed by Quantum mechanical calculations.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: PHYS.P-481

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Synthesis and Luminescence Properties of Ln(III) Complexes with Homoleptic N2O2 and Mixed N2O2 and phen(Ln = Eu, Tb and Dy, N2O2 = 2,2'-(1E,1'E)-(ethane-1,2-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol, and phen =1,10 phenanthroline)**

**정용광 강준길**

충남대 화학과

First, the Schiff base ligand N2O2 was synthesized by nucleophilic addition of ethylenediamine and salicylaldehyde and then lanthanide complexes with homoleptic N2O2 ligand or mixed N2O2 and phen ligands. The chemical formulas of the synthesized compounds were confirmed by IR, NMR, UV EA and ICP. It was found that the efficient sensitized-luminescence of Ln(III) complexes were resulted from the energy transfer from N2O2 to Ln(III). The process of the sensitized luminescence was proposed by Quantum mechanical calculations

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-482**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Synthesis and Characterization of Luminescent Polymer Nanoballs Incorporated with Re(III) Complexes (Re = Eu, Sm, Tb, and Dy)**

**김종문 정용광 강준길**

충남대 화학과

Luminescent polymer nanoballs were synthesized by self-organization process via two steps. First, a solution of a mixture of Re(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) and polysulfone (PS). The size of Re(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.



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장소: 일산KINTEX

발표코드: PHYS.P-483

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A comparative study on the structural and energetic properties of *c*-C<sub>4</sub>F<sub>8</sub> and 2-C<sub>4</sub>F<sub>8</sub>: DFT functional and basis set dependence

최희철 박영춘 백경구<sup>1</sup> 이윤섭

KAIST 화학과 <sup>1</sup>강릉원주대 화학과

Via a series of calculations with various DFT functionals and basis sets, the structural, electronic, and energetic properties of *c*-C<sub>4</sub>F<sub>8</sub> and 2-C<sub>4</sub>F<sub>8</sub> were studied. Especially, we investigated the dependencies of the ring-puckering angle( $\delta$ ) and inversion barrier( $\Delta E_{RP}$ ) of *c*-C<sub>4</sub>F<sub>8</sub> for DFT functionals and basis sets and evaluated the accuracy of DFTs for electron affinities(EAs) of *c*-C<sub>4</sub>F<sub>8</sub> and *trans*-2-C<sub>4</sub>F<sub>8</sub>. The  $\delta$  and  $\Delta E_{RP}$  of the *c*-C<sub>4</sub>F<sub>8</sub> energy minimum can be accurately reproduced by using the long range- and/or dispersion-corrected DFT functionals with Dunning's basis sets. The EAs for *c*-C<sub>4</sub>F<sub>8</sub> and *trans*-2-C<sub>4</sub>F<sub>8</sub> require at least one *f* polarization function to be added to split valence shell type basis functions whereas *g* or higher functions do not noticeably increase the accuracy. In addition, the mechanisms in *c*-C<sub>4</sub>F<sub>8</sub> and 2-C<sub>4</sub>F<sub>8</sub><sup>-</sup> isomerizations were elucidated from the  $\omega$ B97X-D/aug-cc-pVTZ results. In the 2-C<sub>4</sub>F<sub>8</sub> isomerization, its transition state shows the symmetric feature of charge transfer from the C=C bond to the -CF<sub>3</sub> at both ends. The counterpart in the 2-C<sub>4</sub>F<sub>8</sub><sup>-</sup> isomerization has the asymmetric feature of charge transfer from one

side of the C=C bond to another side, resulting in a strengthening of planarity of the C atom on the former and an increase of s-character of C on the latter.



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장소: 일산KINTEX

발표코드: **PHYS.P-484**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **X-ray Structures and Luminescence Properties of 1,2-Bis(4-fluorobenzoyl)-3,4,5,6-tetraphenylbenzene and 1,2-Bis(4-hydroxyphenyl)-3,4,5,6-tetraphenylbenzene**

**김종문 강준길 김환기<sup>1</sup>**

충남대 화학과 <sup>1</sup>건국대 응용화학과

Macro-organic molecules (1,2-BFBTPB and 1,2-BHPTPB), composing of benzene frame substituted by tetraphenyl and bisphenyl containing functional groups, were synthesized, and their structural and photophysical properties were investigated. X-ray structure showed that the compounds had panwheel-type geometries. The photophysical properties of 1,2-BFBTPB and 1,2-BHPTPB were investigated in terms of excitation, luminescence, UV and reflectance. When exposed to UV light, the compounds produced deep blue to green luminescence, depending on the solvent. It was found that the proton transfer from the organic molecule to the solvent played a key role in the observed solvatochromism. Quantum mechanical calculations for 1,2-BFBTPB and 1,2-BHPTPB were also performed to interpret the observed photophysical properties.

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발표코드: PHYS.P-485

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Synthesis and luminescence properties of  $(\text{Ba}_{1-x}\text{Sr}_x)_2\text{SiO}_{4-3y/2}\text{N}_y:\text{Eu}^{2+}, \text{M}^{3+}$  green phosphor for white light emitting diode**

**강봉호 강준길**

충남대 화학과

In the present study, we therefore focused on the preparation and the luminescence properties of  $\text{Eu}^{2+}$ -doped  $\text{M}_2\text{SiO}_2\text{N}_{4/3}$  ( $\text{M} = \text{Ba}$  and  $\text{Sr}$ ) green phosphors, aiming at generating the pure green emission for use in WLEDs. The crystal structures and the luminescence properties of  $\text{M}_2\text{SiO}_2\text{N}_{4/3}$ -type phosphors have not been reported up to now. In this study, we prepared  $\text{Eu}^{2+}$ -doped  $\text{Ba}_2\text{SiO}_2\text{N}_{4/3}$  phosphor and examined the substitution effect of  $\text{Ba}^{2+}$  by other alkali earth ions on the luminescence properties. We found that only  $\text{Sr}^{2+}$  enhanced the luminescence intensity markedly. We prepared  $(\text{Ba}_{1-x}\text{Sr}_x)_2\text{SiO}_{4-3y/2}\text{N}_y:\text{Eu}^{2+}$  in the whole range ( $x = 0$  to  $1.0$ ) and investigated the substitution effects on the crystal structure and the luminescence properties of  $\text{Ba}_2\text{SiO}_{4-3y/2}\text{N}_y:\text{Eu}^{2+}$ . Furthermore, we optimized the green phosphor by co-doping with three valent metal ions and varying the concentration of  $\text{Eu}^{2+}$ . Additionally, we fabricated the phosphor-converted (pc) LEDs by casting the optimized phosphor on a blue InGaN LED chip and investigated the luminescence properties of the fabricated pc-LEDs.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-486**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Critical Temperatures Calculations of Cobalt Orthosilicate by First Principles DFT Calculations

이기학 이창훈<sup>1</sup>

원광대 화학과 <sup>1</sup>포항공과대 화학과

제 1 원리 범밀도 함수 법과 응용 파동함수를 사용하여 Cobalt Orthosilicates 임계온도를 계산하는 식을 유도하였다.

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장소: 일산KINTEX

발표코드: **PHYS.P-487**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## $C_{20}Li_{20}$ 기하구조 이성체의 구조 특성 비교

이기학 황용규<sup>1</sup>

원광대 화학과 <sup>1</sup>원광대 반도체·디스플레이학부

B3LYP/6-31G(d,p) 혼성 범밀도 함수 방법을 사용하여, 2 종류의  $C_{20}Li_{20}$  기하구조 이성체를 얻었다. 2 가지 기하 구조 이성체의 차이를 비교 분석하였다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.P-488**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Photoisomerization dynamics of a styryl dye and its derivatives in oligo(ethylene glycol)

이유민 이민영<sup>1</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학나노과학부

A styryl dye, trans-4-[4-(dimethylamino)-styryl]-1-methylpyridinium iodide (4-DASPI), is a useful fluorescence dye to probe condensed-phase microenvironments. The major nonradiative decay channel in the excited state of 4-DASPI is the internal twisting around the single bond between the aniline ring and pyridylethylene moieties. In this work, we have investigated the photoisomerization dynamics of 4-DASPI and its derivatives in oligo(ethylene glycol) solvents. By varying the molecular weight of oligo(ethylene glycol), it is possible to tune the wide viscosity range up to the gelation point. It was observed that dependence of twisting dynamics of the probing dyes on viscosity is not describable by a simple diffusion equation, and thus the results were interpreted in terms of the solvent size effect as well as its microenvironmental aspect.

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장소: 일산KINTEX

발표코드: **PHYS.P-489**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Energy transfer dynamics of an excited coumarin dye to multiple hemin and cytochrome c molecules**

이혜민 이민영<sup>1</sup>

이화여대 화학나노학과 <sup>1</sup>이화여대 화학나노과학부

This work focuses on the intermolecular fluorescence resonance energy transfer (FRET) between coumarin 334 (C334) and surrounding hemin or cytochrome c (cyt c) molecules. C334 is a good laser dye with high fluorescence quantum yield, excellent photostability, and pH insensitivity. Hemin is the chromophore of cyt c, a small globular heme protein that has served as a paradigmatic case for protein folding. We have measured the fluorescence decay profiles of the FRET donor in the presence of the acceptors in polymer films, which gives information on the distribution of donor-acceptor distances. The FRET data as a function of acceptor concentration showed distinct trends for hemin and cyt c, which was interpreted by applying some existing theories.



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발표코드: **PHYS.P-490**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

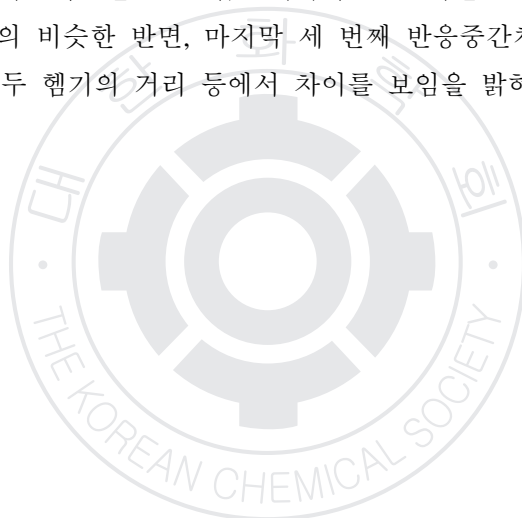
## Investigating Three-Dimensional Structures of Protein Intermediates in Solution Using Time-Resolved Wide-Angle X-ray Scattering

김종구 김태우 김영민 이효철

KAIST 화학과

분자의 거동을 연구하는 데 개발된 많은 물리화학적 측정 기법 및 분석 방법이 눈부시게 발전했음에도 단백질 분자 같은 거대 분자들의 용액상에서의 3 차원 분자구조 변화를 펨토초에서 나노초 영역까지 규명하는 것은 여전히 숙제로 남아 있다. 특히 단백질을 이루는 알파 헬릭스들이 빠르게는 펨토초에서 시간에 따라 어떻게 그 배치가 변하는지와, 피코초 및 그 이후 시간대에서 생성되는 단백질 반응 중간체들의 알파 헬릭스의 재배치 등 매우 상세한 3 차원 구조동력학적 정보를 실험적으로 측정하고 분석하는 일은 학계에 아직 보고된 적 없는 난제 중의 하나다. 시간에 따른 단백질의 3 차원 구조 변화를 측정할 수 있는 방법 중의 하나인 '시간분해 광각 엑스선 산란법(Time-resolved wide-angle x-ray scattering)'을 이용한 단백질의 구조 동력학 연구에 대해 논하고자 한다. '시간분해 광각 엑스선 산란법'은 용액상 단백질의 반응을 레이저 펄스 등으로 개시하고, 특정 시간이 지난 뒤의 구조적 변화에 대한 정보를 용액상 회절 패턴을 통해 얻어낸다. 이렇게 얻어진 시간에

따른 회절 패턴의 변화를 이용하여 '특이값 분해(Singular Value Decomposition)' 라는 선형대수학적 방법을 이용하면 반응중간체들의 회절 패턴에 대한 정보와 반응중간체들의 농도 변화에 대한 정보를 나누어 볼 수 있게 된다. . '특이값 분해'로부터 얻어진 정보들은 실제 실험에서의 반응중간체의 회절 패턴, 그것들의 농도 변화와 회전 변환의 관계이기 때문에 이를 보정해주면 반응중간체들의 고유한 회절 패턴과 반응의 메커니즘, 각 단계 반응의 시간상수에 대한 정보를 도출해낼 수 있다. 이렇게 얻어낸 회절 패턴을 이용해 동종이합체 헤모글로빈 단백질 (Homodimeric hemoglobin)의 광분해 반응 중간에 나타나는 반응중간체들의 3 차원 구조 분석을 시행하였다. 구조 분석은 강체 모델링의 방법을 이용하여 헬릭스를 기본 단위로 한 각 강체들이 실험 결과를 만족하는 동시에 화학적으로 안정한 방향으로 변화되도록 포텐셜을 정의하여 변화하도록 하였다. 또한, 전역 최소점에 위치하는 구조를 찾기 위하여 몬테카를로법을 적용하였다. 구조 분석 결과, 동종이합체 헤모글로빈의 리간드 광분해 이후 나타나는 세 반응중간체의 사차구조적 변화에 대한 구체적인 정보를 얻어낼 수 있었다. 또한, F97Y 변이 단백질의 동역학 연구도 병행하여 특정 아미노산 잔기의 역할과 그에 따른 동역학적 변화에 대하여도 연구하였다. F97Y 단백질의 '시간분해 광각 엑스선 산란법' 데이터를 분석한 결과, 첫 번째, 두 번째 반응중간체의 구조는 거의 비슷한 반면, 마지막 세 번째 반응중간체의 구조가 두 서브 유닛 사이의 물 분자의 개수, 두 험기의 거리 등에서 차이를 보임을 밝혀내었다.



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발표코드: **PHYS.P-491**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Protein Structural Dynamics of Photoactive Yellow Protein in Wild-type and E46Q Mutant Revealed by Pump-Probe X-ray Solution Scattering**

김태우 김종구 김영민 이효철

KAIST 화학과

Photoactive yellow protein (PYP), belonging to the class of photoreceptor protein, plays critical role in receiving external light that give rise to the responses required for biological function. However, the previous studies about the structural dynamics of photoactive yellow protein doesn't show the unified kinetic framework, but also the intermediate structures included in the photocycle under solution phase were rarely explored by the experimental methods. To probe the structural change during the photocycle in solution, we employ pump-probe X-ray solution scattering. By the analysis of both kinetics and structures of intermediates, the structural dynamics of wild-type PYP and its mutant (E46Q) accompanies the characteristic intermediate (pR and pB) and the signaling state (pB) shows the protrusion of N-terminus.

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발표분야: 물리화학

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## Imaging vibrational wavefunctions : Single object scattering sampling method

기호성 김경환 이효철

KAIST 화학과

The reaction process of any chemical reactions involves transition states connecting the reactant to the product. However transition states have never been directly assessable due to its extremely low population and probability. For the same reason, vibrational wavefunctions of even a simple diatomic molecule have never been experimentally measured. By using computer simulations here we explore the possibility to image transition states and/or reconstruct vibrational wavefunctions by incorporating single molecule diffraction with ultrashort intense X-ray pulses, which can be provided by X-ray free-electron-lasers. The idea of single biomolecular imaging experiments using femtosecond X-ray pulses was already suggested in the motivation to overcome the X-ray radiation damage problem and to solve the three-dimensional structure of biological macromolecules. Our perspective is different in that we focus on capturing “rarely populated structures” such as transition states or sampling all structural space to

reconstruct vibrational wavefunctions by single molecule diffraction of a small molecule whose structure in its global minimum is already well known.



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## Study of myoglobin diversity between horse and sperm whale using TR-WAXS

김영민 김종구 김태우 이효철

KAIST 화학과

Structural dynamics of sperm whale and horse Myoglobin coupled to ligand dissociation by laser irradiation were investigated with Time-Resolved wide angle X-ray solution scattering (TR-WAXS). We have identified the horse myoglobin (eMb) transient movements that happen at 840ps, 34ns, 540ns and 230Mm-1S-1, and sperm whale myoglobin (swMb) transient movements that happen at 460ps, 3.5ns, 92ns and 260Mm-1s-1. Comparing both myoglobin kinetics indicate that sperm whale myoglobin have more fast transient movements, but their recovery times are similar. Also the study shows that horse myoglobin does not have geminate recombination, while sperm whale myoglobin has ~13% geminate recombination. In order to find the reason for the difference between transient movements of eMb and swMb we studied the dynamics of swMb R45K-T68V double mutant that has same amino acid as eMb near heme and the swMb R45K-T68V-I28V triple mutant, that has same amino acid residues as eMb near

heme and Xenon site. The results show that the property of amino acids is important factor in the myoglobin kinetics and additionally confirms evolution process between swMb and eMb.



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## Various Al Nanocompounds Obtained by Pulsed Laser Ablation in Liquid-Phase (PLALP)

이슬기 최명룡

경상대 화학과

Various Al nanostructures were prepared by pulsed laser ablation in liquid phase (PLALP) with various surfactants, such as cetyltrimethylammouniumbromide (CTAB) concentrations. Depending on the concentration of surfactants, the size and structures of Al nanocomposites were varied. For example, the size of Al nanostructures decreased as the CTAB concentration decreased. Moreover, the morphology and structural changes of Al nanocompounds were exhibited as function of time, of which transformation was controlled also by the concentration of the surfactant concentration. Proposed mechanisms of the process will be discussed. The structural and morphological properties of the Al nanocompounds were characterized by X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM) and transmission electron microscope (TEM).



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## **Transformation of Titanium Dioxide in Acidic Aqueous Solution: Pulsed Laser Ablation (PLA) in Liquid Phase**

홍성민 최명룡

경상대 화학과

TiO<sub>2</sub> nanostructures were prepared by pulsed laser ablation (PLA) of a Ti metal plate in aqueous solution. TiO<sub>2</sub> nanomaterials were formed to spherical, filamentous and cubic shapes, depending on the PLA experimental conditions. In this study, pure and mixture of anatase/rutile structures of TiO<sub>2</sub> were fabricated by changing the pHs of the solution. 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<sub>2</sub> prepared in this study were investigated and discussed.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nickel and Nickel Oxide Nanoparticles Produced by Pulsed Laser Ablation in Various Solvents

정현진 최명룡

경상대 화학과

Nickel and nickel oxide nanoparticles exhibit useful optical or electrical functions as well as catalytic actions. Among various particle fabrication methods, pulsed laser ablation in liquid phase (PLALP) is currently attracting great interest due to its simplicity and versatility. In this study, nickel and nickel oxide nanoparticles were prepared by PLA in various solvents, such as deionized water, methanol, hexane, tetrahydrofuran (THF), and acetonitrile (AN). A pulsed Nd:YAG laser (1064 nm, 10 Hz, 7 ns) is used to produce the nickel and nickel oxide nanoparticles in deionized water; while pure nickel nanoparticles were produced in methanol, hexane THF, and AN. More interestingly, the crystal structures of Ni were also strongly dependent on the solvents used in PLALP. For example, hexagonal closed packing (hcp) and face centered cubic(fcc) structures of Ni were formed in hexane and THF, while pure hcp and fcc structure were fabricated in AN and methanol, respectively. Nickel and nickel oxide nanoparticles, of which size and composition dependence is demonstrated by the laser fluence, ablation time, and the

nature of the liquid. Size and optical properties of the nanoparticles were characterized by field emission scanning electronic microscope (FE-SEM), X-ray diffraction (XRD) and ultraviolet-visible spectroscopy (UV-vis).



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## Quantum Chemical Calculations of Electronically Excited States :3-Cyanoindole and Its Solvent-Molecule Clusters

안아름 최명룡

경상대 화학과

Indole is an aromatic heterocyclic organic compound. It has a bicyclic structure, consisting of a six-membered benzene ring fused to a five-membered nitrogen-containing pyrrole ring. Also it is a popular component of fragrances and the precursor to many pharmaceuticals. Compounds that contain an indole ring are called indoles. The indolic amino acid tryptophan is the precursor of the neurotransmitter serotonin. In this study, theoretical calculations of 3-cyanoindole and its clusters with various solvent molecules to help in the analysis of spectroscopic data obtained in this laboratory are reported. We calculated the 3-cyanoindole monomer using Møller-Plesset perturbation theory to second (MP2) with a 6-311++G(d,p) basis set and obtained the global minimum structure. We further carried out the excited state calculations on 3-cyanoindole with various solvent molecules using time dependent-DFT (TD-DFT) and configuration interaction singles (CIS). As a result, we obtained the excited state structure and transition energy of 3-cyanoindole-solvent clusters to accommodate the experimental observations.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## REMPI and UV-UV Hole-burning Spectroscopic Studies of Jet-cooled 3-cyanoindole and Its Solvent Clusters

민아름 문철주 안아름 최명룡 김성근<sup>1</sup>

경상대 화학과 <sup>1</sup>서울대 화학부

3-cyanoindole(3-CI) as a derivative of indole has important intrinsic properties for its enormous biological activities in biological systems. In a previous study, we have identified of only one conformer of 3-cyanoindole monomer via the REMPI and UV-UV double resonance spectroscopic studies in the free jet experiments. In this study, we have further investigated 3-cyanoindole-solvent (water, methanol, and ethanol) clusters. For the 3-CI-water (3-CIw) clusters, its REMPI spectrum having a red-shifted origin band compared to that of monomer showed a clear identification of the two conformers of 3-CIw. REMPI and UV-UV hole-burning spectroscopic studies of 3-CI with other solvent clusters will also be presented and discussed.

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## **Resonance Enhanced Multi-Photon Ionization (REMPI) and UV-UV hole-burning Spectroscopic Studies of Jet-cooled Phenacetin**

문철주 민아름 안아름 최명룡

경상대 화학과

Phenacetin is one of the typical synthetic fever reducers as similar to acetaminophen, Tyrenol. In this work, the conformational structures and photochemistry of phenacetin have been studied using one color resonant two-photon ionization and UV-UV hole-burning spectroscopy with a thermal evaporation method. As a result, we have successfully obtained sharply congested REMPI spectra of phenacetin. UV-UV hole-burning spectroscopy is accomplished in order to identify the number of conformers of phenacetin in the molecular beam. Moreover we have calculated the optimized structures of phenacetin by Møller-Plesset perturbation theory to second (MP2). Here, we will compare the previous study of acetaminophen with the present study.

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**Dechlorination of m-dichlorobenzene(m-DCB) using Metal  
Nanoparticles Produced by Pulsed Laser Ablation in Liquid Phase  
(PLALP)**

유이슬 최명룡

경상대 화학과

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. This preliminary study shows the preparation and characterization of the metal nanoparticles used for the effective dechlorination of m-dichlorobenzene (m-DCB). They were prepared by pulsed laser ablation (PLA) in deionized water with a reducing agent. Simple and effective dechlorination of m-DCB using Pd/metal bimetallic nanoparticles will be presented and discussed.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Electron-Nuclear Coupling Strengths of Two Coumarin Conformers Determined Directly by the Coherent Vibrational Wave Packets**

이경진 주태하

포항공과대 화학과

Electronic transition by a light pulse shorter than the vibrational period creates coherent vibrational wave packets. The wave packet motion can be observed by oscillations in various time-resolved spectroscopic signals. Among various methods, time-resolved fluorescence (TRF) has a unique advantage over transient absorption (TA), as it provides information on the dynamics in the electronic excited state exclusively. To launch and to observe vibrational wave packets, however, time resolution must be faster than  $\sim 1/2$  of the vibrational period; for example, it has to be close to 30 fs to observe a  $500\text{ cm}^{-1}$  mode, which is extremely hard to achieve in TRF. In this work, we report the observation of the coherent wave packet motions in the excited state of coumarin153 (C153) directly by TRF. We used fluorescence up-conversion following the excitation by two photon absorption. Then we obtained the TRF of C153 with a time resolution better than 30 fs. Oscillations were observed, which arise from the coherent vibrational wave packet motions in the electronic excited state of C153. Oscillation frequencies were retrieved by the linear prediction



singular value decomposition (LPSVD) method guided by the Fourier transform to yield five frequency components below  $500\text{ cm}^{-1}$ . Analysis of the oscillation components and quantum mechanical ab initio calculations revealed that C153 exists in two conformations, i.e. syn and anti conformers, at room temperature. Normal mode frequencies in the ground and the excited states of two conformers of C153 are calculated, and the electron-nuclear coupling strengths (Huang-Rhys factors) were calculated for the vibrational modes below  $500\text{ cm}^{-1}$  according to the work by Reimers. Especially, considering population ratio of the two conformers of C153 at room temperature, these oscillation frequencies, which have large electron-nuclear coupling strengths matches well with the wave packet oscillations from the experiments. Full theoretical simulation predicts the oscillation spectra reasonably well. The quantum mechanical calculations of the excited state, however, are not accurate enough to reproduce the experiment. Therefore, these results provide a benchmark system to assess a method of quantum mechanical excited state calculation as well as the spectroscopic and dynamical information on the excited state.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **field emission property of double layer coated single walled carbon nantube**

**박태희 이승진 이휘건**

한양대 화학과

We measured the field emission (FE) 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 O<sub>2</sub> gas. The field-enhancement factor,  $\beta$ , was calculated from the Fowler-Nordheim equation of FE results.

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## Gas ionization sensor based on 3-D Single-Walled Carbon Nanotubes network synthesized on ZnO Nanorods

이종택 김희수 이휘건

한양대 화학과

Gas sensors can be classified into a chemical type operated by gas adsorption and a physical type operated by ionization. The chemical types of gas sensor usually utilize an electrical response by the adsorption of gas molecules on the surface of the active layer, which leads to a large change in its electrical resistance. But most of these sensors (except for the CNTs-based sensors) need high working temperatures, for example 300~500 °C. Meanwhile, structures with large surface area may be required for distinguishable detection, which cause problems like high power consumption and pre-heating time. On the other hand, ionization sensors as a physical type gas sensor work by fingerprinting the ionization characteristics of distinct gases. However, this kind of instrument has high power consumption and risky high-voltage operation, and thus cannot be used on site. In this experiment, we synthesize single-walled carbon nanotubes (SWNTs) on zinc oxide (ZnO) nanorods on textured Si substrate using thermal chemical vapor deposition (CVD). By synthesizing SWNTs on ZnO nanorods, the suspended SWNTs

formed on ZnO nanorods can create 3-dim networks structure. After that we fabricate gas ionization sensor using 3-D SWMTs as anode and measure breakdown voltage of gas sensor and degree of stability compared to those of SWNTs film on textured Si. From that result, we confirm that gas ionization sensor using 3-D SWMTs has a better performance than SWNTs film and shows a possibility as practical gas sensor.



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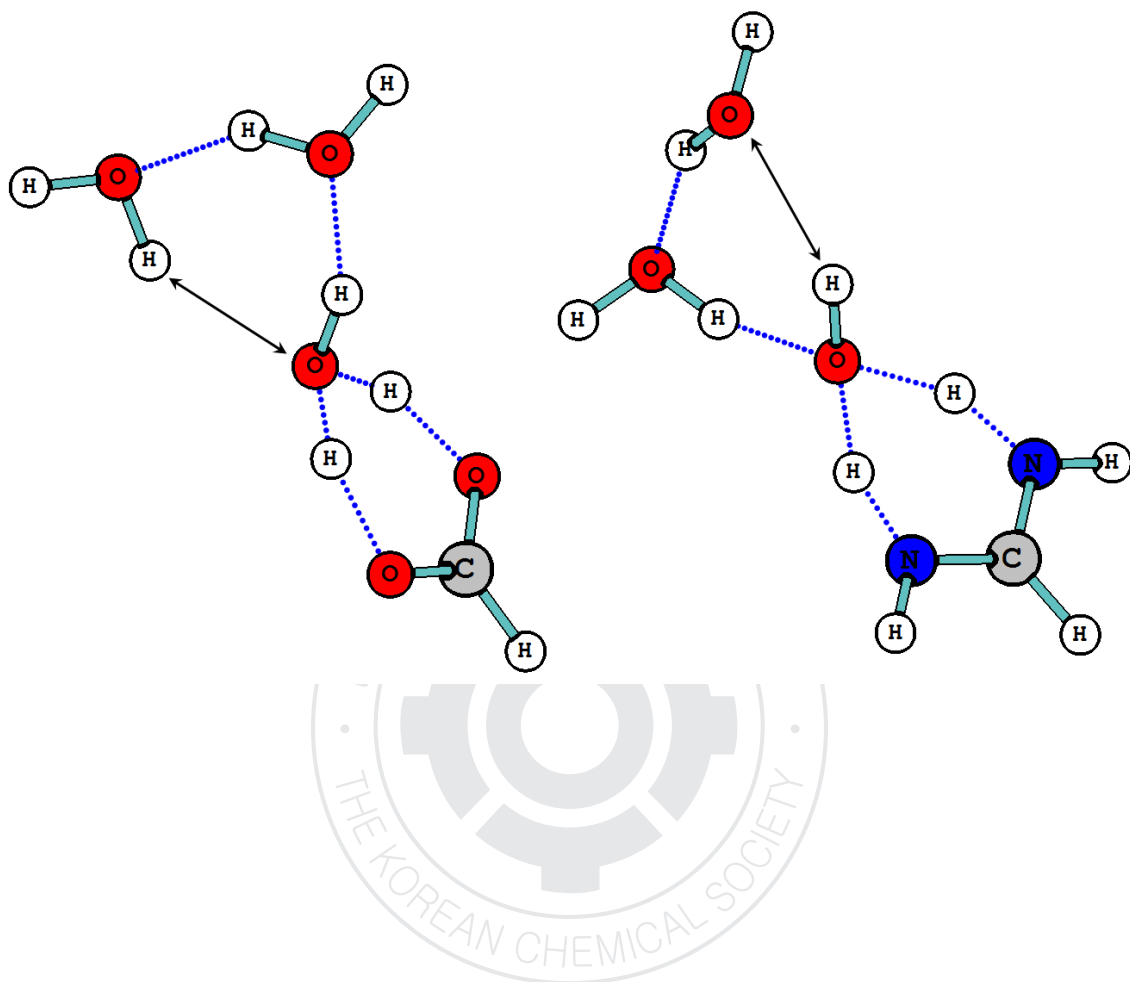
## Effect of Assisted-Waters in Rate Constant and Kinetic Isotope Effects of Tautomerization of Formic Acid and Formamidine: Direct *ab initio* Dynamics Study

Mai Khanh Binh

경희대 Chemistry

The mechanism and dynamics of the double proton transfer in hydrated formic acid (FA) and formamidine (FM) complexes were performed by using direct *ab initio* dynamics approach with variational transition-state theory using multidimensional semiclassical tunneling approximation. Double proton transfer processes of hydrated FA complexes tend to occur in protolysis mechanism. Besides that, solvolysis fashion is the interested one of hydrated FM systems. The effect of assisted-waters, hydrogen bond accepting water - aW - and hydrogen bond donating water - dW - were also investigated. With hydrated FA complexes, aW has a positive effect. It means that aW reduces the barrier height, and the tautomerization process becomes faster. The same effect is also found with dW in hydrated FM cases. On the other hand, dW in hydrated FA and aW in hydrated FM have an opposite trend, increase activation energies and reduce rate constants. Kinetic isotope effects (KIEs) were also calculated. Primary KIEs agree well with experiment values and previous calculated result. Except monohydrated FM system,

tunneling contribution to the primary KIE is not much large. It means that two deuteriums can also tunnel well. Solvent KIEs have small value, because of the hydrogen of assisted-water do not involve directly in proton transfer processes. The quasiclassical effect is the dominant contribution to the primary KIE and solvent KIE, the changing of entropic contribution mostly affect to the KIEs.



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## **NMR Evidence of Motions in Heparin-Binding Domain of VEGF<sub>165</sub> and Its complex with Inhibitor, Triamterene**

정기웅 강동일<sup>1</sup> 김양미

건국대 생명공학과 <sup>1</sup>건국대 화학과

It is known that vascular endothelial growth factor (VEGF) interacts with Ab by binding to heparin-binding domain (HBD) at C-terminal region of VEGF and is accumulated in the senile plaques of Alzheimer's disease patients' brains. In this study, we showed that triamterene (Trm) inhibits VEGF $\gamma$ A $\beta$  interaction without affecting other biological activities of VEGF or A $\beta$ . The results of binding study showed that the loop region (S11-L17) and F18 at the beginning of the first  $\beta$ -sheet in the HBD constitute the inhibitor binding site. Spin relaxation experiments and Model-free analysis showed that the residues in the disordered loop region of the N-terminus exhibited conformational exchanges in free HBD and these flexibility decreased dramatically upon binding to Trm. It suggests that A $\beta$  as well as inhibitor may recognize these unique dynamic features of the HBD. Furthermore, C-terminal residues continued to exhibit slow conformational motions, even in the HBD $\gamma$ Trm complex, implying that these motions of the

HBD might be important for interactions with heparin molecules. The flexibility of HBD should be essential for VEGF function and interaction with other protein partners.





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## Differences in Conformations and Dynamics of Apo, Holo and Acyl Forms of Acyl Carrier Protein

정기웅 김진경 강동일<sup>1</sup> 김양미

건국대 생명공학과 <sup>1</sup>건국대 화학과

Acyl carrier protein (ACP) is a small (~9 kDa) acidic protein whose function is essential for numerous biosynthetic pathways that depend upon acyl group transfer. We investigated structure and dynamic properties of apo, holo, acyl-ACP from *Escherichia coli*. From the observation of chemical shift variations, we confirmed that apo-ACP show only one conformation, while, holo-ACP with  $\text{Ca}^{2+}$  showed two sets of resonances, suggesting that two conformers are in dynamic equilibrium. Also, NMR data of acyl-ACP revealed that changes in the length of the covalently attached fatty acid affect the local conformation and the dynamics of ACP. Acylation stabilizes one conformation and model-free analysis comparing butyryl-, hexanoyl- and octanoyl-ACP indicated that ACP showed increase of structural rigidity upon binding to longer acyl chain. Studies on the interactions between acyl-ACP and the enzymes in FAS such as  $\beta$ -ketoacyl-acyl carrier protein synthase III and  $\beta$ -ketoacyl-acyl carrier protein reductase, showed that large chemical shift perturbations were observed for negatively charged residues in second

helix of acyl-ACP, suggesting that the electrostatic interactions between acyl-ACP and enzymes in FAS are important for elongation reactions of acyl chains.



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## **Inhibitors of $\beta$ -Ketoacyl acyl carrier protein synthase (KAS) III as Broad-spectrum Antimicrobial Agents**

정기웅 강동일<sup>1</sup> 김양미

건국대 생명공학과 <sup>1</sup>건국대 화학과

$\beta$ -Ketoacyl acyl carrier protein synthase (KAS) III is a particularly attractive target for development of antibacterial drug in the type II fatty acid synthetic pathway, since it is central to the initiation of fatty acid synthesis. We performed *in silico* screening in order to find inhibitors of *Escherichia coli* KAS III (ecKAS III), *Staphylococcus aureus* KAS III (saKAS III) and *Enterococcus faecalis* KAS III (efKAS III). Binding study of selected compounds from *in silico* screening was performed by Saturation Transfer Difference NMR spectroscopy and fluorescence experiments, and antimicrobial effect was evaluated against various bacteria. From this study, we found several potent inhibitors of ecKAS III, saKAS III and efKAS III which showed an antimicrobial effect against *E. coli*, *S. aureus* and *E. faecalis* as well as multidrug-resistant bacteria and we confirmed the importance of KAS III as targets for antimicrobial agents. Studies on the interactions between malonyl-ACP and ecKAS III showed that large chemical shift

perturbations were observed for negatively charged residues in second helix of malonyl-ACP, suggesting that the electrostatic interactions are important for elongation reactions of acyl chains.



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## Identifying a intermediate photoproduct of $\text{CHI}_3$ by combining time-resolved X-ray absorption spectroscopy and X-ray solution scattering

김경환 이효철

KAIST 화학과

Identifying intermediate species along a reaction pathway is a first step towards a complete understanding of the reaction mechanism, but this is often non trivial. There has been an on-going debate on which of the two intermediates, the  $\text{CHI}_2$  radical or the  $\text{CHI}_2\text{-I}$  isomer, is the dominant photoproduct. In this communication, by combining time-resolved X-ray scattering (TRXS) and time-resolved X-ray absorption spectroscopy (TR-XAS), we present strong evidence that the  $\text{CHI}_2$  radical is formed rather than  $\text{CHI}_2\text{-I}$  isomer after photolysis at 267 nm in methanol. . The two methods are complementary and capable of monitoring global reaction pathways from their structural sensitivity. The TRXS measurements, conducted using the laser-time-slicing, show no signature of isomer formation. The TR-XAS measurements performed at the iodine L1 and L3 edges are consistent with the conclusion of TRXS. The results exemplify that by combining both methods, give more convincing results and provide a better understanding of the reaction.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Tracing down the exciton relaxation dynamics in macrocyclic oligothiophenes

양재성

연세대 화학과

Functional oligothiophenes have attracted comprehensive interest in the field of materials sciences and have been advanced to be among the most frequently used  $\pi$ -conjugated materials, in particular as active components in organic electronic devices and molecular electronics. The traditional linear oligothiophenes suffer from undesired perturbing end effects on the conjugated chain. To circumvent this problem, in recent years, a multitude of size- and shape-persistent macrocyclic oligothiophenes has been developed and characterized. These macrocycles, in comparison to usual linear oligomers and polymers, have the distinct advantage to ideally combine an infinite defect free  $\pi$ -conjugated chain of an idealized polymer with the advantages of a structurally well-defined oligomer, but excluding perturbing end effects. In this regard, we have prepared a series of macrocyclic oligothiophenes, 5T-N (N = 2, 3, 4, 5, and 6), consisting of 2,5-thienylene, ethynylene, and vinylene units. Single-molecule photophysical properties of 5T-N have been explored with the single-molecule fluorescence detection techniques to reveal size

dependency of their properties. We deal with fluorescence dynamics of them such as photobleaching sequences, fluorescence lifetimes, and collective off-times, in conjunction with excitation energy migration efficiencies.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Structure and Backbone Dynamics Studies of PRL-3: Comparison of the $^{15}\text{N}$ NMR Relaxation Profiles of apo- and holo-PRL-3

강동일 정기웅<sup>1</sup> 김진경<sup>1</sup> 김양미<sup>1</sup>

건국대 화학과 <sup>1</sup>건국대 생명공학과

Phosphatases of regenerating liver (PRL) constitute a novel class of small, prenylated phosphatases with oncogenic activity. In particular, PRL-3 is important in cancer metastasis. With the aim of verifying the functional importance of the inherent structural flexibility of PRL-3, we have investigated the structures and the dynamic properties of apo- and holo-PRL-3 using NMR spectroscopy. Structures of apo- and holo-PRL-3 showed substantial differences in the general acid loop. Cys104, Arg110, and Asp72, participating in the enzymatic reaction, are close with each other and induced closed conformation in holo-PRL-3. When orthovanadate is added to the apo-PRL-3, the NMR signals from the residues in the active site appeared, indicating that the conformation of this region has been stabilized. Ligand binding caused a large conformational rearrangement, influencing on the motional behavior of the loops near the active site. Model-free analysis showed that flexibility of general acid loop is increased while the flexibility of P-loop is decreased upon binding of vanadate ion. Also, Glu82 at  $\alpha 3$  helix showed increase



of flexibility and conformation exchange upon vanadate binding. These results imply that general acid loop and  $\alpha 5$ - $\alpha 6$  as well as P-loop is important in ligand recognition and the difference between the flexibilities of the loops in apo- and holo-PRL-3 controls the protein-ligand interaction.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Altering biomimetic metal Induced aggregation process of F127 block copolymer by phosphate modified mesoporous silica nanoparticles**

남윤우 유창수 장미림 조은범 이동국

서울과학기술대 정밀화학과

Amphiphilic block copolymers composed of hydrophilic poly (ethylene oxide)(PEO) and hydrophobic poly(propylene oxide)(PPO), including (Pluronic?) F-127 (EO99PO65EO99), have been applied in diverse areas such as environment, biomaterials and pharmaceutic[1~3]. The block copolymers are known to form different types of aggregates depending on conditions. Interestingly, the aggregations can be biomimetic. This biomimetic aggregation can be used as a model to understand the aggregating process of biological molecules causing Alzheimer's disease(AD) and Type II diabetes(MD2) [4~6]. Mesoporous silica nanoparticles (MSNs) have been intensively studied due to several attractive features, such as large surface areas and easy surface functionalization [7~9]. In this study, we have synthesized phosphate modified mesoporous silica nanoparticles(PMSNs) and investigated the effect of these nanoparticles on the biomimetic metal induced aggregation process of block copolymer F-127 using biophysical means such as <sup>1</sup>H-NMR, DSC, ITC, UV-VIS and TEM. This biomimetic system is to mimic

peptide oligomerization process accelerated by metal ion, which is believed to be crucial in amyloidosis such as Alzheimer's disease(AD) and Type II diabetes(MD2). P-MSNs show the capability of altering the intrinsic aggregation pathway of F-127 induced by  $Mn^{2+}$  ions. This effect is thought to be mediated by strong electrostatic attraction force between negatively charged phosphate functional group of PMSN and positively charged  $Mn^{2+}$  ion. Results suggest that PMSNs could alter the biomimetic metal induced aggregation process of F127 block copolymer.[1] K. Huang, B.P. Lee, D.R. Ingram, P.B. Messersmith, *Biomacromolecules*. 2002, 3, 397-406. [2] K.H. Bae, Y.H. Lee, T.G. Park, *Biomacromolecules*. 2007, 8, 650-656.[3] T.K. Jain, M.A. Morales, S.K. Sahoo, D.L. Leslie-Pelecky, V. Labhasetwar, *Mol. Pharmaceutics*. 2005, 2, 194-205.[4] F. Ahmed, P. Alexandridis, S. Neelamegham, *Langmuir*. 2001, 17, 537-546.[5] J. Yuan, Z. Xu, S. Cheng, L. Feng, *Eur. Polym. J.* 2002, 38, 1537-1546.[6] C. M. Jan, V. Hest, *J. Mac. Sci.* 2007, 47, 63-92.[7] V.J. Mohanraj, Y. Chen, *Trop. J. Pharm. Res.* 2006, 5, 561-573.[8] I.I. Slowing, J.L. Vivero-Escoto, C.W. Wu, V.S.Y. Lin, *Advanced Drug Delivery Reviews*. 2008, 60, 1278-1288.[9] I.I. Slowing, B.G. Trewyn, V.S.Y. Lin, *J. Am. Chem. Soc.* 2007, 129, 8845-8849.



일시: 2012년 4월 25~27일(수~금) 3일간

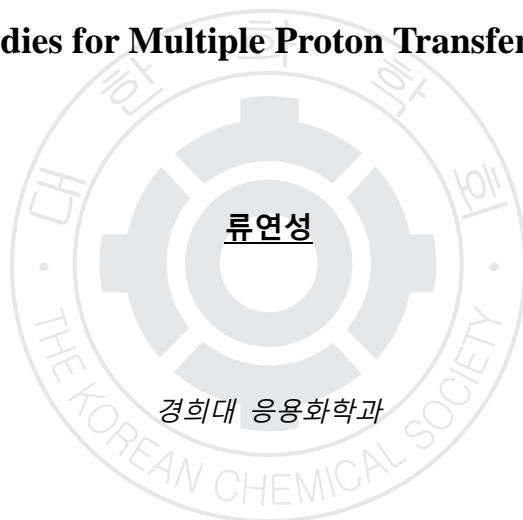
장소: 일산KINTEX

발표코드: **PHYS.P-512**

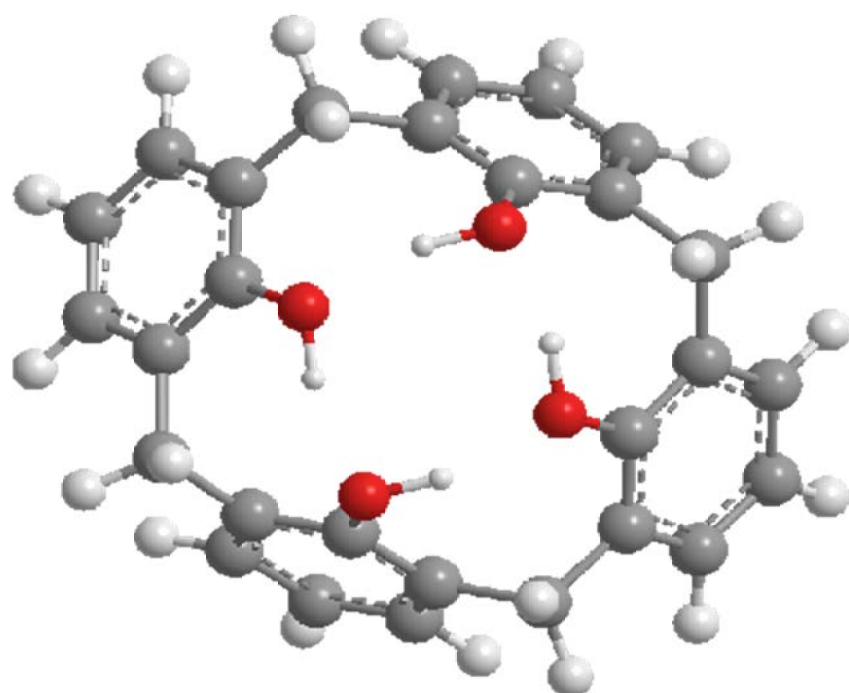
발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Theoretical Studies for Multiple Proton Transfer in Calixarene



Calixarene 은 모방효소, ion sensitive 전극이나 센서에서 적용될 뿐만 아니라 나노기술에서 고해상도 전자빔 리소그래피의 negative resist 로써 사용되는 화합물이다. 본 연구에서는 calix[4]arene 의 내부 양성자 이동을 알아보았다. 반응물과 전이상태, 생성물의 최적화 구조를 M06 계열의 M06-2X DFT 방법과 6-31+G\*\*, MIDIX 의 두 가지 basis set 를 혼합하여 계산하였다. 반응 메커니즘 관찰 결과 산소에 붙어있는 4 개의 수소가 동시에 반응이 일어나는 것을 확인하였다. 다차원 터널링 근사 및 변분법적 전이상태이론으로 반응동역학 계산으로부터 반응속도를 구하고 반응속도론적 동위원소 효과를 확인하였다.



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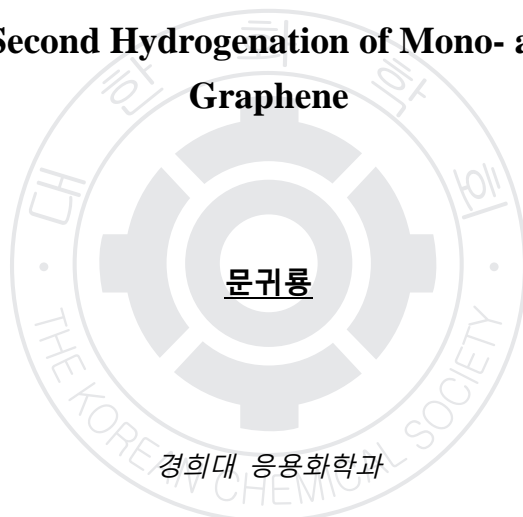
장소: 일산KINTEX

발표코드: **PHYS.P-513**

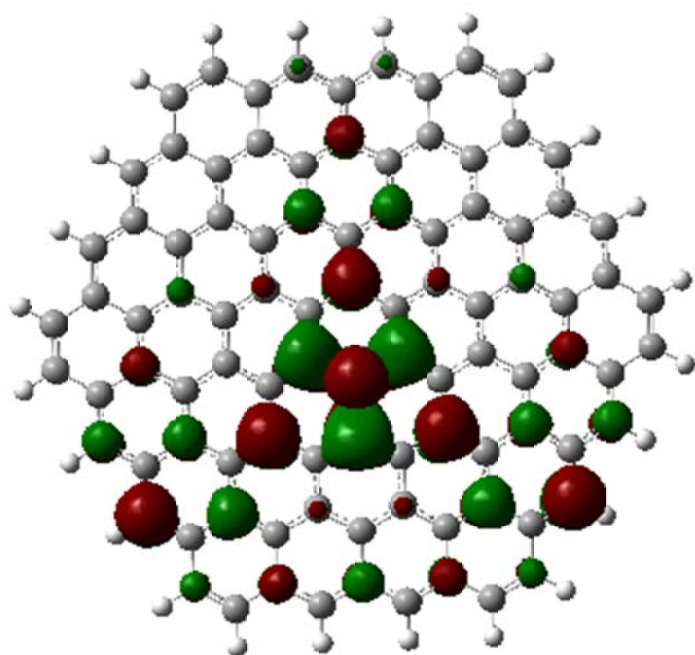
발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Site Dependent Second Hydrogenation of Mono- and Double Layer Graphene



Graphene 은 전기 전도도, 열 전도성, 탄성 등이 뛰어나기 때문에 차세대 신소재로 각광을 받고 있으며, 상온에서 뛰어난 전기전도성을 이용하여 지금까지 고속 트랜지스터 소자에 응용되는 등 구리와 실리콘을 대체할 수 있는 나노전자소자의 유망물질로 고려되고 있다. 본 연구에서는 graphene 에 수소화 반응에서 두 번째 수소가 도입되는 위치에 따른 수소화 에너지의 변화를 계산하였다. 두 번째 수소의 위치가 ortho, para 일 때 가장 안정한 에너지를 보이고, 이런 현상은 spin orbital density 의 분포와 일치하였다. 그리고  $\pi$ - $\pi$  interaction 이 수소화 에너지에 미치는 영향을 알아보기 위해 double layer grapheme 에서 같은 계산을 반복하였다. 이 계산에는 M06-L/6-31G\* 수준의 DFT 방법을 사용하였다.



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발표분야: 물리화학

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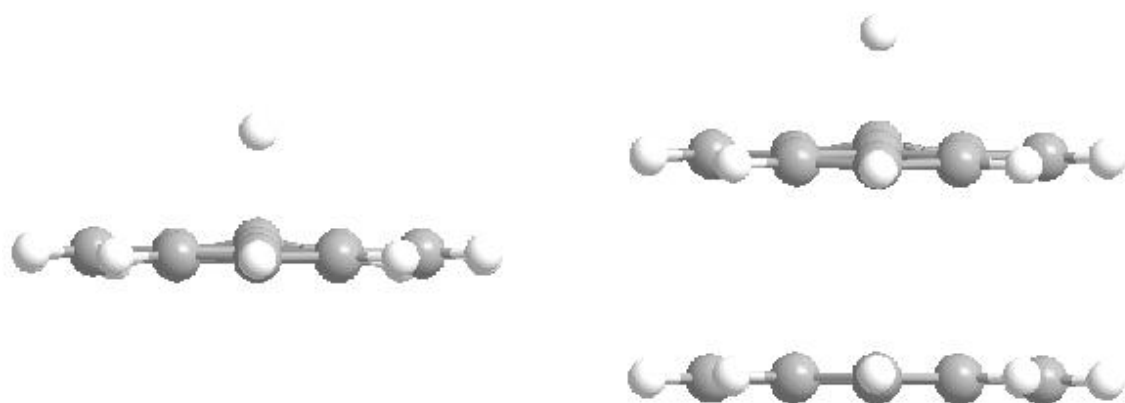
## Reaction Dynamics of Dehydration on Mono- and Double-Layer Graphene

백지혜

경희대 응용화학과

탄소 원자들이 각각  $sp^2$  결합으로 연결된 그래핀은 2 차원 구조로, 벤젠 형태의 탄소 고리가 벌집 형태의 결정 구조를 이룬다. 안전성이 높은 탄소로 구성되어 독특한 전기적, 물리적, 화학적 성질을 갖고 있어 많은 연구가 되고 있다. 본 연구에서는 단층의 그래핀에 첨가된 양성자를 떼어낸 반응에 대한 결과와 두 층으로 된 그래핀에 첨가된 양성자를 떼어낸 것을 비교하여 관찰하였다. 그래핀의 양성자가 첨가되었다가 제거되는 반응의 반응동역학을 알아보기 위해 반응물과 생성물, 전이상태 구조, 포텐셜 에너지를 여러 가지 DFT 방법 중에서 M06-2X/6-31G(d) 레벨로 계산하였다. 그리고 다차원 터널링 근사를 고려한 변분법적 전이상태이론으로 반응동역학 계산으로부터 H 와 D 의 반응속도를 구하고 반응속도론적 동위원소 효과를 얻었다. 다음 두 층으로 된 그래핀의 양성자 첨가 제거 반응도 마찬가지로 계산하였으며 두 층간의  $\pi$ - $\pi$  interaction 이 반응동역학에 미치는 영향에 대하여 연구하였다.





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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The interaction of hydrogen with ZnO surfaces: The effect of surface structure change on low temperature hydrogen adsorption**

**Probir Chandra Roy 김창민<sup>1</sup>**

경북대 화학과 211 호 표면화학 연구실 <sup>1</sup> 경북대 화학과

The interaction of hydrogen with ZnO single crystal surfaces, ZnO(0001), ZnO(000-1), and ZnO(10-10) has been investigated using temperature programmed desorption (TPD) and X-ray photoelectron Spectroscopy (XPS) techniques. When the ZnO single crystal surfaces are exposed to atomic hydrogen at 200 K, all three surfaces show hydrogen desorption at 450 K. The ZnO (000-1) surface does not show any lower temperature hydrogen desorption. In the case of the ZnO (0001) surface, the hydrogen desorption feature at ~260 K is observed as the hydrogen exposure increased. The ZnO (10-10) surface shows low-temperature desorption feature first and the high-temperature desorption feature appears as the hydrogen exposure increases. We will report the adsorption configuration of hydrogen atoms on ZnO surfaces with different surfaces structures.

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발표코드: **PHYS.P-516**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

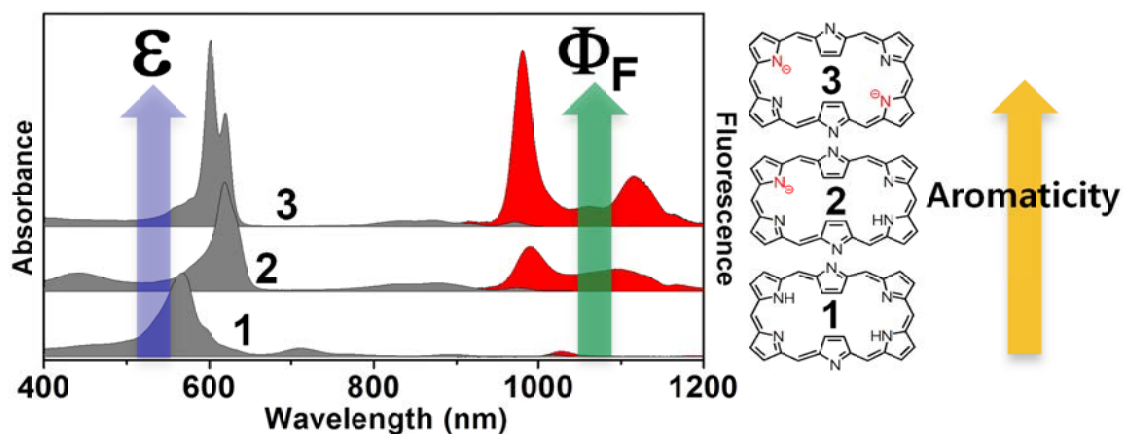
## Deprotonation-Induced Aromaticity Enhancement in meso-Hexakis(pentafluorophenyl) [26]Hexaphyrin(1.1.1.1.1.1)

차원영

연세대 화학과

During the last decade, expanded porphyrins bearing more than four pyrrole rings have attracted considerable attention in light of their rich chemistry such as structural versatility, effective coordination platforms to realize various metal complexes, organic nonlinear optical materials, new near-infrared (NIR) and infrared (IR) dyes, and easy accessibility of  $[4n]$  and  $[4n+2]$  congeners through two-electron oxidation and reduction processes. Throughout the studies on expanded porphyrins, we have consistently observed the correlations between photophysical properties and aromaticity in measurements of the magnetic indices, steady-state absorption and emission spectra, time-resolved excited-state dynamics, and computational calculations including the NICS, HOMA, and AICD. Aromatic expanded porphyrins, regardless of whether they are Hückel- or Möbius-type, exhibit distinct absorption spectra with well-defined, sharp B- and Q-like bands, strong fluorescence, long-lived excited states, and large TPA (two-photon absorption) cross-section values as compared with anti- or nonaromatic expanded porphyrins. as a

part of our continuous efforts to explore novel electronic states of expanded porphyrins, we propose a method for controlling aromaticity of normal [26]hexaphyrin by deprotonation with tetrabutylammonium fluoride (TBAF). Deprotonated monoanion and dianion of hexakis(pentafluorophenyl) [26]hexaphyrin(1.1.1.1.1.1) display sharp B-like bands, remarkably strong fluorescence, and long-lived singlet and triplet excited-states as an indication of enhanced aromaticity. Structural, spectroscopic, and computational studies have revealed that the deprotonation induces structural deformations, which leads to a change in the main conjugated  $\pi$ -electronic circuit as a cause for the enhanced aromaticity.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ultrafast Vibrational Spectroscopic Study on Solvation Structure and Dynamics of 2-Cyanophenol

이주용 조민행

고려대 화학과

2-Cyanophenol (2CP) 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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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dynamics of Solute-Solvent Interaction in Reverse Micelles

이주용 조민행

고려대 화학과

IR probes have been extensively used to monitor local electrostatic and solvation dynamics. Particularly, their vibrational frequencies are highly sensitive to local solvent electric field around an IR probe. Here, we show that the experimentally measured vibrational frequency shifts can be inversely used to determine local electric potential and field distributions and solute-solvent electrostatic interaction energy. In addition, the upper limits of their fluctuation amplitudes are estimated by using the vibrational bandwidths. Applying this method to a core/shell model has often been used to describe water confined to the interior of reverse micelles (RMs). This model is composed of fully deuterated N-methylacetamide (NMA-d<sub>7</sub>) in D<sub>2</sub>O / Aerosol OT / isooctane. Additionally, we could control the size of RMs ( $W_o=2\sim60$ ). Water molecules in confined environments with pools a few nanometers in diameter ( $d_{wp}=2\sim20\text{nm}$ ) or at interfaces undergo hydrogen bond structural dynamics that differ drastically from the dynamics they undergo in bulk water. Therefore, amide I' vibration mode of NMA-d<sub>7</sub> in reverse micelles is influenced by solvent electric field produced by surrounding water molecules, differently for size. Finally, we found

that the solvent electric field produced by surrounding water molecule on the NMA from FR-IR spectra. From the results, we found that solvent electric field is increase as size of RMs decrease. This indicates that the peptide-solvent interactions in nanometer scale water pools are different from the interactions they undergo in bulk solution.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Spin exchange interactions in VOSb2O4

구현주 강은비

경희대 화학과

The spin exchange parameters of VOSb2O4 were evaluated by performing energy-mapping analysis based on density functional calculations. The spin exchange interaction between the nearest-neighbor V4+ ions is strongly antiferromagnetic while other interactions are negligible. Thus, the magnetic structure of VOSb2O4 is best described by a spin-1/2 Heisenberg antiferromagnetic chain with no spin frustration.



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## The physical effects on the formation of polyynes by laser ablation

신승근 박영은 박승민

경희대 화학과

Polyynes were prepared by liquid laser ablation of a graphite target in deionized water at various physical effects, such as, wavelengths (266, 355, 532, and 1064 nm), ablation times (up to 60 min), different laser power (20 and 40 mJ), and identified by analyzing ultraviolet (UV) absorption. In order to examine the physical effects on the linear carbon chain length, we compared to the amount of polyynes and the branching ratios of C<sub>6</sub>H<sub>2</sub>, C<sub>8</sub>H<sub>2</sub>, and C<sub>10</sub>H<sub>2</sub> in the UV-Vis spectra of polyynes, respectively. We concluded that the amount of polyynes produced increased using a laser of long wavelength and the peak intensities of polyynes increased with ablation time and laser power as well.

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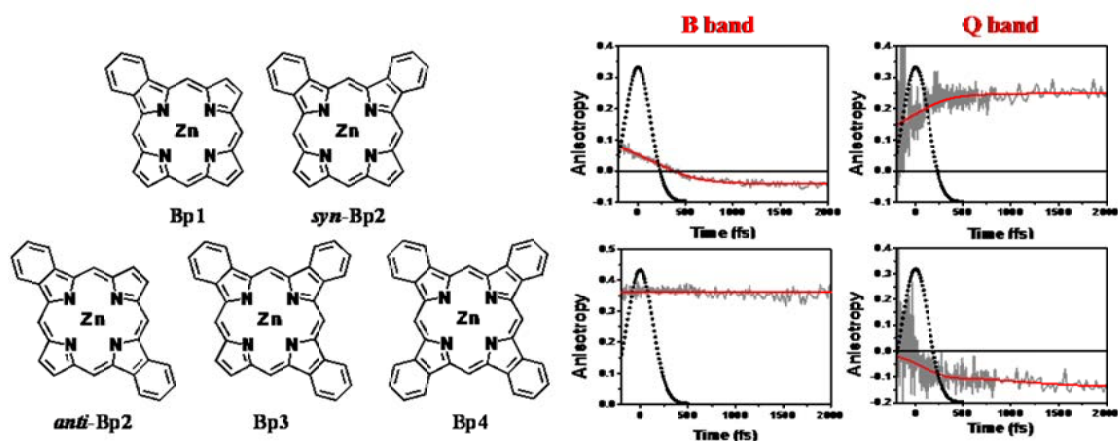
## Ultrafast Intramolecular Energy Relaxation Dynamics of Benzoporphyrins Probed by Femtosecond Fluorescence Upconversion

김표상 김동호

연세대 화학과

Strenuous research efforts have been focused on developing new types of porphyrin chromophores that display certain characteristics for applications such as molecular photonic devices, artificial photosynthesis and dye-sensitizer solar cell. In this context, the detailed understanding of relationship between structure and photophysical properties is crucial for the fabrication of novel porphyrins targeted for specific applications. In this work, we have investigated the role of fused benzo-rings on electronic structures and the intramolecular energy relaxation dynamics in a series of benzoporphyrins (Bp1, syn-Bp2, anti-Bp2, Bp3 and Bp4) by using femtosecond time-resolved fluorescence upconversion technique. Interestingly, despite the same number of fused benzo-rings, while anti-Bp2 shows an obvious splitting of Bx (Qx) and By (Qy) states, syn-Bp2 exhibits degenerate B and Q bands in their absorption spectra. These features provide that anti-Bp2 shows split B and Q bands in the order of  $B_y > B_x > Q_x > Q_y$  which leads a superimposition of Qx (0,0) and Qy (1,0) bands. This overlap generates a strong coupling

between these two states, which results in a direct internal conversion from Bx (0,0) to Qy (0,0). This observation suggests that anti-type fused position of benzo-rings leads to a new mechanism in internal conversion from B to Q state. On the basis of this work, we can obtain further insight into the effect of fused benzo-rings on the photophysical properties of benzoporphyrins, which provides a detailed understanding of the structure-property relationship in a series of benzoporphyrins.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## 염료-감응형 태양전지 응용을 위한 $\text{TiO}_2$ structure(rod, particle)의

### 합성과 특성연구

양희수

성균관대 화학과

염료-감응형 태양전지 응용을 위하여  $\text{TiO}_2$  nanorods 를 autoclave 를 이용하여, FTO 기판위에 수열합성법으로 합성 하였다.  $\text{TiO}_2$  nanorods 는 증류수와 염산, Titanium tetra isopropoxide(TTIP) 전구체의 혼합 용액을 이용하여, 150 - 200 °C 의 온도에서 합성 하였다. 합성된  $\text{TiO}_2$  nanorods 의 두께와 길이, 밀도는 성장시간과 성장온도, 전구체의 양, 염산과 증류수의 비율등의 성장조건 변화를 통하여 조절 하였다.  $\text{TiO}_2$  nanorods 의 결정성과 표면형태를 관찰하기위해 XRD, SEM 그리고 TEM 을 이용하였으며, 광학적 특성을 관찰하기 위해서 UV-Vis 를 측정하였다. 합성된  $\text{TiO}_2$  nanorods 의 형태는 수직으로 성장된 단결정 구조의 rutile 상으로 관찰되었으며. 길이는 약 4 - 6  $\mu\text{m}$  로 관찰 되었다. 고온(200 °C)에서 짧은 시간동안

성장시킨 경우 가장 태양전지에 응용이 유용한 샘플로 성장되었다. 또한, 반응시간과 전구체의 양이 증가할수록  $\text{TiO}_2$  nanorods 의 밀도 또한 증가하였다.



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## Etching effect of AZO film for efficiency improvement of solar cell

정원석 부진효

성균관대 화학과

The etching of glasses in aqueous hydrofluoric acid (HF) solutions is applied in many technological fields. Particularly, the textured transparent conductive oxide (TCO) materials on the glass substrate etched by HF were used to improve the current density of solar cell. In this study, the textured glass substrate has been etched by solution and the Al doped ZnO (AZO) thin films have been prepared on this textured glass substrates by magnetron sputtering method. After the AZO film deposition the surface of AZO has been etched by hydrochloric acid (HCl). We observed morphology in AZO films by using different etchant concentration and etching time. Etched AZO thin films had a lower resistivity and higher haze. The etching rate of AZO film is proportional exponentially to pH value. Increases in the surface root-mean-square roughness of AZO films from 53.78 nm to 84.46 nm enhanced haze ratio in above 700 nm wavelength. The process could be applicable in texturing glass and etching AZO surface to fabricate solar cell in industrial scale.

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## Electron Transport Properties of $\pi$ Conjugated Organic Molecules on Si-Au Heteroelectrode

Pham Thu Hien 최진규 정현담

전남대 화학과

Electron transport through  $\pi$  conjugated molecules has been widely investigated with a simple device structure of molecular junction (metal-molecule-metal sandwich). For the molecular junction, Au has mostly used as the metal electrode due to good adhesion property with sulfur atom from the molecule. In this study, we introduce Si-Au heteroelectrode for the molecular junction with the modification of the nature of the interface by adding more Si electrode which directly connect to the molecule in the absence of sulfur atom. The electron transport properties were studied using nonequilibrium Greens' function/density functional theory (NEGF-DFT) formalism in ATK package. We expect that Si-Au Heteroelectrode is a promising candidate for simulations of electronic transport in nanoscale devices.

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## Electron Trapping and Transport Properties of 1-D and 3-D Quantum Well Polymers

최진균 Dao Duy Tung 이돈성 손흥래<sup>1</sup> 정현담

전남대 화학과 <sup>1</sup>조선대 화학과

Quantum well polymers (QWPs) are defined as polymers of QW electronic structures created by alternating molecular units of low and high HOMO-LUMO energy gaps in a polymer. The difference in HOMO-LUMO gaps may give an interesting QW electronic structure, in which the high HOMO-LUMO gap acts as the energy barrier. Recently, we introduce two kinds of QWPs: (1) 1-D QWPs; poly(tetraphenyl)silolesiloxane (PSS) and silole-neopentasilane (SNPS) hybrid, (2) 3-D QWP; C<sub>60</sub>-organosiloxane (C<sub>60</sub>OS) nanocomposite. Because the silole and the C<sub>60</sub> are well known to have low-lying LUMOs, the 1-D and 3-D QWPs are realized by alternating them with siloxane linkage of high energy gap. The electron trapping in the QWPs thin films was confirmed by the capacitance-voltage (C-V) measurements performed within the metal-insulator-semiconductor (MIS) device structure. The electron transport properties of the QWPs were studied by the combination of theoretical calculations using



Gaussian03 and ATK packages and current-voltage (I-V) measurements in metal-insulator-metal (MIM) device structure.



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## Silicon Quantum Dots with Conjugated Organic Shell

Mai Xuan Dung 정소희<sup>1</sup> 정현담

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Various silicon quantum dots (Si QD) terminated with different capping molecules including heptene (Hept), trimethylsilylacetylene (TMSAc), Phenylacetylene (PheAc), and Dimethylphenylsilylacetylene (MPSAc) were synthesized by post hydrosilylation the as-prepared hydrogen terminated Si QDs with the corresponding capping molecules. All of the Si QDs have diamond crystal structure, similar size distribution, and average size of about 1.75 nm. The quantum yields are in the range from 4 to 12% by comparison with 2-aminopyridine, which has standard quantum yield of 60%. The decay of photoluminescence (PL) can be fitted with two component exponential function  $I_t = A_1 \exp(-t/\tau_1) + A_2 \exp(-t/\tau_2)$  where  $\tau_1$ ,  $\tau_2$  are in the range from 1 to 6 ns. The rate of radiative and non-radiative decay pathways are about  $10^7$ - $10^8$  s<sup>-1</sup>, which are comparable with the transition rate in CdSe QDs. Interestingly, the optical gap of Si QD is decreasing in the order Hept-Si QD, TMSAc-Si QD, PheAc-Si QD, MPSAc-Si QD, from 3.45 eV to 3.32, 3.16 then 3.10 eV. From simple “particle in a box” model, the decrease in the optical gap

of Si QD can be attributed to the relaxation of exciton from the Si QD core into the capping layer shell induced by the reduction in potential height of the barrier.



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## Simultaneous Determination of Sibutramine, Phentermine and other weight loss substances in Weight loss functional foods

우현경

식품의약품안전청 첨단분석팀

A simple, specific, accurate and precise reverse-phase high performance liquid chromatographic method was developed and validated for simultaneous determination of sibutramine and other weight loss substances in weight loss functional foods. Chromatography was carried out on a Eclipse XDB C18 (Agilent, 4.6mm x 250mm, 5  $\mu$ m) Column with 0.5mM Sodium-1-hexane sulfonate in 0.1% phosphoric acid and 95% acetonitrile (90:10 v/v) at a flow rate of 1.0mL/min to gradient elution and UV detector was set at 210nm. A linear response was observed in the range of 2.5-25  $\mu$ g/ml ( $R^2=1.000$ ) for sibutramine and 2.5-25  $\mu$ g/ml ( $R^2=1.000$ ) for phentermin, respectively. The limit of detection (LOD) was observed in sibutramine 0.545  $\mu$ g/ml and phentermin 0.5185  $\mu$ g/ml in weight loss functional food sample.

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## Enzymatic Digestion of Single-DNA Molecules at Different Environment of Nanopores

이승아 강성호

경희대 응용화학과

The enzymatic digestion of individual DNA molecules in three dimensional controlled-environments was investigated at the single-molecule level. To trap individual lambda-DNA and enzyme molecules, the platform deposited gold within solid-state nanoporous polycarbonate membrane was used. The surfaces of deposited gold were modified with L-cysteine and mercaptoethanol to investigate the environment-dependent enzyme digestion of single DNA molecules. The enzyme digestion rates were found to increase as decreasing the diameter of nanopores. The digestion rates with the L-cysteine chemisorbed nanopores were 2.1-2.6 times faster than with the mercaptoethanol chemisorbed nanopores, even though these nanopores had equivalent interspacial areas. These results prove that the environmental factor as the chemical property of the surface in confined nanopores strongly affects the enzyme digestion rates.

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## Multi-Channel Microchip Electrophoresis for High-Efficient Analysis of GM-Rice

He Nan 강성호<sup>1</sup>

경희대 대학원 화학과 <sup>1</sup>경희대 응용화학과

A multi-channel microchip electrophoresis (MC-ME) system with a laser-induced fluorescence detector was developed for fast simultaneous detection of rice knockout mutants as a model of genetically modified (GM)-crop. Three parallel separation channels were fabricated on a glass microchip to investigate the possibility of high-throughput screening at the same time. The MC-ME system simultaneously analyzed amplified-PCR products representing wild type rice and mutants on all channels using an expanded laser beam, a band-pass filter, specific designed electrodes, and a charged couple device camera. Under a programmed electric field strength and a sieving gel matrix of 0.7% poly(ethyleneoxide) ( $M_r = 8\,000\,000$ ), the T-DNA inserted rice mutagenesis as well as two standard wild type rice and six rice knockout mutants were analyzed within 4 min at three parallel channels on the microchip. Comparing to conventional single-channel microchip electrophoresis, the MC-ME method provided a valid practical way to effectively analyze multiple samples in parallel for the identification of

GM-rice without any loss of resolving power and reproducibility. The MC-ME method was also more than 15 times faster than a traditional slab gel electrophoresis. It proved the feasibility of MC-ME system as a powerful tool for high-throughput screening of GM-rice with high sensitivity, efficiency and reproducibility.



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## Postsource Decay of Peptide Ions Produced by Laser Desorption/Ionization on Amorphous Si Surfaces

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융합연구단

We investigated the thermal mechanism involved in laser desorption/ionization (LDI) of thermally labile molecules from the flat surfaces of amorphous Si (a-Si) and crystalline Si (c-Si). a-Si was chosen for this study because due to its thermal property, particularly its low thermal conductivity, it was predicted to be highly susceptible to laser-induced surface heating. By virtue of lack of surface nanostructures, the flat surfaces offer a simple model system to focus on the thermal mechanism, avoiding other effects including possible non-thermal contributions that can arise from the physical existence of surface nanostructures. For the energetics study, the internal energies of substituted benzylpyridinium ions produced by LDI on the bare and coated surfaces of a-Si and c-Si were obtained using the survival yield method. The results including LDI thresholds, ion yields, and internal energies all suggested that the LDI mechanism would be indeed thermal, which is most likely promoted by thermal desorption caused by laser-induced surface



heating. In addition, the LDI process driven by laser-induced thermal desorption (LITD) was also found to be capable of depositing an excessive internal energy in resulting LDI ions, giving rise to a metastable dissociation. It exhibited the essentially same features as in postsource decay (PSD) caused by MALDI using CHCA matrix. Thereby, we report that the LDI process by LITD offers not only a way of intact ionization but also a facile means for PSD of peptide ions, which this work demonstrates well suited to peptide sequencing using TOF/TOF mass spectrometry.



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## Path trace contamination through the tracking of phosphate dissolved in freshwater

조보배 조원제 유국현

동국대 화학과

Nonpoint source is extensive regional pollutants on collective called the words, agricultural, urban, forest, mining, etc. that occur fertilizer, hybriicides, pesticides, chemicals, various pollutants, including, from air pollution, sedimentation, too, nonpoint source pollution as can contain. Nonpoint source pollution in watersheds that occurs, but the emissions from the source to reach the final outflow point for many of the physical, chemical and biological mechanisms are exposed to certain pollutants is difficult to grasp for. Water management should be considered urgently, especially in terms of causal pathogens of pollutants that may be. If phosphorous is the isotope analysis not because it is one kind of phosphorous combines with oxygen isotope ratios depending on the region using two different points in the form of phosphorous  $\text{Ag}_3\text{PO}_4$  ammonium phosphate and the final processing of this heat and Carbon in the  $\text{CO}_2$  or CO as Mass spectroscopy analysis to change is

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## Investigation of SERS Spectra Features under Localized Electric Field

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Novel SERS measurement by molecular dynamics modulation with surface localized electric field has been investigated. Applied localized electric field gives an influence on molecular dynamics of target molecules, resulting in control of Raman activities. This leads to enhance the resolution of SERS analysis and make it possible to distinguish target molecules in mixture into the individuals by virtue of a different degree of changes in molecular dynamics under the same electric field. In this study, anodic aluminum oxide (AAO) templates fabricated by an electrochemical anodizing process have been modified to modulate the surface localized electric field. An additional gold layer acting as an electrode (the other electrode is an aluminum itself) and a SERS active layer was deposited on AAO templates with keeping intact the open pore structure, and target molecules were dispersed. Subsequently, Raman measurement has been conducted with applying external voltages on the electrode of AAO templates. With increasing the external applied voltage, the surface localized electric field changes from 0 V/m to ~107V/m.

Consequently, applied localized electric field on SERS active AAO substrate would be a developed SERS analysis method that can be applied for the multi-detection in diverse analytical fields.



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## **Effect of Ionization Modifiers on the Simultaneous Analysis of All Classes of Phospholipids by Nanoflow Liquid Chromatography/Tandem Mass Spectrometry in Negative Ion Mode**

**방대영 문명희**

연세대 화학과

In this study, the effect of modifier added to mobile phase solutions of nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS3) on the simultaneous analysis of all phospholipid (PL) classes at negative ion mode has been investigated. 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 mixture of 0.05% ammonium hydroxide and 1 mM ammonium formate added to the mobile phase provided effective ionization for all classes of PLs.

The optimized conditions were applied to 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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## **Top-down approach for protein study by using an on-line chip-type flow field-flow fractionation/ESI-MS-MS**

**김기훈 문명희**

연세대 화학과

A chip-type design asymmetrical flow field-flow fractionation (AF4) channel has been developed for high speed separation of proteins and top-down proteomic analysis using on-line coupled electrospray ionization mass spectrometry (ESI-MS). The new miniaturized AF4 channel was assembled by stacking multilayer thin stainless steel (SS, 1.5 mm each) plates embedded with an SS frit in such a way that the total thickness of the channel assembly was about 6 mm. The use of aqueous MS-compatible buffer and desalting and purification of proteins achieved during the AF4 operation by the action of a crossflow were advantageous for on-line coupling of the chip-type AF4 with ESI-MS. Its analysis of proteins exhibited an increased signal to noise ratio compared to that of direct ESI-MS analysis. The capability of on-line coupling of AF4 and ESI-MS was demonstrated for the high speed separation and identification of carbonic anhydrase (29 kDa) and transferrin (78 kDa) by full scan MS and for the first top-down identification of proteins with AF4-ESI-MS-MS using collision induced dissociation (CID). The presence

of intact dimers (156 kDa) of transferrin was confirmed with the determination of molar mass by AF4-ESI-MS via size separation of transferrin dimers from their monomers.





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## Qualitative Analysis of the Oxidized Phospholipids in Human Lipoprotein by Nanoflow LC-ESI-MS-MS

이주용 문명희

연세대 화학과

Low-density lipoprotein (LDL), responsible for transporting fats from liver to other parts of the body via blood vessel, is known as a major biomarker of coronary artery disease (CAD). Many studies have proven that the size and lipid composition of LDLs in CAD patients differ from those of healthy normal people. Metalloprotein hemoglobins (Met-hemoglobin) are the transformed type of normal hemoglobin when the charge of an iron ion changes from +2 to +3. They promote a production of oxidized LDL by changing intact properties of phospholipids (PL) and apolipoprotein. According to the studies that have been published in the past decade, the existence of oxidized LDLs is more critically associated with CAD than any other factors due to their lack of ability to carry out an important role of digesting macrophages. This leads to inflammation in arteries, which risks a development of CAD. In this study, collision induced dissociation (CID) patterns obtained from nanoflow LC-ESI-MS-MS of the oxidized phospholipids were analyzed to investigate the standard oxidized LDL. The standard phospholipids and LDLs used in this

study were artificially oxidized by using 10 mM of CuSO<sub>4</sub> in PBS buffer. A comparative analysis of PLs from the oxidized LDLs in CAD patients and normal people was carried out.



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## Discovery of Biomarkers of Coronary Artery Disease by Flow Field- Flow Fractionation and Nanoflow LC-ESI-MS-MS

변슬기 이주용 문명희

연세대 화학과

Phospholipids (PL) and lysophospholipids (LPL) have been reportedly manifested as biomarkers of human diseases in numerous studies recently. Among various cardiovascular diseases, coronary artery disease (CAD) is one of the most common diseases and also results significantly high number of deaths annually around the world. Regarding the fact that high accumulation of low-density lipoprotein (LDL) particles, which are as known as bad cholesterol, is one of the main risk factors of developing cardiovascular diseases such as CAD, a closer examination at PL and LPL profiling of high-density lipoprotein (HDL) and LDL is necessary to discover biomarkers of CAD. In this study, HDL and LDL from human plasma were separated according to the particle size by multiplexed hollow fiber flow field-flow fractionation (MxF5), a separation technique that eluted particles in order of size, smallest to largest. Intact PLs and LPLs were extracted from HDL and LDL using a modified lipid extraction with methyl-tert-butyl ether and methanol. Followed by comprehensive qualitative analyses of PLs and LPLs from

CAD patients and control using nanoflow liquid chromatography electrospray ionization-tandem mass spectroscopy (nLC-ESI-MS-MS), further analyses were performed to investigate the identified PLs and LPLs quantitatively.



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## A Software Tool for Automated Structural Characterization of Glycerophospholipids Using Raw Mass Spectra from nLC-ESI-MS-MS

임상수 이주용 변슬기<sup>1</sup> 문명희

연세대 화학과 <sup>1</sup>연세대 화학

Lipidomics is drawing a great attention with the development of mass spectrometry-related techniques. However, conventional analysis of CID spectra of lipid classes is manually processed and severely laborious. Although various sophisticated algorithms are currently used in proteomics field for facile comprehension of raw mass spectra, programmed analysis of mass spectra of lipidomes has a lot to be developed. A structural analysis tool (LiPilot) for the identification of phospholipids (PLs) including lysophospholipids (LPLs) and cardiolipins (CLs) from mass spectra is introduced. This algorithm utilize raw mass spectra generated 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 generated from data-dependent, collision-induced dissociation(CID). In addition, library files addressing the typical fragmentation patterns of PLs from an LTQ-Velos ion trap mass spectrometer to characterize PL or LPL molecular species by comparing the experimental fragment

ions with theoretical fragment ions in the library file were implemented. Identification is processed by the calculation of a confidence score newly developed in our laboratory to maximize identification efficiency which encloses 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. The software 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 and 3 CLs.



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**Dual Lectin/Size Based Enrichment Strategy for Targeted N-linked  
Glycopeptides Using Asymmetrical Flow Field-Flow  
Fractionation: Applications to Profiling of Lung Cancer Biomarkers**

**김진용 문명희**

연세대 화학과

N-linked glycosylation, one of the most common post-translational modifications (PTMs) in protein synthesis, has been widely studied because of its crucial roles in many physiological functions and biological pathways such as protein folding, cell-cell interaction, cell signaling, cell recognition, and cell proliferation. Recently, it is reported that an erroneous glycosylation of proteins is related to various type of diseases including neurodegenerative diseases, immune deficiencies, and cancers. In spite of the importance of characterizing glycoproteins as a latent biomarker, there are some limitations when analyzing glycoproteins from complicated biological samples, such as blood serum, urine, tissue, and vesicles, since the amount of glycoproteins is as low as 2 ~ 5% of total amount of proteins. Therefore, the enrichment of glyco-proteins/-peptides is an essential step for glycoproteomics. In this study, a new lectin-based enrichment method for glycopeptides using dual lectins (WGA and SNA) was developed by

using asymmetrical flow field-flow fractionation (AF4), which is a size-separation technique. Application was made to human blood serum to determine relative regulation of targeted glycopeptides between lung cancer patients and healthy controls.. A mixture of two lectins was mixed with serum peptides and they were separated by AF4. Glycopeptides bound to each specific lectin were collected by AF4 and treated with PNGase F in order to characterize the deglycosylated peptides using nanoflow liquid chromatography-tandem mass spectrometry.





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**Clindamycin phosphate-coated zirconia monolith as the chiral  
stationary phase for capillary electrochromatographic  
enantioseparation**

**김은주 박진명 박정학**

영남대 화학과

Clindamycin phosphate (CMP)-coated zirconia monolith (ZM) was used as the chiral stationary phase (CSP) in capillary electrochromatography (CEC) for separation of a set of six chiral compounds. Retention and chiral selectivity were measured in mobile phases of varying composition of ammonium acetate and methanol. CMP-ZM provided good enantioseparations for the six compounds studied. Optimum mobile phase composition was found to be 10 mM ammonium acetate and 35 v% methanol.

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## Analysis of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) by direct infusion electrospray ionization-mass spectrometry (ESI-MS)

박세환 고성석<sup>1</sup> 이성만<sup>1</sup> 고은미<sup>2</sup> 조수경<sup>2</sup> 김정권

충남대 화학과 <sup>1</sup>(주)센서테크 연구소 <sup>2</sup>국방과학연구소 국방신기술센터

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) is one of the most widely used explosives. In this study, we investigate HMX in negative ion mode using electrospray ionization-mass spectrometry (ESI-MS), where HMX was directly infused into a ESI-MS system. The HMX stock sample was prepared in a concentration of 1 mg/mL in acetonitrile (ACN). Then, the HMX stock sample was diluted in ACN (100-fold dilution) prior to the analysis. Direct infusion of the diluted HMX sample provided an adduct ion of  $\text{HMX} + \text{HCOO}^-$  where  $\text{HCOOH}$  is believed to be originated from the decomposition of HMX. In positive ion mode, no HMX signal was observed in the current direct infusion ESI-MS analysis. The HMX samples spiked with acetic acid or benzoic acid were also analyzed, which provide an adduct ion of  $\text{HMX} + \text{CH}_3\text{COO}^-$  ( $m/z$  355) or  $\text{HMX} + \text{C}_6\text{H}_5\text{COO}^-$  ( $m/z$  417). Analysis of HMX spiked with ammonium acetate also generated an adduct ion of  $\text{HMX} + \text{CH}_3\text{COO}^-$  ( $m/z$  355). The detailed experimental procedures and results will be provided during the presentation.

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## **Sensitive Arsenic Analysis by Carrier-Mediated Counter Transport Single Drop Microextraction Coupled with Capillary Electrophoresis**

성인혜 정두수

서울대 화학부

A sensitive analytical technique for arsenic compounds based on single drop microextraction (SDME) coupled in-line with capillary electrophoresis (CE) was developed. In SDME, a drop of an acceptor phase covered with an organic layer is hung at the inlet tip of a separation capillary. By pH adjustment, analytes in the neutral form in an aqueous donor phase are first extracted into the organic layer, and then back-extracted into the acceptor phase. However, the hydrophilic nature of the arsenic compounds, hampering the first extraction into the organic layer, lowers or even eradicates the efficiency of SDME. This problem can be solved by employing the scheme of carrier-mediated counter transport using  $\text{CH}_3(\text{C}_8\text{H}_{17})_3\text{N}^+\text{Cl}^-$  (Aliquat 336) as a carrier in the organic layer. Aliquat 336 enhances the transport of the arsenic compounds across the organic layer by forming hydrophobic complexes. The arsenic enrichment is driven by the concentration gradient of hydroxide or chloride ion in counter with the arsenic extraction from the donor phase of low hydroxide or chloride concentration to the acceptor phase of high concentration of

hydroxide or chloride. The gradient of hydroxide concentration yielded high enrichment factors for arsenic compounds including As(III) which could not be extracted with the gradient of chloride only. After extraction, a portion of the enriched acceptor drop is injected and the arsenic compounds are separated by CE. Thus the whole procedures of SDME and CE can be performed in an in-line mode using a commercial CE instrument. Using the acceptor phase of pH 13, the enrichment factors obtained for a sample in unbuffered water with 15 min extraction were 120, 250, 730, and 930 for As(III), dimethylarsinic acid (DMA), monomethylarsonic acid (MMA), and As(V), respectively. The limits of detection ( $S/N = 3$ ) with absorbance detection at 200 nm were 0.3, 0.5, 0.2, and 0.2  $\mu\text{M}$  for As(III), DMA, MMA, and As(V), respectively.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Resolution of the Tocainide and Their Analogues on Crown Chiral Stationary Phase

김상준 진형아 현명호

부산대 화학과

Enantiomer separation is considered as a most attractive research area in both institution and industry. Especially, the separation of chiral drugs consisting of two enantiomers has been considered as most important one, because each enantiomer shows different pharmacological activity in living systems. Recently, the enantiomers of the chiral drugs were efficiently resolved by using chiral stationary phases (CSPs) in high performance liquid chromatography systems. In our laboratory, recently, we developed (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid based CSP containing thiol ester linkage. The new CSP was found to show very good chiral recognition efficiency for the enantiomers of various racemic primary amino compounds than the CSPs containing amide linkage. In other hand, tocainide is known to be one of the effective antiarrhythmic drugs, and R-form of the tocainide drug gives better medicinal effect than S-form. In this study, we applied the new CSP to the resolution of tocainide and their analogues. The resolution was found to be dependent on the composition of aqueous mobile phase.

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## 페놀의 실시간 검출을 위한 나노바이오융합형 SPR 센서

김엄지 이해진

경북대 화학과

본 포스터에서는 미량의 노출 및 유입만으로도 극심한 생태계 및 인명 피해를 줄 수 있어 연속적으로 신속하게 측정할 수 있는 분석 기술들이 요구되는 페놀을 검출하는데 있어 신속성, 실시간 검출 및 시료의 사전처리를 필요로 하지 않는 새로운 페놀 맞춤형의 고감도 나노융합형 SPR 바이오센서 기술 개발에 관해 발표하고자 한다. 이를 위해 우리는 실시간 분석이 가능한 Surface Plasmon Resonance (SPR)에 바이오기능성을 도입한 금 나노파티클을 융합한 표면센드위치 검출방식을 도입하여 고감도로 페놀을 검출하려 하였다. 먼저 SPR 금 박막 칩은 Prolinker B 를 이용하여 아민기 말단의 페놀 항체(UGT1A6 monoclonal antibody)를 공유 결합시켜 페놀 맞춤형의 항체칩을 만들었다. 제작한 페놀항체칩 위에 페놀을 먼저 흘려준 다음, 페놀과 선택적으로 결합하는 또 다른 페놀 항체(UGT1A6 rabbit polyclonal antibody)로 코팅한 약 50 nm 지름의 다각형 모양의 금 나노파티클(Au NP)을 흘려줌으로써

Anti-phenol/phenol/Anti-phenol-Au NP 샌드위치 복합체를 형성함을 통해 SPR 신호를 증폭시켜 미량의 페놀 농도 검출을 시도하였다.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Biofunctionalized quasi-spherical gold nanoparticles for electrochemical sandwich detection of protein biomarker

장혜리 이해진

경북대 화학과

본 포스터 발표에서는 고감도 및 고선택적으로 단백질 바이오마커 검출을 위한 새로운 전류법 기반의 나노바이오융합형 샌드위치 분석법을 개발하고자 하였다. 모델 단백질로 적어도 두 개 이상의 서로 다른 리간드들의 결합사이트를 갖는 트롬빈(thrombin, Th)을 모델 단백질 바이오마커로 선택하여 이를 좀 더 고감도로 검출할 수 있도록 표면에 샌드위치 복합체를 형성하여 전기화학적으로 검출하는 방안을 고안하였다. 이를 위해 먼저 트롬빈 앵타머(Th-aptamer)로 코팅한 다각형의 금나노입자(NP)를 전극에 고정하였고 이에 타겟인 트롬빈 단백질을 흘려주고 alkaline phosphate(ALP)와 결합된 트롬빈 항체(ALP-anti-Th-NPs)를 흘려주어 특이적으로 전극 표면에 Th-aptamer/Th/ALP-anti-Th-NPs 샌드위치 복합체를 형성한 후 위 전극을 4-aminophenylphosphate 기질과 반응시켰다. 위 반응 결과 APP 가 ALP 에 의해 산화되어 두 개의 전자를 내놓게 되고 이를 순환전류법과 시차펄스전류법을 이용하여 검출한 결과에 대해 논의하였다.



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## Highly Sensitive SERS-based Immunoassay on a Disk Chip Using Hollow Gold Nanospheres

전향아 이상엽<sup>1</sup> 주재범<sup>1</sup>

한양대 바이오테크놀로지학과 <sup>1</sup>한양대 생명나노공학과

A highly sensitive surface-enhanced Raman scattering (SERS)-based immunoassay technique, using hollow gold nanospheres (HGNs) and glass beads, has been developed for sensitive blood analysis. Innovative laser irradiated ferro-wax microvalves and centrifugal microfluidic flow techniques have been utilized for effective suspension of glass beads, and the SERS detection has been used for highly sensitive immune-sensing of target biomarkers on the disc. Here, glass beads and HGNs were used as supporting substrates and SERS probes, respectively, for the formation of the immunocomplex. All the necessary reagents are preloaded on the disc and total processes, including the plasma separation, incubation with target specific antigen- or antibody-coated microbeads, multiple steps of washing, probe reactions with substrates and indirect Raman detection, could be finished within 30 minutes. Three well-known cardiac markers, troponin I, myoglobin and creatine kinase-myoglobin (CK-MB) have been used as target markers for the validation of simultaneous SERS-based multiplex immunoassay. This SERS-based

optofluidic immunoassay on a disk chip is expected to be a powerful clinical tool for early diagnosis of cardiac disease.



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## Investigation of Chiral Self-Recognition of 3,5-Dinitrobenzoylleucine Derivatives

이원재 황호

조선대 약학대학

We have investigated the separation of the enantiomers of N-DNB leucine ester and amide derivatives on two  $\pi$ -acidic CSPs and described a proposed chiral recognition mechanism between  $\pi$ -acidic DNB leucine derivatives and  $\pi$ -acidic DNB leucine derived CSP as well as enantioselective chiral self-recognition. For systematic studies on the resolution of DNB leucine derivatives on DNB leucine derived CSPs, we performed the separation of enantiomers of  $\pi$ -acidic DNB leucine as esters and amides on CSPs 1 and 2 derived from  $\pi$ -acidic (S)-DNB N-propylamide and N,N'-dipropylamide, respectively. From the chromatographic results, it is proposed that the carboxamide oxygen of the CSP interacts with DNB N-H of the analyte for a hydrogen bonding interaction. Also it is proposed that the C-terminal carbonyl oxygen of the analyte is associated with DNB N-H of the CSP for another hydrogen bonding interaction. Interestingly, by chiral-self recognition, (L)-DNB leucine N,N'-diethyl amide behaves like the corresponding dimer. In terms of chiral recognition rationale, all chromatographic and X-ray structure

data show consistently not only dual intermolecular hydrogen bonding interactions with a  $\pi$ - $\pi$  interaction between  $\pi$ -acidic DNB groups but also the chiral self-recognition of DNB leucine amide.



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## Electrochemically Inducible Surfaces for Patterning Distinct Biomolecules

최인성 여운석

건국대 생명공학과

Stimuli-responsive surfaces that change their properties upon external stimuli have been actively harnessed for various applications such as basic cell studies, biochips, sensors, and arrays of biomolecules. Another important research theme in these applications is a development of selective surface modification methods for the patterning in microscale. In practice, several multicomponent patterning strategies have been reported, including e-beam lithography, UV-photopatterning, and dip-pen nanolithography. In this poster, we report on a new patterning method based on electrochemically induced surface reactions on bifunctional self-assembled monolayers (SAMs) on gold. The gold chip was modified with the two electrical inducible molecules which can be activated by different electrical potentials. The resulting functional groups, amine and alkyne, then play a role of chemical handles to introduce biomolecules by way of bioorthogonal chemistries. We verified our strategy using cyclic voltammetry (CV), X-ray photoelectron spectroscopy (XPS), fluorescence and selective cell adhesion.

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## Detection of BCR/ABL Chimeric Protein Using Biochips and MALDI-TOF MS

홍설혜 여운석

건국대 생명공학과

Chronic myelogenous leukemia (CML) is a myeloproliferative disease, arising from translocation between chromosome 9 and 22 known as Philadelphia Chromosome. This translocation leads to a juxtaposition resulting in a BCR-ABL fusion gene that codes for BCR-ABL transcripts and fusion proteins with abnormal tyrosine kinase activity. Therefore, The BCR/ABL fusion protein acts as a biomarker for diagnosis of CML; however, only few efficient methods have been reported for the detection of BCR-ABL in protein level. In this poster, we present a new detection method of BCR-ABL chimeric protein in cell lysates using hollow gold nanoparticles (HGNs) and a biochip. The BCR-ABL chimeric protein was captured by two antibodies, anti-BCR on HGNs and anti-ABL on a biochip, through a sandwich assay format. The presence of BCR-ABL in cell lysates was then verified by MALDI-TOF MS signals of small molecules, called Am-tag, which existed in large excess on HGNs and therefore,

played a role for amplifying the biological events. Our strategy clearly observed BCR-ABL chimeric protein in cells and, as a further study, will be applied to real samples for the diagnosis of CML.



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## Combination of Mass Signal Amplification and Isotope Labeled Alkanethiols for the Multiplexed Detection of miRNAs

강현욱 홍설혜 여운석

건국대 생명공학과

In this poster, we extended our ultrasensitive detection strategy which combines self-assembled monolayers (SAMs) on gold and laser desorption/ionization time of flight mass spectrometry (LDI-TOF MS) for the multiplexed miRNAs without the need of PCR or a labeling. In our strategy, gold nanoparticles (AuNPs) were decorated with a large number of small molecules (Am-tag) and a probe oligonucleotide, and the gold chip was prepared to contain another probe oligonucleotide. The target miRNA was captured by the immobilized probe oligonucleotides on the AuNPs and the gold chip with sandwich assay format. The presence of miRNAs was then verified by amplified LDI-TOF MS signals of Am-tag on AuNPs. For the multiplexed detection, we designed and synthesized four Am-tag molecules containing 0, 4, 8, 12 isotopes so that they have same molecular properties but different molecular weights. As a model case, we tested four miRNAs, mir-365, mir-142-3p, mir-1207-3p, and let-7c. miRNAs in samples were easily discriminated by observing different Am-tag signals at  $m/z$  553, 561, 569



and 577, and the relative amounts of miRNAs were quantified. We believe that this strategy will provide a biological important tool for accurate, sensitive, rapid, and low-cost multiplexed detection of miRNAs.



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## Development of SERS-based aptasensor for Thrombin Detection Using Magnetic Beads and Gold Nanoparticles

윤지연 박세휘<sup>1</sup> 주재범<sup>2</sup>

한양대 바이오테크놀로지학과<sup>1</sup> 한양대 바이오나노공학과<sup>2</sup> 한양대 생명나노공학과

Aptamers, single-stranded DNAs or RNA sequences, have increasingly become important tools for medical diagnostics. They can bind specifically to their target molecules of interest with high affinities and specificities. A variety of aptamer-based immunoassay methods for the biomolecules detection have been studied in these days. Among these, thrombin has been known as an important target for the early diagnosis of thrombotic disease such as cardiac infarction or pulmonary embolism. In this presentation, we report the application of SERS-based aptasensor, using magnetic beads and gold nanoparticles, for a highly sensitive detection of thrombin. Two thrombin-binding aptamers, TBA<sub>15</sub> and TBA<sub>29</sub>, interact with different epitopes in the thrombin molecule, respectively. Here, magnetic beads and gold nanoparticles are capturing substrates and sensing probes, respectively. Using this SERS-based immunoassay technique, a highly sensitive immunoanalysis of thrombin could be possible. This new conceptional method shows a strong potential for the clinical diagnosis of a diagnosis.

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## Highly sensitive detection of multiple proteins using surface-enhanced Raman spectroscopy coupled with gold-patterned microarray chip

김인설 주재범<sup>1</sup>

한양대 바이오테크놀로지와 <sup>1</sup>한양대 생명나노공학과

We report a highly sensitive immunoassay using surface-enhanced Raman scattering (SERS) platform. For this purpose, a gold-patterned microarray chip has been fabricated and used as a SERS detection template. Here, a typical sandwich immunocomplex protocol has been adopted. Polyclonal antibodies are immobilized on gold patterned substrates, and then antigen solutions and certain Raman reporter-labeled hollow gold nanospheres (HGNs) are sequentially added for the formation of sandwich immunocomplexes. Antigen biomarkers can be quantitatively assayed by monitoring the intensity change of a characteristic SERS peak of a reporter molecule. Under optimized assay conditions, the limit of detections (LODs) were determined to be 10fg/mL for human IgG and 100fg/mL for rabbit IgG, respectively. This SERS-based immunoassay technique fulfills the current needs of high sensitivity and selectivity which are essential for the clinical diagnosis of a disease.

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## Home-built Solid-state NMR Probe with Specialized Coil

최성섭 정지호 박유근 김용애

한국외국어대 화학과

Analysis of membrane protein using solid-state NMR on lipid bilayer or bicelle samples, membrane-like environment, is valuable for these with a predominantly helical secondary structure. Most of biological lipid samples have high dielectric property due to containing large amounts of water and salts. This electrical property cause a loss of probe efficiency from severely reducing the probe Q-factor and significantly shifting the tuned frequency down. For these reasons, a specific probe with high efficiency and high capability is required to study these biological samples by using solid-state NMR, and several probe designs have been developed in a recent research to improve the probe efficiency. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil to prevent heating by high RF power. This probe provides short pulses, high power capability, and good RF homogeneity. 1H-15N 2D SAMMY spectra from a single crystal and membrane proteins in oriented phospholipid bicelles was successfully obtained by using this

home-built solid-state NMR probe. Inspired by the natural and technical similarities between membrane proteins in lipid bilayers and liquid crystals in Liquid Crystalline Display (LCD) panels, we employed solid-state NMR methodologies originally developed for the study of membrane proteins in lipid bilayers for the in-situ analysis of LCD panels. Thus, we also present a home-built 500 MHz narrow bore (NB)  $^{19}\text{F}$ - $^{13}\text{C}$  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.



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## Covalent protein immobilization with parylene-H film for MALDI-TOF mass spectroscopy

김조일 고희 변재철

연세대 신소재공학과

MALDI-TOF mass spectroscopy has been used for the analysis of receptor-ligand interactions. The receptor-ligand interaction has been analyzed by the following steps: immobilization of receptor proteins, binding of ligand molecules, and analysis with MALDI-TOF mass spectroscopy (MS). For this study, the parylene-H, which is a modified polymer of para-xylene to have formyl groups on the surface, was used as a receptor binding surface. In order to apply parylene-H film for the immobilization of receptor proteins, the parylene-H was thermally deposited on the target plate to be less than 50 nm thick by microprocessor controlled parylene coater. The thickness and the roughness of parylene-H film were determined by the AFM, and the rms deviation of the surface roughness was estimated to be  $\pm 2$  nm within the area of  $5 \times 5 \mu\text{m}^2$ . In order to analyze the receptor-ligand interaction, streptavidin and biotinylated CCP were used as a receptor protein and ligand molecule, respectively. As the first step, streptavidin was immobilized to the parylene-H film by dipping the parylene-H coated target plate to the

streptavidin solution, and then analyzed by MALDI-TOF MS. From the results, no significant mass peak was found at the mass spectrum, because streptavidin was covalently immobilized to parylene-H film by forming imine bond. As the second step, the ligand molecule, biotinylated CCP in this study, was treated to the immobilized receptor proteins on the target plate. The target plate with covalently immobilized streptavidin resulted in the far higher mass signal of biotinylated CCP than physically adsorbed streptavidin target plate. These results show that the parylene-H film is feasible for the analysis of receptor-ligand interaction with MALDI-TOF MS.



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## Identification of Volatile Components from Wine using Needle Trap Device and GC/MS



Analyzing volatile components is important in many different fields such as food, perfume and environment. Particularly, identifying fragrances from flowers could be used to develop perfume and cosmetic products. Analyzing odor and aroma of wine could be used simply to evaluate the wine's quality as well as to find out the orange of the wine. There is a need to develop an easy and fast way to sample volatile components to avoid loss or potential change of fractions of released odors and aromas, and to reduce the number of volatiles under scope for some reasons. We used a needle trap device packed with DVB particles to sample and analyze volatile components from flowers and red wine. Simple sample transfer technique by internally expanded desorptive flow was used to transfer volatile components trapped on the DVB sorbent particles packed needle trap device into a separation column of a GC. Identification was carried out based on MS library and the linear temperature programmed retention index (LTPRI). ~20 volatile components were tentatively identified using NTD-GCMS.



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**Top-down synthesized TiO<sub>2</sub> nanowire assisted laser  
desorption/ionization mass spectrometry for quantitative analysis of  
small molecules**

**김조일 변재철**

연세대 신소재공학과

In the previous work, we reported semiconductor nanowires synthesized by VLS mechanism could be applied for matrix-free laser desorption/ionization ? time of flight analysis called nanowire-assisted laser desorption/ionization mass spectroscopy (NALDI-MS). By using this method, the quantitative analysis of small molecule could be achieved without adding organic matrix molecules. In order to apply TiO<sub>2</sub> nanowires to NALDI-TOF MS, the nanowires were synthesized by mild hydrothermal process directly on the surface of Ti plate. For this study, the sample target plate was patterned to have 81 TiO<sub>2</sub> nanowire zones on the surface. The morphology of the synthesized TiO<sub>2</sub> nanowires were observed to be a diameter of 30 nm by SEM, and the crystal structure was determined to be a mixture of anatase and rutile phases by XRD. The feasibility of applying the synthesized TiO<sub>2</sub> nanowires to NALDI-TOF MS was tested by the quantitative analysis of bradykinin fragments 1-7 and P<sub>14</sub>R synthetic peptide. Mass spectrometric

analyses of the compounds mainly showed  $[M+H]^+$  and  $[M+K]^+$  ion peaks by using  $\text{TiO}_2$  nanowires, and the sums of the two peaks was considered to be signals for the quantitative analysis. The summed signals from bradykinin fragments 1-7 were exponentially increased with a correlation coefficient of 0.997 in a concentration range of 5 ? 100 nmol/mL. Similarly, P<sub>14</sub>R synthetic peptide showed exponentially increased signals in the same concentration range. The results show that the synthetic  $\text{TiO}_2$  nanowires could be applied to laser desorption/ionization MS, and the quantitative analysis of small compounds by using top-down synthesized  $\text{TiO}_2$  nanowires were feasible.



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## **New interfacial platform for the electrochemical immunoassay based on pyridine-functionalized redox probe at the modified NiNPs/ ITO electrodes**

**이금옥 김남혁<sup>1</sup> 최영봉<sup>2</sup> 김혁한<sup>2</sup>**

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A novel interfacial platform for the electrochemical immunoassay based on the pyridine-functionalized osmium (Os) redox probe at the nickel nanoparticles (NiNPs) modified indium-tin oxide (ITO) electrode is presented for the detection of urinary hippuric acid (HA). This is the first report on the use of pyridine moieties to immobilize strongly on nickel nanoparticles (NiNPs) modified indium-tin oxide (ITO) electrode. As an electrochemical redox probe, [Os(4,4'-dimethoxy-2,2'-bipyridine)<sub>2</sub>(4-aminomethylpyridine-HA)(4,4'-bipyridine)]<sup>2+/3+</sup> (Os-HA-Bpy) was successfully synthesized and immobilized onto the nickelnanoparticles (NINPs) midified ITO electrodes. The interaction between Os-HA-Bpy conjugate antigens and antibody-HA (anti-HA) was performed by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The most stable configuration for pyridine on the Ni-edge surface is the end-on adsorption through Ni<sup>2+</sup>-N bonding. Electrocatalytic oxidation of hippuric acid on the

surface of the modified electrode were investigated with cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques. The redox currents of osmium complexes were linearly proportional to urinary HA in the range of 0.1 ~ 5.0 mg/mL, which is sufficient for use as an immunosensor using a cutoff concentration of 2.0 mg/mL in urine samples. The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.



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## Attachment of Osmium-hippuric acid conjugate on carbon nanotubes: Synthesis, characterization and electrochemical immunoassay

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The successful attachment of Osmium-hippuric acid conjugate to carbon nanotubes through a simple, one-step procedure is reported. Amine-functionalized osmium-hippuric acid (Os-HA) can be covalently linked to the carboxylic acid-modified carbon nanotubes. Hippuric acid (HA), the target small organic molecule of this study, is a major urinary metabolite in toluene-exposed humans with a molecular weight of 180 Da. Toluene is readily available, and widely used for chemical synthesis, paints, thinners, detergents, adhesives, and as a main solvent in petroleum industries. The interaction between CNT-Os-HA conjugate antigens and antibody-HA (anti-HA) was performed by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). As this assay relies on the relative affinity of the HA antibody for the electrode surface bound CNT-Os-HA relative to the affinity for the target analyte (HA) in solution. The redox currents of osmium complexes were linearly proportional to urinary HA in the range of 0.01 ~ 5.0 mg/mL, which is sufficient for use as an immunosensor using a cutoff concentration of 2.0 mg/mL in

urine samples. The proposed electrochemical method can be extended to the applications to detect a wide range of different small antigens in the health care area.



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## **Biocompatible nanoparticles doped polydopamine film: electrochemical aptamer based competitive thrombin detection**

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분석과학기술과

A gold nanoparticles-encapsulated poly-dopamine (AuNP-PD) film-based electrochemical thrombin aptamer sensor has been fabricated for the competitive detection of thrombin (TB). The TB aptamer sensor is fabricated by immobilizing a thiolated TB binding aptamer onto the AuNPs-PD film. The poly-dopamine/AuNPs surface was characterized using AFM, SEM, XPS, and electrochemical impedance techniques. The electrochemical activity of the poly-dopamine/AuNPs film was studied using cyclic and square wave voltammetry techniques. The thrombin detection is based on the competition binding between methylene blue-labeled thrombin and free thrombin. Square wave voltammetric (SWV) responses before and after competition between free and labeled-thrombin suggested that thrombin can be successfully detected with the biocompatible AuNP-PD platform.

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## 조선시대 회곽묘 출토 미라 조직의 안정동위원소 분석으로 생애 주기에 따른 식생활 변화 추적

강다영 신지영

국립문화재연구소 보존과학연구실

우리가 섭취한 음식은 옛날 사람들이 살았던 시대의 식생활, 환경, 질병 등에 관한 중요한 정보를 제공할 수 있다. 이 중에서도 음식물을 섭취했던 사람 생체조직의 탄소와 질소 안정동위원소 분석을 통해 직접적인 식료 섭취에 관한 정보 제공이 가능하다. 특히 미라의 경우 뼈뿐만 아니라 머리카락, 피부, 손톱 등 생애 기간 중 서로 다른 시기를 반영하는 생체 조직 분석이 가능하다. 본 연구에서는 문경 흥덕동 조선시대 회곽묘 출토 미라에서 추출한 뼈 콜라겐, 피부 콜라겐, 머리카락 케라틴, 손톱 케라틴의 탄소와 질소 안정동위원소 분석을 수행하여 생애 주기 동안 식생활의 변화를 추적하고자 한다. 시간이 지나도 그 비율이 변하지 않는 안정동위원소 정보를 바탕으로, 뼈 콜라겐으로부터는 약 10~30 년 사이의 평균 식생활, 그리고 손톱과 머리카락, 피부의 정보로부터는 죽기 전 며칠에서 몇 달 전의 식생활



복원이 가능하다. 지금까지 우리나라에서 출토된 미라를 통해서 고기생충 연구, 복식사, 질병 등 의학적인 연구는 활발하게 이루어져왔으나, 식생활을 위해 직접 조직의 안정동위원소 분석을 수행한 사례가 없었기 때문에, 본 연구는 매우 의미 있는 시작이라 할 수 있다. 예비 결과를 살펴보면, 뼈 콜라겐과 머리카락 케라틴의 질소 안정동위원소비에서 유의미한 차이를 나타냈으며, 뼈 콜라겐의 평균값은  $\delta^{13}\text{C} = -19.0\text{‰}$ ,  $\delta^{15}\text{N} = 11.5\text{‰}$  (N=4), 머리카락 케라틴의 경우  $\delta^{13}\text{C} = -21.5 \sim -20.9\text{‰}$ ,  $\delta^{15}\text{N} = 13.4 \sim 15.0\text{‰}$  기기의 분석 정밀도(precision)는  $\pm 0.2\text{‰}$ 이다.  $\delta^{15}\text{N}$ 의 경우 가장 높은 질소 값을 나타내는 머리카락과 뼈의 차이가 2.5‰로 육류섭취량 등에서 한 단계 정도의 영양 상태 차이를 나타낸다. 즉, 생애 전반에 걸친 영양 상태보다 죽기 전 몇 달 동안 육류 등으로 인한 단백질 섭취량이 높았다고 추정되며, 추후 관련 연구 결과들이 활발하게 진행된다면, 조선시대 식생활 복원을 위한 의미 있는 자료들이 축적될 것이라 기대된다.



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## Analytical methods to determine phthalates in foods

성준현

식품의약품안전평가원 첨가물포장과

Phthalic acid esters(dialkyl or alkyl aryl esters of 1,2-benzenedicarboxylic acid), known as phthalates, are primarily used as plasticizers to soften poly(vinyl chloride)(PVC) products. They have also been widely used in the industrial products. Thus, phthalates have widely ubiquitous environmental contaminants due to leaching from their widespread applications. With the decrease of their usage in food packaging materials, contamination of the environment has become a more important source for phthalates in foods. Also it is important to determine levels of phthalates in foods to provide data for human exposure assessment. Like other chemical contaminants, the determination of phthalates in food involves sample preparation and detection. Extraction and cleanup are the most challenging parts for phthalates analysis in food and are often the critical steps in deciding the levels of detection limits of the overall method. Gas chromatography-mass spectrometry(GC-MS) is most widely used routine detection method, and liquid chromatography-tandem mass spectrometry(LC-MS/MS) method is also reported recently. In this study, the analytical methods to determine high-molecular weight phthalates, such as di-(2-ethylhexyl)

phthalats(DEHP), di-n-butyl phthalats(DBP), and benzyl-n-butyl phthalats(BBP), were reviewed. And to minimize the blank levels of phthalates for existing methods, the sample preparation steps were developed.



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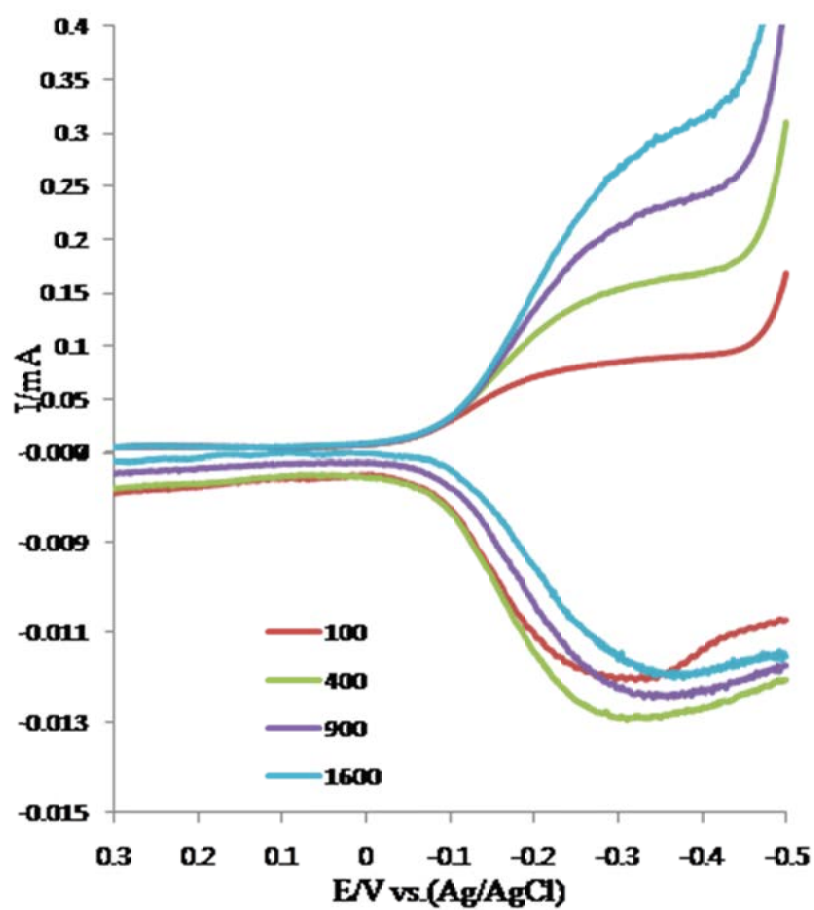
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## ORR catalyzed by active graphene-gold nanocomposite in basic media

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The electrocatalyst for reduction of dioxygen ( $O_2$ ) has been synthesized and employed as doping agent. The surface of multi walled carbon nanotubes (MWCNT) was modified by gold (Au) in the chemical process. The  $O_2$  reduction had done by several MWCNT-Au modified glassy carbon electrode (GCE), denoted as MWCNT-Au/GCE. The synthesis of MWCNT?Au nanoparticles matrix was investigated by XPS, TEM and EDX. The electrocatalytic reduction of  $O_2$  was investigated via cyclic voltammetry (CV), and rotating ring disk electrode (RRDE) techniques in 0.1 mol l<sup>-1</sup> KOH aqueous solutions. The electrocatalytic reduction of  $O_2$  at the MWCNT-Au/GCE established a pathway of two and/or four-electron transfer reduction to hydrogen peroxide ( $H_2O_2$ ) and  $H_2O$  respectively. Especially, hydrodynamic voltammetry revealed the modified electrode was catalyzed effectively by the 4 electron reduction of dioxygen to  $H_2O$  and the minimal generation of  $H_2O_2$  in the process of  $O_2$  reduction. The MWCNT-Au showed the significant efficient electrocatalytic performance. Figure: RRDE voltammograms for MWCNT-Pt/GCE at 100, 400, 900, 1600, 2500 rpm at scan rate of 20 mV/s in 0.1 M KOH.



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## Identification of various explosive materials using Raman spectroscopy and PCA analysis

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Recently, the development of a fast and sensitive explosive detection system is strongly needed for security screening, criminal investigations, and other applications. A promising analytical technique for the identification of unknown explosive materials in the field is not still available. Some of the greatest improvements during the last years have been made in the area of Raman spectroscopy. In this work, we selected 14 species of representative explosive materials, and measured their optimal Raman spectra. For a systematic database of these Raman spectra, the baseline correction and the noise reduction have been performed for raw spectral data. In addition, a principal component analysis (PCA) has been done using a feature extraction technique. A software algorithm to automatically identify with unknown explosives will be developed on the basis of this Raman spectral database in the near future. In this presentation, a

novel identification method of various explosive materials using Raman spectroscopy and their feature extraction-based PCA analysis will be discussed.



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## Size and surface charge effects on the cellular uptake of nanoparticles

최서연 권동욱 박민선 양누리 박종훈 윤태현

한양대 화학과

As the production of manufactured nanomaterials increased, more concerns are being raised on the potential biological and environmental risks of nanoparticles (NPs). For the beneficial use of NPs, it is essential to have a clear understanding on the impacts of various physicochemical properties of NPs on the cellular uptake and resultant cytotoxicities. In this study, cellular uptake and cytotoxicity of various NPs (i.e., ZnO and SiO<sub>2</sub>) with different sizes and surface charges were investigated. First of all, viability of HeLa cells exposed to positively and negatively charged ZnO and SiO<sub>2</sub> NPs were evaluated by using MTT and PI (propidium iodide) assay. Then, the effects of particle size, surface charge on the cellular uptake were investigated by using flow cytometry, TEM, ICP-OES and XRF. In HeLa cell, cellular uptake were preferred for NPs with positive surface charge, while relatively strong cytotoxicity was observed for NPs with smaller size. In this poster, we will also present that the cellular uptake and cytotoxicity of NPs is closely related to their physicochemical properties (i.e., surface charge, and size), and these physicochemical properties play important roles in the mechanisms of cellular uptake of NPs



and following cell death process. Acknowledgement: The research was supported by a grant (10182KFDA991) from Korea Food & Drug Administration in 2010.



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## Colloidal Mobility of Iron Oxide Nanoparticles in Porous Media

전수경 권동욱 윤태현

한양대 화학과

Recent advancement of nanotechnology may result in significant release of manufactured nanomaterials into the environment (e.g., air, soil, water, and etc.). Colloidal properties of these novel materials are closely related with their transport behaviors in the environment. Therefore, laboratory studies and theoretical modeling on the colloidal mobility of nanoparticles (NPs) may provide important knowledge in understanding transport behaviour of NPs in the soil environment. Particularly, column studies with well-defined porous media are suitable for this purpose and often used to explore the governing transport mechanisms of chemicals in the environment, since general dynamics and mathematical basis for these systems in porous media are relatively well understood. In the present study, to understand transport behaviour of NPs released into the environment, we investigated the transport behavior of iron oxide nanoparticles with different sizes (i.e., 20~60nm and Bulk) and crystal phases(i.e., Hematite ( $\alpha$ - $\text{Fe}_2\text{O}_3$ ) and magnetite ( $\text{Fe}_3\text{O}_4$ )) in a saturated porous medium. Then, experimental observations were compared

with the results from theoretical modeling to test prediction capability of current theoretical models for NPs.



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발표코드: ANAL.P-565

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cellular uptake, ROS formation, and cytotoxicity of ZnO and SiO<sub>2</sub> nanoparticles in various cell lines

박민선 최서연 박종훈 권동욱 윤태현

한양대 화학과

Recently, wide range of nanoparticles (NPs) have been used for various industrial applications, such as medicine, cosmetics, and food additives. But, their potential adverse effects on human health and environment has not been well understood yet. In this study, cellular uptake, ROS(reactive oxygen species) generation and cytotoxicity of ZnO and SiO<sub>2</sub> NPs were investigated by using flow cytometry. More specifically, viabilities of three different cell lines (i.e., Raw264.7 :mouse leukaemic monocyte macrophage, U373MG :human caucasian glioblastoma astrocytoma, and HaCaT :human keratinocyte) were tested by MTT assay in 96well plate. Then, cellular uptake and ROS formation were investigated by using flow cytometry. Here, we found that cellular uptake and ROS formation are closely related to the cytotoxicity on these three cell lines. Particularly, positively charged NPs generated more ROS and resulted in significant cytotoxicity than negatively charged NPs. AcknowledgementThe research was supported by a grant (10182KFDA991) from Korea Food & Drug Administration in 2010.

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발표코드: ANAL.P-566

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparison of antioxidant activities in different *Capsicum annuum* L. varieties

이미성 김해경 김미진 현명호<sup>1</sup> 신성철<sup>2</sup> 진종성

한국기초과학지원연구원 부산센터 <sup>1</sup>부산대 화학과 <sup>2</sup>경상대 화학과

*Capsicum annuum* L. contains plenty of phenolic compounds that have antioxidant activity owing to OH functional group and aromatic structure. Antioxidant activity can be assessed in vitro methods for example DPPH, ABTS, FRAP. Results vary with condition such as wavelength of measurement, pH, solvents and temperature. So it is desirable to compare antioxidant activities by various means. Proportional to the antioxidant activity, absorbance decreases. We assessed ABTS, DPPH assay for estimating antioxidant activity in different *Capsicum annuum* L. varieties. And total phenolics content was determined.

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발표코드: ANAL.P-567

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Microfluidic Image Cytometry(uFIC) assessments of silver nanoparticle cytotoxicity

박종훈 윤태현

한양대 화학과

Recently, due to increasing concerns on their potential hazards to human health and environment, cytotoxicity assessments of manufactured nanomaterials have received great attention. However, current platforms for cytotoxicity assessments (e.g., microplate reader and FACS) are typically labor-intensive and/or extremely expensive. Thus there has been increasing needs for microfluidic devices (uFD), which have been recognized as potential platforms for future cell-based HT-HCS assays, since they are capable of reducing experimental costs, increasing assay throughput and shrinking the physical dimensions of current instruments. In this study, cytotoxicity assessments of silver nanoparticle were performed by using MTT-based microfluidic image cytometry (uFIC). Additionally, cytotoxicity assessments of silver ion and silver nanoparticle were performed in conventional 96 well plate and compared with LC50 value measured by image cytometry (IC) and uFD. As a result of this study, we have confirmed that LC50 values measured by conventional microplate reader or IC are similar with each other (for silver ion, and

silver nanoparticle: 3.06, 63.4 mg/L for IC and 2.86, 58.1 mg/L for microplate reader, respectively), which means that IC approach is suitable for cytotoxicity assessment. However, LC50 value measured with uFIC was appeared as 47.7 mg/L, which is approximately 85% less than that measured from 96 well plate. In this presentation, we will demonstrate benefits and limitations of the current MTT-based uFIC and discuss about future applications of these novel platform technology.



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발표코드: ANAL.P-568

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Quantitative Analysis of Enrofloxacin and Ciprofloxacin using FITC doped nanoparticles

김수지 고정아<sup>1</sup> 박지현<sup>1</sup> 임흥빈<sup>1</sup>

단국대 자연과학대 화학과<sup>1</sup> 단국대 화학과

Enrofloxacin and Ciprofloxacin have been increasingly used in veterinary medicine to reduce, suppress microbe activity and treat microbial infections. However, Enrofloxacin and Ciprofloxacin are banned in several countries due to its potential negative effects on the environment and human health. Numerous methods have been reported for the determination of antibiotics using techniques such as liquid chromatography(LC), Gas chromatography (GC) and high-performance thin-layer chromatography (HPTLC). However, those systems 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 for the determination of Enrofloxacin and Ciprofloxacin using Dye doped silica nanoparticle that involves minimal sample pre-treatment and rapid analysis times. The nanoparticles have uniform shape and are modified several functional group like amine and carboxylic acid. In this work 46.19 (+/- 4.59)nm size of the nanoparticles doped with FITC (fluorescein isothiocyanate, Eab=494nm, Eem=521nm) were synthesized by



microemulsion method. For quantitative detection, we use a lab-built laser induced fluorescence microscope (LIFM) with Photomultiplier tube(PMT) and 473nm DPSS BLUE Laser(with 500nm~550nm interference filter). The results showed that the detection limit (LOD) for the two compounds was 45 pg/mL and it was lower than detection limit of ELISA method (LOD = 1ng/mL).



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발표코드: ANAL.P-569

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A comparison study on adsorbents for PCB adsorption from PCB-laden insulation oil**

**유건상 최종하<sup>1</sup> 홍용표 정선영**

안동대 응용화학과 <sup>1</sup>안동대 화학과

Activated carbon has been known as an attractive technology for removing a variety of non-polar organic pollutants from wastewater. Hence, this adsorbent can be used as an effective remover of PCBs which are relatively non-polar. However, due to its high-cost, there is a necessity for developing and testing other adsorbents. Loess and fly ash may be used as alternative adsorbents replacing activated carbon for the removal of PCBs. The adsorptive capability of loess for organic compounds was reported by several literatures. Fly ash, a combustion by-product generated from a thermal power plant, has been widely used in a range of applications and particularly as filler for cement in concrete. A lot of researcher studied on the adsorptive properties of fly ash and concluded that it has a significant adsorption capacity for the removal of organic compounds and dyes from aqueous solutions. The aim of the present study is to explore the possibility of utilizing loess and fly ash as well as activated carbon for the adsorptive removal of PCBs in insulation oil. Here, we investigated the effect of various factors such as temperature, contact

time, adsorbent dose and concentration on adsorption of PCBs in details. The equilibrium adsorption data were fitted to the Freundlich and Langmuir isotherm equations. The kinetics of PCBs adsorption in transformer on each adsorbent was analyzed by fitting various kinetic models.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 리튬 회수 흡착제의 흡착 특성 비교

유건상 최종하<sup>1</sup> 심훈

안동대 응용화학과 <sup>1</sup>안동대 화학과

리튬은 리튬전지, 합금원소, 내열유리의 배합제, 핵융합로, 항공우주 재료 등에 널리 쓰이고 있으며 최근 산업의 발달로 리튬에 대한 수요가 점차로 증가하고 있다. 그러나 국내에서 사용되는 리튬은 전량 국외에서 수입하고 있으며 2008 년 한해만해도 수입액이 대략 6 억 달러였다. 이에 따라 우리나라도 국가차원에서 리튬을 확보하기 위한 다각적 방안을 모색하고 있는 중이다. 현재 국내의 경우, 리튬을 회수할 수 있는 분말형태의 흡착제를 개발하였으나 실적용 시 흡착제의 수거와 재사용이 곤란하여 상용화 단계에는 이르지 못하고 있다. 본 연구는 이의 문제점을 극복하기 위해 현장 적용 시 물리·화학적으로 안정하고 취급이 용이하며 반복적 사용이 가능한 흡착젤 개발 중이며 이 기술이 성공한다면 증가추세에 있는 리튬의 수요 충족에 일익을 담당할 수 있으며 리튬 관련 사업에 미치는 경제적, 기술적 파급효과는 매우 클 것으로 예상된다.

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발표코드: ANAL.P-571

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemical dechlorination treatment of PCB-laden oil by PEGs

유건상 홍용표 안찬주

안동대 응용화학과

Practical disposal of transformer insulation oil laden with PCBs (polychlorinated biphenyls) by a chemical treatment has been studied in field work. The transformer insulation oil containing PCBs was treated by the required amounts of PEG (polyethylene glycol) and KOH, along with different reaction conditions such as temperatures and times. The reaction of PEG with PCBs under basic condition produces arylpolyglycols, the products of nucleophilic aromatic substitution. Removal efficiencies of PCBs in insulation oil before and after chemical treatment were examined. The removal efficiency of PCBs was very low at lower temperatures of 25 and 50oC. Under the reaction condition of PEG 600/KOH/100oC/2hr, removal efficiency of PCBs was approximately 70%, showing completely removal of PCBs containing 7 ~ 9 chlorines on biphenyl frame which appear later than PCB IUPAC Number 183 (2,2',3,4,4',5',6-heptaCB) in retention time of GC/ECD. However, when increasing the reaction temperature and time to 150oC and 4 hours, removal efficiency of PCBs reached 99.99% without any formation of PCDDs/PCDFs during the process. Such reaction conditions were verified by several

official analytical institutions. In studying the reaction of PEG with PCBs, it confirmed that the process of chemical treatment led to less chlorinated PCBs through a stepwise process with the successive elimination of chlorines.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Quantitative analysis of enrofloxacin and ciprofloxacin by enhanced chemiluminescence system

안정원 권민혁<sup>1</sup> 임흥빈<sup>2</sup>

단국대 자연과학대학 화학과 <sup>1</sup>단국대 <sup>2</sup>단국대 화학과

Fluoroquinolone (FQ) antibiotics have been widely used in the prevention and treatment of diseases in humans and animals. Several FQs, for example, enrofloxacin (ENR) and ciprofloxacin (CIP), were specifically developed for veterinary use in food-origin animals such as cattle, pigs, and poultry. But possibility of abuse or misuse of FQs present potential hazards to human health, such as the emergence and spread of drug-resistant bacteria and possible induction of cancer. Therefore a method for the residue analysis of ENR and CIP in foods is required. In this work, we used enhanced chemiluminescence (ECL) method based on the HRP-luminol-H<sub>2</sub>O<sub>2</sub>-*p*-iodophenol system for rapid and accurate analysis. For extraction and concentration of the analytes from food sample, we synthesized and modified magnetic nanoparticles. Calibration graphs had linear range from 1.0 to 70 ng/mL for ENR and CIP. The limits of detection for ENR and CIP were 0.84ng/mL and 0.34ng/mL respectively. The ECL system could perform

faster and more sensitive detection than former method such as Enzyme-linked immunosorbent assay (ELISA).





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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Profiling analysis of catecholamines, serotonin and their metabolites  
in mouse brain tissue by gas chromatography - tandem mass  
spectrometry**

**홍주연** **표희수<sup>1</sup>** **홍종기**

경희대 약학과 <sup>1</sup>KIST 융합오믹스센터

Catecholamines, serotonin, and their metabolites are closely related in neural diseases and cancers as neurotransmitters. The ability to monitor them provides an important key to understand the roles in body, and a possibility of simple and accurate diagnosis of neural diseases. Serotonin, catecholamines and their metabolites in brain tissues were extracted from control or MPTP-treated mice based on centrifugation and MCX-SPE method. For the sensitive and selective detection of catecholamines, a two-step derivatization with MSTFA and MBHFBA was applied. The GC-MS/MS was used to monitor the ultra-trace level of neurotransmitters in brain tissues. The isotopic-labeled internal standards (DA-d<sub>3</sub>, HVA-d<sub>5</sub>, and E-d<sub>6</sub>) were used for the quantitation of neurotransmitters. By the MCX-SPE cleanup, acidic and basic neurotransmitters were separately collected in the variation of pH value of SPE elution solvent. Basic neurotransmitters and acidic metabolites were eluted at pH 5 to 7 and pH 9 to 10, respectively. The pH

variation could lead to high recoveries (> 90%) of acidic and basic neurotransmitters and significant minimization of matrix effect. To improve the chromatographic properties and detection sensitivities of 10 neurotransmitters used in this study, trimethylsilylation (TMS) and heptafluorobutylacylation (HFBA) derivatization were applied. Base peaks of their chemical derivatives were selected as selected ions and precursor ions in the GC/MS-SIM and GC/MS/MS-MRM analysis, respectively. By using GC/MS/MS-MRM, the selectivity and sensitivity of neurotransmitters could greatly improve approximately over 10 folds, compared to GC/MS-SIM mode. Moreover, the neurotransmitters showed good linearity (> 0.99), LODs (> 0.1 ng/mL), and LOQs (> 0.5 ng/mL) enough to determine ultra-trace level of neurotransmitters presented in biological fluids. The developed method was successfully applied to the control and MPTP-treated mouse brain tissue, respectively. From the profiling data of ten neurotransmitters in brain tissues, some catecholamines showed significant decreases of homovanillic acid, DOPAC, and dopamine levels for comparison group.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparative profiling analysis of various Fangchi species using UPLC-UV and LC-MS/MS

김지희 유세미 홍종기

경희대 약학과

Fangchi Radix, one of the most commonly used herbal drugs, is derived from the Aristolochiaceae (*Aristolochica fangchi*) and Menispermaceae plants (*Sinomenium acutum*, *Stephania tetrandra*, *Cocculus trilobus*). A simple and rapid method was performed for determination of the bioactive compounds such as alkaloids, lignans and furans. Several compounds including (hydroxymethyl)-2-furaldehyde, sinomenine, isosinomenine, magnoflorine, fangchinoline, tetrandrine, syringaresinol, liriioresinol A, and aristolochic acid A in various Fangchi extracts were successfully separated by C18 column UPLC with a gradient elution consisting of 10 mM ammonium acetate and methanol. Based on the established UPLC conditions, the determination of marker compounds was performed to find marker compounds in various Fangchi species with different origins. As results, sinomenine and magnoflorine were found to be major compounds in *Sinomenium acutum*. Fangchinoline and tetrandrine were found to be major characteristic compounds in *Stephania tetrandra* and *Aristolochica fangchi* contained aristolochic acid A. The structural

characterization of bioactive compounds in Fangchi species was performed by LC-electrospray ionization (ESI) tandem mass spectrometry. For the identification of minor bioactive compounds, MS/MS spectral patterns of authentic compounds were investigated preferentially to find the diagnostic ions according to structural characteristics. This study will be helpful for the understanding of Fangchi metabolism and elucidation of unknown bioactive compounds.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Elucidation of change occurred to spilled oil at the molecular level by high resolution mass spectrometry

ISLAM ANANNA 김성환<sup>1</sup>

경북대 <sup>1</sup>경북대 화학과

During the Hebei Oil spill on December 2007 a Tanker carrying almost 209000 tons of crude oil collided with another crane barge, splitting three different kind of oil through the west coast of South Korea covering about 37m km of area. The oils were UAE Upper Zakum crude (UZC), Kuwait Export crude (KEC) and Iranian Heavy crude (IHC). Once the crude oil is stranded and exposed to weather that goes through different chemical processes resulting different compounds that may appear to be toxic. After the incident the oil samples for this investigation were collected from different area at different times. The oil samples were separated into saturates, aromatics, resins, and asphaltenes (SARA) fractions. The fractions were characterized by positive-ion atmospheric pressure photo ionization (APPI) coupled to Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). Double-bond equivalent (DBE) vs. Carbon numbers plots were used to identify different chemical class species. The distribution patterns of HC, S<sub>1</sub>, S<sub>2</sub>, N<sub>1</sub>, O<sub>1</sub>S<sub>1</sub>, and O<sub>1</sub> class species in the saturates and aromatics fractions are almost similar for

the samples with slightly disappearances of  $S_1$  and HC classes. Sulfur compounds are dominant in most of the subfractions. However more oxygenated compounds were present in resin and asphaltene fractions in the oils that were collected well ahead. The relative abundance plots of double-bond equivalent (DBE) vs. Carbon numbers were also used to see the differences between the samples.



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발표코드: ANAL.P-576

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Detection of Explosive Materials at a distance using Raman Spectroscopic Analysis

정진혁 조수경<sup>1</sup> 주재범<sup>2</sup> 백성준<sup>3</sup>

국방과학연구소 국방신기술센터 융복합기술부 <sup>1</sup>국방과학연구소 4-2부 <sup>2</sup>한양대 생명나노공학과 <sup>3</sup>전남대 전자컴퓨터공학부

Terrorist activities using improvised explosive device (IED) have been one of the major concerns of modern societies. IED could be used not only in regular warfare but also in any cities over the world. One of the approaches to the solution of this problem is stand-off detection of explosives. There are many technologies under research to achieve this goal. Raman spectroscopy is one of the emerging methods for this purpose, since its spectrum can provide crucial information for the identification of unknown materials, and can differentiate explosives and harmful materials from others. For this purpose, we tried to analyse a dozen of explosive materials used to be utilized to make IEDs including TNT, RDX, and HMX in stand-off environment, where these materials located several meters away from both the laser source and detection system. More than 15 species of possible IED components including major explosive powders and inflammable chemicals are successfully analysed by this method. the stand-off

Raman spectroscopy results using pulse laser will be presented, and compared with the results measured with the confocal microscope.





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발표코드: ANAL.P-577

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Level variation of arabidopsis polyphenols under the irradiation of sound wave

박세민 정성우<sup>1</sup> 서온누리 이지은 신성철

경상대 화학과 <sup>1</sup>경상대 원예학과

Mechanical stimuli such as gravity, wind and touch influence on plant development and growth. Metabolism associated with the mechanical stimuli provides new information, which is related to pathogen defense system. Recently, sound wave stimulation has shown to affect significantly the product of callus growth in chrysanthemum and the product of genes in Arabidopsis. In this works, the variation of polyphenols profile in Arabidopsis plants grown under sound wave treatment or non-treatment was investigated for the first time using a liquid chromatography with electrospray ionization tandem mass spectrometry (LC ESI-MS/MS). The chromatographic separation was achieved INNO C<sub>18</sub> RP- column (250 x 2mm, i.d. 5  $\mu$ m) with 0.1 % acetic acid aqueous solution and acetonitrile gradient.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Optimization and development of a process to produce biodiesel from algae and quantitative evaluation of the process by GC-MS

정지은 김성환

경북대 화학과

In a previously published paper<sup>1</sup>, a procedure to generate biodiesel was reported. The procedure was based on extraction method described by Bligh and Dyer<sup>2</sup>. In the procedure, extraction of biodiesel compound is performed by chloroform : methanol mixture and the extract was isolated, dried, re-dissolved with hexane and converted to biodiesel by transesterification reaction. However, the procedure is difficult to be implemented for a larger scale production because it includes a drying step which is difficult to be automated and requires usage of a large volume of chloroform which is known to be toxic. Therefore, in this study, a new procedure which does not include chloroform and drying step was developed. Briefly explained, hexane was used as an extraction solvent and the hexane extract was for transesterification reaction without further process. Since drying step is removed, the extraction and transesterification can be done in one reaction vessel, and this provides an advantage for automation. Experimental parameters for the new procedure were optimized. The parameters include sample to

extraction solvent ratio, temperature for transesterification, and the amount of catalyst. The effect of sonication was also investigated. Finally, GC-MS and GC-FID was performed to quantitatively evaluate and determine extraction efficiency of the newly proposed procedure. 1. Injoon Yeo et al., Bull. Korean Chem. Soc., 2011, 32, 2830. 2. Bligh, E. G.; Dyer, W. J. Can. J. Biochem. Physiol. 1959, 3, 911.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ANAL.P-579

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The influence of different LEDs spectrum on the flowering response and the phenolics variation of chrysanthemum ‘Gaya Yellow’**

**정성우 박세민<sup>1</sup> 서온누리<sup>1</sup> 이지은<sup>1</sup> 신성철<sup>1</sup>**

경상대 원예학과 <sup>1</sup>경상대 화학과

Chrysanthemum represents a facultative short day plant which flowers at or below the critical day lengths in a natural light condition. Photomorphogenesis and physiology in ornamental crops are strongly influenced by light quality composition, and as well as a light duration. However, little information is available on the relationship between the light quality and the flowering response associated with metabolism. In the present study, it was investigated the influence of light quality composition: blue, green, red and white LEDs, respectively, on the flowering response of chrysanthemum, and determined the variation of phenolic compounds in their leaves using LC-MS/MS.

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장소: 일산KINTEX

발표코드: ANAL.P-580

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Position of hydrogen in toluene molecule is used to generate protonated PAH ions during APPI process

AHMED ARIF 최철호<sup>1</sup> 김성환<sup>1</sup>

경북대 Chemistry<sup>1</sup> 경북대 화학과

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<sup>+</sup> for APPI when only toluene was used as a solvent. However, there still remain many questions unanswered. For example, the source of H<sup>+</sup> when common solvents such as H<sub>2</sub>O and MeOH coexist with toluene is not known. In this study, APPI mechanism, especially, the source of H<sup>+</sup> during the generation of protonated PAH compounds were studied by combination of quantum mechanical calculation and mass spectrometry analysis. Density functional theory with B3LYP functionals was utilized in combination with an all-electron 6-31G(d,p) basis set. Minimum energy reaction paths were determined by first optimizing the geometries of the minima and transition states.

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발표코드: ANAL.P-581

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Oligomeric States of hIAPP and the Effects on Fibrillation in the Model Membrane System: Conformational Analysis Using Mass Spectrometry and Spectroscopic Tools**

**이신정 김준곤**

포항공과대 화학과

Human islet amyloid polypeptide (hIAPP) is one of the amyloid proteins, which can form  $\beta$  structure fibrils and trigger degenerative disorders, including Alzheimer, Parkinson's disease, type II diabetes, and so on. As an intrinsically disordered protein, hIAPP represents random coil structure in solution phase, but lipid molecules are known to induce  $\alpha$ -helix transition at the membrane interface. To elucidate the conformational dynamics in the lipid membrane, we use solutions composed of different organic solvent ratios as a model membrane system which has similar influences on the protein structure. Utilizing an electrospray ionization mass spectrometry, we observe the specific oligomer formation in the solutions with low dielectric constants. To figure out the role of this oligomer in the fibrillation pathway, the kinetics of conformational changes are monitored by using fluorescence and circular dichroism spectroscopy. The structural analysis of hIAPP is expected to be a meaningful step to clarify the linkage

between the change in intramolecular interaction involved in helicity of the protein and its effects on the  $\beta$  fibril formation by inter-molecular interaction.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Spectroscopic Analyses of Rotational Barriers in Tertiary Aromatic Amides

원다운 서지혜 민지은 정기주 안상두

중앙대 화학과

The barrier to rotations about the N-CO and Ar-CO bonds in tertiary aromatic amides was investigated by variable temperature NMR and FT-IR spectroscopy. NMR studie showed that the C-N bond rotation in N,N-diethylpyrene-1-carboxamide and N,N-diethyl-1-naphthamide would occur rather more slowly than the Ar-CO bond rotation. Calculated Gibbs energy changes of the rotational barriers were in good agreement with results using coalescence temperature (TC). The bond rotational properties were also evaluated by using FT-IR spectra acquired with temperature variation and molecular simulations.



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발표코드: ANAL.P-583

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Convection Flows on PGSE-NMR Self-Diffusion Measurements: Investigation on the Effect of Sample Height

서지혜 정기주 안상두 천아영 원다운 민지은

중앙대 화학과

Diffusion coefficients of acetone-d<sub>6</sub> and pyridine-d<sub>5</sub> solvents were measured in range of various temperatures by the PGSE NMR method to investigate the effect of convective flow during the diffusion NMR experiments. To examine the effects of liquid volume (height) in NMR tube, diffusion experiments were conducted with samples of different volumes. Above 288K, the convective flows increased as the height of sample liquid increased. In contrast, as the height increased the convective flows seemed to decrease below 288K. It is thought that this difference might come from the different sources of convection, i.e., buoyancy which overwhelms above room temperature and the variation of surface tension which may be superior at low temperature.

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발표코드: ANAL.P-584

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparison of GC/MS and LC/MS methods for the determination of propofol and its metabolites in human urine

이선영 박나현 홍종기

경희대 약학과

Propofol and its phase I and II metabolites were determined by gas chromatography-mass spectrometry (GC/MS) and liquid chromatography-mass spectrometry (LC/MS) in human urine. Urine samples were collected at 0, 6, 12, 18, 24, and 48 hr after an intravenous injection. For GC/MS analysis, acidic hydrolysis, liquid-liquid extraction (LLE), and trimethylsilyl (TMS) derivatization procedure were subsequently applied. For LC-ESI-MS/MS analysis, a simple sample treatment based on centrifugation and dilution was applied. In case of GC/MS, overall amount of propofol and phase I metabolites obtained without hydrolysis were much lower than those after acidic hydrolysis. From this observation, most of these compounds might be presented as glucuronide or sulfate conjugated form in urine. Moreover, the detection sensitivity of propofol and its metabolites was improved after TMS derivatization. The linearity ranges by GC/MS scan mode was 1-2000  $\mu\text{g/mL}$  for propofol TMS derivatization. The limits of quantitation (LOQ) for propofol TMS derivatization was 325 ng/mL at S/N of 10. In case of LC-MS/MS,

five conjugated metabolites were identified by the interpretation of their tandem mass spectral data and LC elution patterns. On the other hand, propofol and its unconjugated metabolites could not well observe due to its low MS detection sensitivity in both positive and negative ion modes. The linearity ranges by LC-ESI-MS-MRM mode was about 5-2000 ng/mL for propofol-glucuronide(PG). The limit of quantitation (LOQ) obtained by LC-MS-MRM mode for PG was 0.48 ng/mL. In addition, time profile of urinary excretion of propofol and its metabolites was presented using GC/MS and LC/MS. Based on this study, comprehensive assessment of propofol and its metabolites was compatible with GC/MS and LC-ESI-MS/MS.



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발표코드: ANAL.P-585

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Determination of polyphenolic components in *Scutellaria baicalensis* Georgi using high-performance liquid chromatography coupled with tandem mass spectrometry**

서온누리 박세민 이지은 신성철 정성우<sup>1</sup>

경상대 화학과 <sup>1</sup>경상대 원예학과

*Scutellaria baicalensis* Georgi has been routinely used in the treatment of bronchitis, hepatitis, allergy, inflammation, arteriosclerosis. Flavonoids such as baicalein, wogonin and their glycosides are the major and effective components in *S. baicalensis* Georgi. The principal objective of the present study was to characterize in detail the polyphenol compounds of the different tissues (leaf, flower and stem) of *S. baicalensis* Georgi using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) in the negative and positive mode with selected ion monitoring (SIM).

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발표코드: ANAL.P-586

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Forensic comparison of soil samples from three different regions

민지숙 허상철 김기욱 장유림<sup>1</sup>

국립과학수사연구소 화학분석과 <sup>1</sup>이화여대 화학나노과학과

Small-scale(<1m<sup>2</sup>) spatial variability in soil properties was investigated at three locations around the NFS area in Seoul Korea. At each site, ten samples were collected sequentially in a square grid pattern(5 sites). The samples were compared in terms of four properties: major and minor element composition of the 53-500  $\mu\text{m}$  size fraction determined by X-ray fluorescence and LA-ICP-MS, stable carbon isotope ratios and carbon amount of the bulk <53  $\mu\text{m}$  fractions determined by isotope ratio mass spectrometry(IRMS), and colour of the 53-500  $\mu\text{m}$  fractions determined by spectrophotometry. Results showed that analytical and within-site variations were much smaller than between-location variations, and that the three sampling localities could be readily distinguished using any of the four soil properties. Significant within-site variation in the elemental composition was found at all eight localities. Colour properties and carbon isotope ratios and carbon amount showed relatively low variability at three sites. Considering the data as a whole, the three localities could be readily differentiated on the basis of a two sample from each site, using a minimum of ten comparison criteria. However, in order to adequately assess the potential

variability at this scale it is recommended that a minimum of three, and preferably five or more, samples should be taken to assess variation within a localized area of forensic interest. Additional samples should also be taken from the wider surrounding area for purpose of comparison.



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발표코드: ANAL.P-587

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization of phenolic compounds in *Aronia melanocarpa* (Michx.) Elliott using HPLC-MS/MS

이지은 서온누리 박세민 정성우<sup>1</sup> 신성철

경상대 화학과 <sup>1</sup>경상대 원예학과

Black chokeberries, *Aronia melanocarpa* (Michx.) Elliott, belongs to a Rosaceae family, and is a natural shrub in Northern America. The dark berries have been used by native Americans both as a food resource and a traditional medicine for treatment of cold. In recent years, black chokeberries have been highlighted with respect to its potential use as a source for valued phytonutrients. However, little information is available on the variation of phenolic compounds of its fruit depending on developmental stage (immature fruit, mature fruit). In this study, we analyzed phenolic compounds in *Aronia melanocarpa* (Michx.) Elliott using high-performance liquid chromatography coupled with tandem mass spectrometry.

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발표코드: ANAL.P-588

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Investigation of Mercury Ion Induced Deprotonation of Diamide Derivatives by Solution NMR spectroscopy

천아영 안상두 원다은 서지혜 민지은 정기주

중앙대 화학과

A series of diamide derivatives was prepared by the condensation of 3,6-dioxaoctanedioic acid with various aromatic subunits having benzene, naphthalene, anthracene, and pyrene ring systems, and their complexation properties with mercury ion were investigated by NMR spectroscopy. When these diamide derivatives react with mercury, mercury ion induces deprotonation of the amide group next to aromatic rings. As a result, we could observe the changes in the chemical shift of those aromatic rings in  $^1\text{H}$  NMR spectra before and after the complexation with mercury ion. In addition, disappearance of the amide proton resonance signal was also observed as diamide derivatives react with excess of mercury ion, except diamide derivatives of benzene ring. The selective deprotonation by mercury ion was also confirmed through  $^{13}\text{C}$  NMR as well as  $^1\text{H}$  NMR. The structural change on the deprotonation process and the assigning of each peaks were carried out through 2D NMR methods such as COSY, HMBC, and



HSQC. From all these experiments, it could be concluded that the deprotonation process strongly depends on the size and intrinsic property of aromatic subunits.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Microfluidic Flow Cytometry Study on the Cellular Interaction with Nanoparticles

양누리 박종훈 박민선 윤태현

한양대 화학과

The miniaturization, and integration of cell-based assays is one of the most important tasks for enhancing efficiency and reducing costs of many in vitro cytotoxicity assays. Microfluidic device ( $\mu$ FD) is considered as one of the most promising approaches capable of improving current in vitro cell-based assays. In this study, by using simple microfluidic device, we have set-up a microfluidic flow image cytometry system and performed real-time monitoring of the interactions between HeLa cell and ZnO nanoparticles. The cells interacting with nanoparticles were flowing through microchannel of the microfluidic device and microscopic images of flowing cells were acquired and analysed. Our results demonstrated the feasibility of microfluidic flow image cytometry in studying cellular interaction NPs and resultant cytotoxicity.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thiol-ene multilayer film deposition for gas sensor applications using surface plasmon resonance

장성우 박상수<sup>1</sup> 박찬량

국민대 화학과 <sup>1</sup>원익머트리얼즈 개발팀

The thiol-ene multilayer films with multi-armed thiols and vinyls(or acrylates) were successfully deposited on the gold substrates using UV-induced thiol-ene reaction. The angle shifts of surface plasmon resonance curves were measured for the molecular multilayers produced from three or four-armed monomers. The density of each layer has been controlled by adding the single-armed monomers to the multi-armed monomers and the growth kinetics were determined using the simulated SPR curves. For comparison, the amorphous films were also produced from photopolymerization of thiol-ene mixtures and tested using SPR. Potential applications of these polymer films to the gas sensors were discussed.

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발표코드: ANAL.P-591

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemical and physical properties study of fluorocarbon films by plasma polymerization

이지혜 임원철 김강진<sup>1</sup> 이연희

KIST 특성분석센터<sup>1</sup> 고려대 화학과

Fluorine-containing thin films were obtained by two different plasma methods : inductively coupled plasma (ICP) and pulsed plasma (PP). Fluorine-containing plasma polymers are formed as a hydrophobic film on the substrate. Three kinds of fluorine-containing gases such as  $C_2F_6$ ,  $C_3F_8$ , and  $c-C_4F_8$  were used to generate plasma polymer films. Process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, pulse frequency, and processing time were investigated. Surface analytical instruments, XPS, TOF-SIMS, and FT-IR were used to provide useful information about the chemical properties such as surface composition and functional groups. And, AFM result showed the surface roughness and morphology of fabricated film and FE-SEM was used to measure the film thickness and deposition rate. Wear-test and peel-test were performed in order to confirm physical properties of films such as abrasion resistance and adhesion strength.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Detection of gaseous Xylene based on SPR and QCM using MIPs and SURMOFs

진성일 조영호<sup>1</sup> 박찬량

국민대 화학과 <sup>1</sup>국민대 생명나노화학과

Miniaturized portable SPR gas sensor adapting CMOS was constructed to detect some VOCs. Various types of sensing layers including MIPs(Molecularly Imprinted Polymers), SURMOFs(Surface Metal Organic Frameworks) were fabricated on gold thin film. Sensing characteristics depending on the film thickness and density were studied using SPR. Due to the limitation of film thickness in SPR sensing, home-made QCM sensors which allows much thicker sensing layers were also constructed. Using Xylene, sensitivity of the sensor films manufactured by various processes were measured and compared.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Multi-Component Analysis of Vitamin B Mixtures by UV-Vis Spectrophotometer

박소영 노경원 강인성

(주)신코 중앙연구소

혼합물의 구성 성분 분석은 제약, 식품, 염료, 페인트처럼 다양한 분야에서 사용되고 있다. 일반적으로 HPLC, GC, UV-Vis Spectrophotometer 등을 이용하는데, 각 성분마다 추출, 분리, 발색 등 시료를 전처리 하는데 있어 많은 시간이 소요되는 단점이 있다. 특히 기존의 UV-Vis Spectrophotometer를 이용할 경우, 단일 성분마다 발색시켜 정량을 해야 하는 번거로움이 있다. 하지만 Multi-component analysis (MCA, 다성분 분석) 기능을 이용하면 다른 분리 과정 없이 개별 성분의 정량 분석이 가능하다. 다성분 분석은 구성 성분비가 다른 다성분 표준 시료들의 스펙트럼을 측정한 후 미지 시료를 측정하여 구성 물질의 개별 농도를 측정하는 방법이다. 본 연구에서는 UV-Vis Spectrophotometer로 혼합물의 구성 성분 정량을 위해, 한번에 최대 4개 성분의 정량 분석이 가능한 Multi-component analysis software를 개발하였다. 이 소프트웨어와 190 ~ 1100 nm의 전 파장을 동시에 측정할 수 있는 광다이오드 어레이

(photo-diode array) 타입의 분광광도계를 이용하여 Vitamin B 군 혼합물의 성분을 분석하고, 이 소프트웨어를 활용한 제약 및 응용 분야를 소개하고자 한다.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Monitoring Bioluminescence Resonance Energy Transfer using Fluorescence Spectrometer

정원빈 정병도 강인성 노경원

(주)신코 중앙연구소

분자간의 에너지 전달은 일반적으로 전자기파에 의한 복사전이로 이루어진다. 하지만 다른 종류의 형광체가 수 ? 단위로 가까워지면 복사전이 없이 공명에 의해 에너지가 전달되는 공명에너지전이 (RET, Resonance energy transfer) 현상이 발생한다. 대표적인 RET 현상으로 FRET (Förster resonance energy transfer)이 있다. FRET에서는 에너지 전달자인 donor를 들뜨게 하기 위해 강한 빛을 조사하는데, 이 과정에서 의도치 않은 여러 잡광들이 발생하고, 형광성질을 서서히 잃는 광표백 (Photobleaching) 현상이 일어나 감도를 떨어뜨린다. 이를 보완하기 위해 donor를 생물학적 발광 물질로 대체한 BRET (Bioluminescence resonance energy transfer)을 활용한다. BRET은 직사광이 없어 잡광들의 생성을 차단하고 광표백 현상을 막아준다. BRET은 감도가 좋아 이미징 장비로의 관찰은 효율적이지만, 발광 광량이 작고 수명이 짧아 분광광도계를 사용하여 스펙트럼을 구하기 쉽지 않다. (주) 신코에서 개발한 형광 분광광도계 (FS-2)와 발광 마이크로 셀 홀더 (Luminescence Microcell Holder) 액세서리는



BRET 측정에 최적화 되도록 설계하였다. 본 연구에서는 액세서리를 활용하여 바다 펜지 추출물을 변이시킨 발광물질 Luc8 을 donor 로 사용하고, Quantum Dot 을 acceptor 로 사용하여 자사와 타사 장비의 BRET 측정 수율을 비교하였다. 또한 다양한 파장의 Quantum Dot 들을 사용하여 각각의 BRET 스펙트럼과 측정 수율을 확인하였다. 형광 분광광도계에서 BRET 액세서리는 다양한 생체 내, 생체 외 기초 연구와 임상 연구에 응용될 수 있을 것으로 기대된다.



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## Stearic Acid monolayer isotherm investigation on different cation subphases

Yalda Hozhbari Pooladi Nezhad 신관우<sup>1</sup>

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

Fatty acid Langmuir monolayers like Stearic acid monolayers on pure water have been well studied and pressure ? area isotherms have been investigated. But pictures for fatty acid salts are still far from complete. In this study, stearic acid monolayer structure and collapse behavior on different aqueous subphases is going to be studied in presence of different divalent cations such as Ni, Co, Ca and Fe. It's also of interest to measure the isotherm by varying the temperature, compression rate and PH. In order to investigate the temperature, compression rate and PH effect on the isotherms and as a result on the monolayer and collapse structures.

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## Trace Metal Analysis for Determination of the Source of Physical Evidence

민지숙 김기욱 허상철 장유림<sup>1</sup>

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Using 7 certified reference materials, we investigated for the reasonable analytical method for the determination of elemental content of metal samples. Those methods included are (1) inductively coupled plasma-optical emission spectrometry(ICP-OES), (2) inductively coupled plasma-mass spectrometry(ICP-MS), (3) Laser ablation-inductively coupled plasma-mass spectrometry(LAICP-MS), (4) X-ray fluorescence spectrometry(XRF). Each method has its own characteristics in sensitivity, ruggedness, easiness etc. ICP-OES is accurate for the most elements but requires time, labor and exposes some dangerous chemicals to put through. ICP-MS is the most sensitive so trace element in the metal samples can be determined most exactly but easy to be detracted for the wrong end. LAICP-MS is the most convenient method among the investigated methods with accuracy and precision. XRF is a good screening step procedure for the more accurate results.

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## **A study on the extraction and determination of vanadium species ( $V^{4+}$ and $V^{5+}$ )**

**김나영 남상호 CUI SHENG**

목포대 화학과

Vanadium compounds were prescribed as therapeutic agents for anaemia, chlorosis, tuberculosis and diabetes. vanadium was also used as an antiseptic. Clinical feature of poisoning shows a broad spectrum of toxic effects of vanadium on the respiratory, circulatory and central nervous systems, the digestive organs, kidneys, and skin. Toxic and biological effects of vanadium depend not only on the total concentration of vanadium but also on the chemical species of vanadium in a sample. 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). Thus, an accurate determination of each species is typically critical to evaluate the environmental and biological risks. In this study, we have focused on speciation method of vanadium species ( $V^{4+}$  and  $V^{5+}$ ) using ICP-OES coupled with IC (Ion Chromatography). The 2.5 mM EDTA was used for the extraction of vanadium species from various samples.

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## Nanoparticle tagging for sample treatment to determine ceruloplasmin using ICP-MS

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단국대 자연과학부 화학과 <sup>1</sup>단국대 화학과

Fluorescence spectrometry is one of the most common techniques to determine proteins accompanied with fluorescent tagging. Recently metal-ligand tagging technique has been also developed. However, these techniques sometimes confronted with difficulties of multi target analysis, lack of sensitivity, poor quantitative results due to photobleaching, etc. In this research, we developed nanoparticle tagging ICP-MS technique (NPT-ICP-MS) to determine bio targets tagged by nanoparticles instead of fluorescence tagging. TiO<sub>2</sub> nanoparticles and Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles were synthesized for tagging and separation to determine ceruloplasmin(CP) using ICP-MS. TiO<sub>2</sub> nanoparticles were modified with IgG antibody and react with the target CP. IgG modified Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles were used to separate CP bound TiO<sub>2</sub> particles from sample. The molar relation of TiO<sub>2</sub> particles and CP was determined by measuring <sup>48</sup>Ti signal using flow injection (10  $\mu$ L) ICP-MS. Linear regression coefficient of the curve obtained by plotting CP concentration vs. <sup>48</sup>Ti signal was 0.9834. This newly developed NPT method

enhanced sensitivity and specificity compared to the single metal ion tagging in ICP-MS can be potentially extended to various biomaterials.



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## Microchip-Based Analysis System for Wastewater Monitoring

안재훈 나고은 조경호 한종훈

포항공과대 화학과

We have developed a sensitive, simple and continuous microchip-based analysis system for monitoring of pollutants in wastewater. In this system, typical analysis steps such as a chemical reaction and detection, are continuously carried out in a microchip. The microchip is fabricated with black poly(dimethylsiloxane) (PDMS) which can block the stray light and decrease the noise. First, we have developed a microchip-based analysis system for continuous monitoring of chromium (Cr) in wastewater. The Cr analysis using chemiluminescence reaction is based on the measurement of the intensity of light emitted when luminol is oxidized by hydrogen peroxide in the presence of Cr(III). Therefore, the analysis system for Cr simply consists of the microchip and a photomultiplier tube (PMT) as a detector. Cr(VI) is completely converted to Cr(III) by selective injection of the reductant and we can determine the total Cr and Cr(III). Second, nitrite ( $\text{NO}_2^-$ ) and orthophosphate ( $\text{PO}_4^{3-}$ ) in water have been determined by colorimetric methods. The system can be miniaturized by containing a light emitting diode (LED) and PMT as a light source and detector respectively. The liquid core waveguide made of Teflon AF-2400 was used to extend a light path

length of absorbance detection system. The interference filter was positioned in front of the PMT to define the wavelength of maximum absorption. The miniaturization of microchip-based analysis system for water quality monitoring is capable of portability as well as fast analysis and low reagent consumption. Furthermore, the system integrated with wireless communication will be particularly suited for environmental monitoring requiring high spatial or temporal resolution.





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## Colorimetric Sensor Based on Neutral Receptors

이은빈 김동완 김관겸 박세빈 김재상

경상대 화학과

The tripodal receptors( $L^1$ ,  $L^2$  and  $L^3$ ) bearing Schiff-base groups as selective colorimetric sensor for ascorbic acid has been synthesized. The selectively binding ability of the receptors to ascorbic acid over other acids tested was demonstrated by UV-Vis. spectroscopy in DMSO. Comparing with other acids studied, the UV-Vis spectrum in DMSO shows significant response toward ascorbic acid with high selectivity, and color change is observed from yellow to dark-red( $L^1$ ,  $L^2$ ) or orange( $L^3$ ) in the presence of ascorbic acid ( $5 \times 10^{-4}$  M). Also, upon addition of citric acid to receptors ( $L^1$  and  $L^3$ ) in DMSO, the appearance of the solution of receptors showed a fluorescence enhancement at  $\lambda=380\text{nm}$ . Whereas, in the addition of other acids, no change in the absorption and emission spectrum of given receptors.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Determination of $\text{Cu}^{2+}$ using an electrode modified with receptor self-assembled gold nanoparticles on the ITO electrode

김동완 김관겸 박세빈 이은빈 김재상

경상대 화학과

A new type indium tin oxide (ITO) electrode is developed for sensing  $\text{Cu}^{2+}$ . The ITO film was modified with gold nanoparticles (AuNPs) functionalized with a self-assembled film of 2-(((3-mercapto-1*H*-1,2,4-triazol-5-yl)imino)methyl)phenol (I) or 2-((5-mercapto-1,3,4-thiadiazol-2-yl)methyleneamino)phenol (II). The resulting ITO film was characterized by scanning electron microscopy (SEM), UV-Vis spectra, X-ray diffraction (XRD) and electrochemical methods. Also, cyclic voltammetry (CV) and linear sweep voltammetry (LSV) of  $\text{Cu}^{2+}$  on the modified electrode were performed. The modified electrode showed particularly a significant selectivity toward copper ions, even in the presence of other metal cations. Moreover, the electrode exhibited high sensitivity and reproducibility.

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## Highly Sensitive and Selective $\text{Be}^{2+}$ Colorimetric Sensor Based on 2-((5-mercapto-1,3,4-thiadiazol-2-yl)methyleneamino)phenol-functionalized Gold Nanoparticles

박세빈 이은빈 김관겸 김동완 김재상

경상대 화학과

We report herein the development of a highly sensitive and selective colorimetric detection method for  $\text{Be}^{2+}$  based on 2-((5-mercapto-1,3,4-thiadiazol-2-yl)methyleneamino)phenol (I)-functionalized gold nanoparticles (II) which were characterized by IR, UV-vis spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). In the presence of  $\text{Be}^{2+}$ , receptor (I) could rapidly induce the aggregation of gold nanoparticles, thereby resulting on olive-to-lightsteelblue color change. The concentration of  $\text{Be}^{2+}$  can be determined by monitoring with naked eye or a UV-vis spectrometer. This method exhibits excellent selectivity for  $\text{Be}^{2+}$  over other alkali, alkaline earth metals. The assay is simple, inexpensive, and highly sensitive. Also, seed-mediated growth of gold nanoparticles on glassy carbon (GC) surfaces was developed. The as-prepared GNP/GCE was modified by I. The modified electrode (I/GNP/GCE) was then used as a voltammetric sensor in detecting the  $\text{Be}^{2+}$ .

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## Molecular Recognition of Sodium Salts Using a Ditopic Receptor

김관걸 김동완 이은빈 박세빈 김재상

경상대 화학과

A ditopic receptor with adjacent anion and cation binding sites is able to extract a range of monovalent salts. The sodium salts are bound to the receptor as contact ionpairs, with the metal cation located in the receptor's crown ether ring and the anion bonded to the Zn(salphen) complexes. The complexed were characterized by NMR, UV-Vis, X-ray analysis. The receptors bound specific anion in a ditopic fashion with a color change, and in contrast other sodium salts bound to the receptors in a monotopic fashion without a color change.

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## Laser desorption ionization FT-ICR MS applied to heavy crude oil analysis

조윤주 김성환

경북대 화학과

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is one of the powerful techniques that can cope with the complexity of crude oils. However, even with FT-ICR MS, complete understanding of crude oils' chemical composition is not currently available. One of the problems limiting our knowledge is the discrimination occurring during the ionization process. No single ionization technique has capability to ionize all different variety of compounds existing in crude oils. Therefore, it is beneficial to be able to use as many ionization techniques as possible and hence there have been many researches devoted to utilize various ionization techniques such as ESI, APPI, and APLI. In this study, laser desorption ionization (LDI) coupled to FT-ICR MS was applied to study crude oils at the molecular level. Molecular ions were major types of ions detected by (+) mode and deprotonated and radical anions were major ones observed by (-) mode LDI FT-ICR MS. N1 and hydrocarbon classes were dominant in the class distribution plots obtained by (+) mode but other heteroatom classes including Ox and S1 were

also abundant in ones by (-) mode. However, O<sub>2</sub> classes were exception because nonaromatic and aromatic O<sub>2</sub> compounds could be detected at the same time. It has been shown that abundance of O<sub>2</sub> nonaromatic compounds (presumably naphthenic acids) has correlation with TAN numbers but O<sub>2</sub> compounds with condensed structures has not. It is important to note that vanadyl- and Ni-porphyrine compounds were detected by LDI FT-ICR MS directly from an unfractionated crude oil. Overall, the research describe in this study clearly shows that LDI FT-ICR MS can be a powerful technique to study crude oils at the molecular level.



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## development of nanostructre surface and magnetic bead to improve sensitivity measurement of LDI-TOF analysis

김병준 진장미 김성환

경북대 화학과

Laser desorption ionization (LDI) with organic matrix is widely used for analysis of biomolecules and polymers. However, this approach can be limited because peaks originating from the matrix can be abundant in lower  $m/z$  ranges and may overlap with peaks from samples. Therefore, particles or surfaces with nanostructures have been combined with LDI to improve ionization efficiency and reduce matrix interference. Although many studies have employed nanostructures to improve LDI efficiency and selectivity, relatively few reports have examined how the nanostructure is related to LDI efficiency. In this study, LDI efficiency obtained from four surfaces with different gold (Au) nanostructures were compared, and the dependence of LDI efficiency on the surface areas was evaluated.

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## Effect of composition and flow rate of carrier liquid on retention of microparticles in gravitational field-flow fractionation (GrFFF)

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Field-flow fractionation (FFF), a group of elution-based separation techniques, is capable of separating and characterizing nano or micro colloids, polymers, and biological macromolecules. Gravitational field-flow fractionation (GrFFF) uses the Earth's gravity as the external field and is relatively simple in principle and operation. In this study, the effect of the viscosity, composition and flow rate of the carrier liquid on the retention, and thus the size-based selectivity ( $S_d$ ) and the zone-broadening of microparticles in GrFFF were investigated using polystyrene (PS) latex beads as the model particles. In order to adjust the viscosity of carrier liquid, various amounts of (hydroxyl propyl) methyl celluloses (HPMCs) were added to the aqueous carrier liquid. The effect of the carrier viscosity on size-based size selectivity ( $S_d$ ), ionic strength ( $I$ ), retention ratio ( $R$ ), and the plate height ( $H$ ) was investigated at various flow rates ranging from 0.5 to 4 mL/min. Results suggest that particles were rapidly eluted as the carrier viscosity increases due to increase in the flow rate-induced lift forces ('hydrodynamic lift forces', HLF). This study



has shown that the influence of carrier liquid viscosity on HLF must be taken into account in GrFFF analysis of micron-sized particles. It also indicates that carrier viscosity is an important variable that may be exploited in GrFFF to improve the resolution and to reduce analysis time of microparticles.



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## Synthesis and Characterization of Rod-Shaped FeOOH Nanoparticles Using Asymmetrical flow-Field flow fractionation

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한남대 BK21<sup>1</sup> 한남대 화학과

The size and shape of nanoparticles play important roles in determining their various physical properties. In case of magnetic nanoparticle, their morphology strongly influences their chemical and physical properties, and especially their magnetic and electrical properties. Magnetic nanoparticles have shown its applicability in various fields such as nanoparticle-based imaging, cell-receptor actuation, cancer diagnosis, solar cell, lithium ion battery and water treatment, etc. Asymmetrical flow field-flow fractionation (AsFIFFF) is an elution-based excellent separation tool that has been widely applied to separation and characterization of various biological components, polymers, and particles over broad mass and size ranges. In this study, rod-shaped FeOOH nanoparticles were synthesized. Then AsFIFFF was applied for separation and analysis of the FeOOH nanoparticles. It was found that the size (or the length) of the FeOOH particles vary with the sample preparation method as well as the synthesis condition. The AsFIFFF method used for analysis of FeOOH nanoparticle may also be used for analysis

of  $\text{Fe}_2\text{O}_3$  magnetic nanoparticles having similar sizes and shapes. The effect of sonication time during sample preparation for the rod-shaped  $\text{FeOOH}$  nanoparticle was also studied. Increasing the sonication time resulted in reduction in the mean size of the nanoparticles and an increase in the population of smaller particles. Similar sample treatment method may be used for characterization of monodispersed  $\text{Fe}_2\text{O}_3$  magnetic particles.



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## OPTIMIZATION OF ASYMMETRICAL FLOW FIELD-FLOW FRACTIONATION (ASFLFFF) FOR ANALYSIS OF QUANTUM DOT (QD)

최재영 이승호

한남대 화학과

Quantum Dot (QD) is a semiconducting nano-crystal that can emit light. Their optical properties show great potential in many areas of applications such as optical technologies, media industries and photovoltaic devices. The color of the emitting light usually depends on the size of the QD, and thus the quality control of QD requires accurate determination of the size distribution of QD. Flow field-flow fractionation (FIFFF) is a versatile chromatography-like separation technique that is well suited for the characterization of colloidal particles. The asymmetrical version of FIFFF, called 'asymmetrical FIFFF' (AsFIFFF), has certain advantages over conventional FIFFF (called 'Symmetrical FIFFF') in terms of the separation efficiency. It uses only one pump, instead of two, to generate both the longitudinal and the cross-flow, and allows the focusing of the injected sample before the elution begins. There are a few experimental parameters in AsFIFFF including the type of the surfactant which is usually added in

AsFIFFF analysis as a dispersing agent, the ionic strength of the carrier liquid, and the cross-flow rate. In this study, CdS QD complex was synthesized. Then, in order to optimize AsFIFFF conditions for analysis of the QD's, the influences of the various experimental parameters on the elution behavior of the QD were investigated. Among the surfactants tested, anionic surfactant tends to give better elution profile than cationic or neutral surfactants. AsFIFFF provides separation based on the hydrodynamic diameter ( $d_H$ ) of the sample components, thus allows direct measurement of  $d_H$  from their retention times. The size distributions obtained from AsFIFFF were compared with those from other means such as dynamic light scattering (DLS) and electron microscopy (EM).



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## Fluorinated monolithic column for capturing of perfluorooctane sulfonate

황효진 오한빈<sup>1</sup>

서강대 <sup>1</sup>서강대 화학과

With an aim of effectively separating fluorinated analytes of interest, we prepare fluorinated monolithic column using a modified procedure of Richard D.Oleschuk et al. Since monolithic columns generally provide far higher mass transfer efficiency than particle-based stationary phases, our column is expected to show high permeability, low back pressure, and high efficiency. In the present study, we performed LC-MS experiments in negative ion mode with the prepared fluorinated monolithic column. Our column showed a good efficiency in capturing inorganic perfluorooctane sulfonate, i.e., PFOS(perfluorooctane sulfonate), which is widespread in the environment. This persistent pollutant, which has an increasingly risk of causing chronic kidney diseases, was found to be well separated using our fluorinated monolithic column. Our method holds a good promise for use in monitoring this type of fluorine-rich persistent pollutants in the environment. Furthermore, we plan to use this fluorinated monolithic column in

enrichment of fluoro-tagged nitrated peptides, which is one of important posttranslational modifications. The further details of the experimental results and procedure will be presented in the conference.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Application of Asymmetrical Flow Field-flow Fractionation for Characterization of Cyclotrimethylene Trinitramine (RDX) Particles

DouHaiyang 이승호

한남대 화학과

High energy materials such as explosives and propellants are used extensively for both civilian and military applications. The need for the development of high performance and insensitive explosives is increasing, due to the need to lower their explosive self-vulnerability caused by unintentional explosion and the increasing demand for high explosives. The size, shape and internal defects are important properties of explosives crystals. Field-flow fractionation (FFF) is one of versatile separation techniques in the field of analytical separation sciences. Asymmetrical flow FFF (AsFIFFF), one of members of FFF family, provides separation of components based on their hydrodynamic sizes. AsFIFFF is regarded as a powerful tool for characterization of particles and polymers. To date, there has not been a report on the characterization of cyclotrimethylene trinitramine (RDX) particles using AsFIFFF. In this work, AsFIFFF was employed, for the first time, to determine the size distributions of RDX particles. The micron-sized RDX particles were prepared using a supercritical anti-solvent recrystallization process. The influence of



the pressure drop on the size and shape of the recrystallized RDX particles were investigated. It was found that the mean diameter of recrystallized RDX particles decreases as the pressure drop increases, mainly due to the reduction in population of larger particles. Also the size distribution tended to become narrower with increasing the pressure drop by the same reason. Near-spherical RDX particles with relatively narrow size distribution were obtained at the pressure drop of 11 MPa. The mean diameters of RDX particles determined by AsFIFFF were in reasonable agreements with those obtained by optical microscopy (OM). AsFIFFF seems to provide a useful tool for the separation and characterization of RDX particles.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

**APPLICATION OF THERMAL FIELD-FLOW  
FRACTIONATION/MULTI-ANGLE LIGHT SCATTERING  
(THFFF/MALS) FOR MICROGEL CONTENT DETERMINATION  
OF STYRENE-BUTADIENE RUBBER**

**최유진 이승호<sup>1</sup>**

한남대 생명나노과학대학/화학과 <sup>1</sup>한남대 화학과

Thermal field-flow fractionation (ThFFF) is a separation technique that is particularly suited to the characterization of ultrahigh-molecular weight (UHMW) polymers and macromolecules in an organic solvent that are difficult to analyze by SEC. The open channel geometry, which is one of unique features of ThFFF, minimizes nonideal phenomena such as adsorption and shear degradation of the UHMW polymers. It also allows the passage of microgel particles through the channel. ThFFF has been used for analysis of microgel-containing polymers. Styrene-butadiene rubber (SBR) is a copolymeric rubber, and usually shows good mechanical and dynamic properties and good aging stability when it is protected with appropriate additives. SBR is widely used in automobile tires, where it is usually blended with natural rubber and butadiene rubber. It is known that SBR contains components having 3-dimensional cross-

linked network structure called microgel. In this study, ThFFF combined online with multi-angle light scattering (MALS) was employed for physical characterization of various sources of SBR. ThFFF provides separation of the microgels from the soluble polymers (sol), allowing determination of the microgel content. The light scattering detection provides enhanced sensitivity for the microgel particles, and allows determination of the size distribution of the microgel particles. The results from ThFFF/MALS were compared with those obtained from size-exclusion chromatography (SEC). It was found that the MW's obtained by SEC are generally lower than those from ThFFF, which is probably due to lower resolution of SEC for high MW components of the sample. Unlike ThFFF, SEC was unable to show the presence of the microgels because the sample solutions are filtered prior to the injection. It seems ThFFF/MALS can provide a useful tool for analysis of various types of microgel-containing materials such as SBR.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Zinc-finger and DNA noncovalent interactions studied by intensity-fading MALDI mass spectrometry**

**박선희 오한빈**

서강대 화학과

Zinc-finger 와 DNA noncovalent interaction 을 intensity-fading MALDI-TOF-MS 통해 확인했다. Zinc-finger sample 로 Sp1-1 (QHICHIQGCG KVGKTSHLR AHLRWHTGER), Sp1-3 (KFACPECPCR FMRSDHLSKH IKTHQNKK), CF2II-4 (PYTCSYCGKS FTQSNTLKQH TRIHTGEK) , CF2II-6 (PYTCP YCDKR FTQRSALTVH TTKLHPL)을 사용하였다. DAN sample 농도를 증가하며 실험한 결과 Zinc-finger peak 이 점차 사라짐을 확인하였다. ESI-MS 를 통해 Zinc-finger 와 DNA noncovalent interaction 한 실험값과 일치하는 데이터가 확인되었다.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## MALDI In-source decay (ISD) characteristics of PAMAM and DAB dendrimers

소혜림 한상윤<sup>1</sup> 오한빈

서강대 화학과 <sup>1</sup>한국표준과학연구원 나노바이오융합연구단

We investigated MALDI in-source decay (ISD) characteristics of synthetic dendritic polymers such as polyamidoamine (PAMAM) and polypropylenimine (DAB) dendrimers. The ISD studies of dendrimers offer a unique opportunity to understand the MALDI-ISD behavior of monodisperse polymers with amide or imine functionalities. In experiments, high laser fluence gives internal energy to the analyte that favors the backbone fragmentation. In this experiment, comparison was also made for the results obtained using various matrix chemicals such as  $\alpha$ -cyano-4-hydroxycinnamic acid (CHCA), 2,5-dihydroxybenzoic acid (2,5-DHB), 5-aminosalicylic acid (5-ASA), 5-formylsalicylic acid (5-FSA), 5-nitrosalicylic acid (5-NSA), 1,5-diaminonaphthalene (1,5-DAN), and sinapinic acid (SA). Furthermore, the ISD results will also be compared with the results obtained previously with electron capture dissociation mass spectrometry. The details of the experimental results will be discussed in the symposium

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of capillary electrophoresis inductively coupled plasma mass spectrometry for quantitative analysis of phosphate

방수경 이경석<sup>1</sup> 임용현<sup>1</sup> 김태규<sup>2</sup>

한국표준과학연구원 분석화학표준센터, 부산대 화학과 <sup>1</sup>한국표준과학연구원 분석화학표준센터 <sup>2</sup>부산대 화학과

Adenosine phosphates are energy carriers of cell and participate in a metabolic phosphorylation as essential ingredients. Besides, it is possible to get information about specific metabolic pathways through ATP/ADP ratios. For this reasons, their quantitative analysis is very important in biochemical field. Here, we report the development of inductively coupled plasma mass spectrometry (ICP/MS) hyphenated to the capillary electrophoresis (CE) for quantitative analysis of adenosine phosphates. The CE has been applied to separate adenosine tri-phosphate (ATP) and adenosine di-phosphate (ADP). Then, their accurate concentrations were determined through phosphorus measurement by ICP/MS. In addition, metrological traceability to SI has been introduced in the fields of measurement for biomolecules. The limit of detection and dynamic range of phosphorus measurements in these adenosine phosphates by the developed CE-ICP/MS method have been also studied. It is considered as a promising technique in

analysing biomolecules owing to its excellent detection limits and selectivity with providing traceability to SI.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Removal of phenol from aqueous solution by adsorption to  
hydroxyapatite**

**유구용**

삼육대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.



일시: 2012년 4월 25~27일(수~금) 3일간

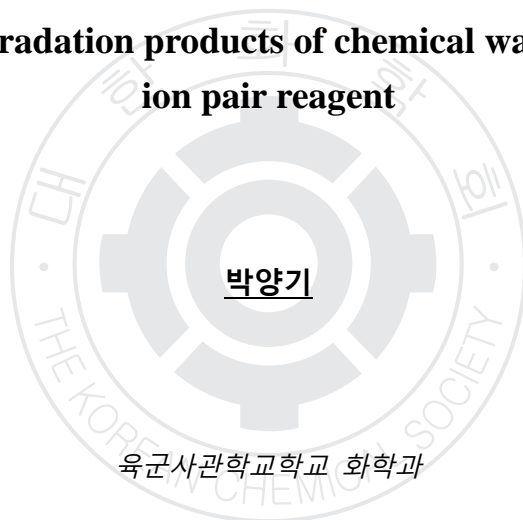
장소: 일산KINTEX

발표코드: ANAL.P-616

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Extraction of degradation products of chemical warfare agents using ion pair reagent



The chemical warfare agent degradation products have been successfully extracted using ion pair reagents. The target analytes in the sample solution were converted into thier ion pair complexes with cetyltrimethylammonium bromide(CTAB) and then extracted.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Identification of flavonoid content change in citrus varieties caused by green mold(*Penicillium digitatum*) employing LC-MS/MS

김해경 이미성 김도연 신성철<sup>1</sup> 진종성

한국기초과학지원연구원 부산센터<sup>1</sup> 경상대 화학과

Green mold is caused by the fungus *Penicillium digitatum* which is ubiquitous to all citrus growing regions. It is the most common and serious postharvest disease of citrus. The green mold induces the change of the flavonoid component distribution in citrus fruit. This studies on the role of these compounds in resistance to and on the resistance conferred by flavonoid in Citrus. It was confirmed by LC-MS/MS that as procedure of disease, while the content of hesperidin (HPD) increases, hesperetin (HPT) decreases. According to the literature *Penicillium* produces hesperidinase which hydrolyzes HPT to afford HPD.

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발표코드: ANAL.P-618

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Sensitivity Enhancement of Small Molecules Immunoassay by Electrokinetic Concentration on Microfluidic Chip

한동훈 김양래 김솔지 정택동

서울대 화학부

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 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.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Surface Probing on Various Substrates by Extraordinary Enhanced Raman Scattering based on a Single Gold Microshell

김솔지 한동훈 정택동

서울대 화학부

We report finely tuned gold microshell with self-contained “hot spots” and demonstrate that gold microshell acts as a surface-enhanced Raman scattering (SERS) probe on any substrate. The optimized gold microshell is obtained by controlling of several variables, such as the number of gold reducing steps and the aging time of gold nanoparticle solution. When the gold microshell is sprinkled on p-aminophenyltrimethoxysilane (p-APhTMS) monolayer modified substrate, the SERS spectrum on various substrates are clearly obtained. These results indicate extraordinary potential of gold microshell for surface probing on any substrate, application to semiconductor industrial processes and in situ electrochemical SERS on any electrode which is not consisted of coinage metals.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and characterization of a novel nanodiamond based sponges with entrapped enzyme

Shanmuga sundaram Komathi A.Gopalan<sup>1</sup> 이광필<sup>2</sup>

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Nanodiamond (ND) based conducting sponges (ND-NS) were prepared through one-step enzymatic polymerization process. A “modular approach” has been demonstrated for the preparation of (ND-NS) with entrapped enzyme (Horseradish peroxidase, HRP) (ND-NS(HRP)). ND-NS was prepared with a mixture of ND, aniline, cross linker and HRP. HRP induces the formation of sponge and simultaneously be entrapped within ND-NS to result ND-NS(HRP). Field emission scanning electron microscope image of ND-NS(HRP) reveals sponge like suprastructure comprising of interconnected nanospheres with numerous openings/pinholes/cavities. The electronic state was determined by UV-visible spectroscopy. The other physico-chemical characteristics of ND-NS(HRP) is carried out. The electrochemical characteristics of ND-NS(HRP) was evaluated and the electron transduction capability between the enzyme and electrode was analyzed. ND-NS(HRP) shows the characteristics of establishing direct electrochemistry and usefulness as a matrix for electrochemical determination of biomolecules.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## New hydrogel network for environmental application

정재홍 M. Francklin Philips<sup>1</sup> A.Gopalan<sup>2</sup> 이광필<sup>3</sup>

경북대 일반대학원 과학교육학과 <sup>1</sup>경북대 차세대에너지기술연구소 <sup>2</sup>경북대 화학과 <sup>3</sup>경북대  
화학교육과

Poly(acrylamide-co-acrylicacid)/poly(aniline-co-4-vinylaniline-co-2-amino benzonitrile) (P(AAm-co-AA)/P(ANI-co-VA-co-2ABN) hydrogels were prepared by free radical polymerization of the monomers, acrylamide, acrylic acid, aniline, 4-vinylaniline, 2-aminobenzonitrile and N,N'-methylenebis(acrylamide) by using ammonium persulfate as the initiator. The new hydrogel network (NHGNW) was used loaded with palladium nanoparticles (Pd NPs) by reduction of Pd ions using sodium borohydride as reducing agent. The morphology and microstructure of the NHGNW-Pd NP composite were analyzed by field emission scanning electron microscope and X-ray diffraction analysis, respectively. The structural characteristics and thermal stability of the NHGNW-Pd NP composites were characterized by Fourier transform infrared spectroscopy and thermogravimetric analysis (TGA), respectively. This NHGNW-Pd NP composite is suited for the removal heavy metal ions.

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발표코드: ANAL.P-622

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of composite membranes based on Sulfonated poly(ether ether ketone) and high proton conducting particles

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The organic - inorganic composite membranes were prepared with the incorporation of high proton conducting functional particles into Sulfonated poly(ether ether ketone) (SPEEK). The organic phase consisted mainly of SPEEK with different degree of sulfonation. The inorganic phase was limit with one or two functional particles that can improve the performance of membrane towards fuel cell proton exchange membrane application. The new composite membranes was designated as SPEEK-CM(F)s. The incorporation of functional particle was ascertained by Fourier transform infrared spectroscopy and X-ray diffraction analysis. SPEEK-CM(F)s were characterized for their thermal and physical properties. The membrane stability, i.e. liquid uptake in water and in aqueous methanol solution, oxidative stability as well as mechanical and thermal stability were tested. SPEEK-CM(F)s posses characteristics as the promising electrolyte in direct methanol fuel cells.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of new interpenetrating polymer network hydrogels

김민경 A.Gopalan 이광필<sup>1</sup>

경북대 화학과 <sup>1</sup>경북대 화학교육과

New interpenetrating polymer network hydrogels (IPNHG), comprising of poly(N-isopropylacrylamide) (P(NIPAAm)), polyacrylic acid (PA), poly(2-acrylamidomethyl propanesulfonic acid) (PAMPSA) and gold nanostructures (GNS), were prepared using ammonium persulfate (APS) as an initiator at 60°C. IPNHGs were prepared by varying the proportion of the individual components. The morphology of IPNHGs was investigated by scanning electron microscopy. Lower critical solution temperature of IPNHG was determined by differential scanning calorimetry. Physicochemical properties of IPNHGs, such as swelling ratio and drug release capacity, were reported.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Identification of Degradation Products of Lincomycin and Iopromide by Electron Beam Using LC-MS/MS

함현선 명승운

경기대 화학과

In recent years, pharmaceuticals in the environment are of growing concern and scientific interest worldwide. Identification of degradation products of pharmaceuticals is a challenging task because they are present in very low concentrations. It is led to need for the development of its metabolites and degradation products, as well as parent pharmaceuticals. Identification of the degradation products of lincomycin (antibiotic pharmaceuticals) and iopromide (iodinated X-ray contrast media (ICM)) under electrical beam was performed by LC-MS/MS. Electron beam (10 MeV, 1 mA and 10 kW) experiments for the spiked aqueous sample, which in fortified with lincomycin and iopromide, were performed at the dose of 10 kGy. The separation of its degradation products, lincomycin and iopromide was carried by C18 column (2.1 × 100 mm, 3.5 μm and 4.6 × 100 mm, 3 μm, respectively), using gradient elution with 20 mM ammonium acetate or 0.1% formic acid and acetonitrile. Some degradation products of lincomycin and iopromide were identified by interpretation of mass spectra by mass spectrometry.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Effective Analysis of Gibberellic acid ( $GA_3$ ) using HPLC/UV-vis

마경나 명승운<sup>1</sup>

경기대 자연과학부 화학과 <sup>1</sup>경기대 화학과

Gibberellins (GAs) are a class of plant growth hormones that exert profound and diverse effects on plant growth and development such as seed germination, fruit external ripening and fruit development and others. GAs are increasingly applied in agriculture to improve crop quality and yields. But, there is no regulation of GAs in Korea. On the other hand, the MRL(Maximum residual limits)s of Gibberellic acid ( $GA_3$ ) in Japan and EU are 200  $\mu\text{g/kg}$  and 500  $\mu\text{g/kg}$ , respectively. Determination of  $GA_3$  by HPLC/UV-vis has always been extremely difficult because  $GA_3$  has little ultraviolet (UV) absorbance. Therefore, in this study, the analytical method, which is sensitive and selective on HPLC/UV-vis, was developed. Derivatization of  $GA_3$  with benzyl alcohol was performed and the derivatized  $GA_3$  was effectively analyzed by HPLC/UV-vis. The HPLC/UV-vis was equipped with C8 column (4.6 mm I.D.  $\times$  150 mm, 3.5  $\mu\text{m}$ ) using a binary solvent system composed of containing 0.1% formic acid water and acetonitrile and flow rate was 0.8 mL/min. The established method can be applied to more effective analysis of  $GA_3$  from plant and food.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Derivatization of Cholesterol and Cholesterol Oxidation Products (COPs) for HPLC/UV-Vis Analysis

이진주 조현우 명승운

경기대 화학과

Free cholesterol is an unsaturated alcohol susceptible to oxidation in the presence of light, oxygen and high storage temperature. This autooxidation involves a free-radical reaction which leads to the formation of cholesterol oxidation products (COPs). COPs turned out to have a variety of potentially atherogenic, cytotoxic, mutagenic and possibly carcinogenic affects in humans. Nevertheless, HPLC/UV-Vis are not sensitive enough to separate and quantify free cholesterol and COPs simultaneously. In this study, significant improvements are realized by increasing the UV absorption of compounds through derivatization attaching a chromophore to the functional groups of cholesterols. Effective and sensitive derivatization of free cholesterol and COPs (25-hydroxycholesterol, 7-ketocholesterol, 5,6 $\alpha$ -epoxycholesterol, 5,6 $\beta$ -epoxycholesterol, cholestane-3 $\beta$ -5 $\alpha$ -6 $\beta$ -triol) that differentiate from traditional methods, which are more complex derivatization procedure, was performed. The devatized cholesterol and COPs were separated simultaneously on a C18 column (2.1 $\times$ 100 mm, 3.5  $\mu$ m) using a mobile phase

of water and acetonitrile. The derivatized cholesterol and COPs showed the increased sensitivity and selectivity on HPLC/UV-Vis.



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## **Fabrication of a Chemiluminescence Microfluidic Sensor on a Chip with the Co(II) Immobilized CNT-Nafion Composite to Determine Amino Acids**

**MD.KAMRUZZAMAN ALAM MD AL MAHMNUR 이상학 Dang Trung Dung<sup>1</sup>**

경북대 화학과 <sup>1</sup>경북대 기계공학부

A novel chemiluminescence (CL) sensor with a microfluidic chip system has been presented based on the immobilization of Co(II) on the functionalized carbon nanotube (CNT)-Nafion composite membrane. CNT- Nafion composite was constructed by solution casting using 5 wt% CNT in 5% Nafion solution. Co(II) was immobilized on the CNT-Nafion composite membrane by solution impregnation using  $\text{CoCl}_2$  solution as precursor. Co(II) grafted CNT-Nafion composite exhibited excellent catalytic activity towards the oxidation of luminol in the luminol- $\text{NaIO}_4$  CL reaction. Co(II) immobilized sensor on a microfluidic chip was fabricated by a soft-lithographic procedure using polydimethyl siloxane (PDMS) with a 500 nm wide, 250 nm deep and 82 mm long microchannel. L-phenylalanine (L-PA) was sensed by the CL reaction between luminol and  $\text{NaIO}_4$  in the presence of Co(II) immobilized MWCNT-Nafion composite on the PDMS chip. The fabricated CL sensor on the PDMS chip provides sensitive determination of L-

PA with long lifetime without any special pretreatment of the sample. Due to the ease of operation and excellent catalytic properties of the proposed sensor, it may be a potential amino acid sensor to determine amino acid in real samples.



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## **Spectrofluorometric Determination of Bovine Serum Albumin by Enhanced Fluorescence of Terbium Nanoparticles**

**ALAM MD AL MAHMNUR MD.KAMRUZZAMAN 이상학**

경북대 화학과

A new spectrofluorometric method has been developed for the determination of bovine serum albumin (BSA) using terbium nanoparticles (TbNPs) as fluorescence (FL) probe. TbNPs was synthesized by tannic acid reduction method and stabilized by sodium dodecyl benzene sulfonate (SDBS). The average size of the nanoparticles was found as 70-80 nm in transmission electron microscope (TEM). TbNPs emits maximum FL emission at the wavelength of 402 nm upon excitation at 225 nm. When BSA was added to the colloidal solution of TbNPs, a remarkable enhancement of emission spectrum was observed at the emission wavelength. Under the optimized condition, the FL emission intensity of the TbNPs-BSA system exhibited a linear correlation with the BSA concentration. Linearity was observed in the range of 4-120 nM of BSA with a limit of detection (LOD) of 0.76 nM. The precision of the method was tested at the concentration level of  $1 \times 10^{-8}$  M for 11 replicate measurements giving relative standard deviation (RSD) values of 1.25 %.

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## Drug release monitoring from monodisperse drug-loaded PLGA microparticles using lanthanide ligand-sensitized fluorescence

김경민 이상학 김환곤<sup>1</sup>

경북대 화학과 <sup>1</sup>경북대 기계공학부

A drug release monitoring method has been presented for the determination of two model drugs, L-dopa (LD) and enoxacin (ENX), which released from monodisperse drug-loaded polylactic-co-glycolic acid (PLGA) microparticles prepared by solvent evaporation technique using a microfluidic chip device. The presented method is more sensitive and selective than the conventional UV-Vis absorption method since the highly enhanced fluorescence (FL) emission of Tb(III) at 544 nm is induced by ligand-sensitized effect of the LD and ENX. The FL enhancement showed a good linear relationship with the concentration of two model drugs. The effects of Tb(III) concentration and pH were investigated and optimized for the drug release monitoring as well as the determination of LD and ENX using a standard calibration curve. Drug release profiles from monodisperse PLGA microparticles were investigated and compared with UV-Vis detection method. The results of relationship between PLGA particle concentration and FL intensity showed that the proposed method is reliable and precise to monitor drug release.



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## Detection of biomarker protein OjaMT using Single Chain Variable Fragment antibodies

정덕호 민경미 권영은

동국대 의생명공학과

The expression of metallothionein in *O.javanicus* (OjaMT) increases as a result of heavy metal exposure. Measuring the level of OjaMT expression in *O.javanicus* can be a good monitoring method for heavy metal contamination of environment and their toxicity. Previously, western blotting and ELISA methods were used to monitor the level of OjaMT expression and these methods requires long detection time and gives high level of background. Also, it was rather difficult to achieve quantitative measurement of OjaMT. Here, we set-up an assay to quantitatively detect OjaMT using surface plasmon resonance (SPR) system. We have used OjaMT specific antibody for the SPR based label free detection of OjaMT. Also, we have constructed OjaMT specific scFv using the total RNA of antibody generating hybridoma cells using jumping PCR. The generated scFv's exhibited specific binding activity to OjaMT in solution. ScFv's were immobilized to gold substrate using a 3-Cys tag introduced during the cloning vector

construction. The performance of two different probes were compared and the amount of OjaMT was measured quantitatively.



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## **Analysis of pharmaceuticals in environmental sample using three-phase hollow fiber-liquid phase microextraction (HF-LPME)**

차용병 명승운

경기대 화학과

There has been an increasing interest in sample pretreatment (extraction & clean-up). Liquid phase microextraction is one of simple techniques in Analytical Chemistry because it only needs to a little amount of organic solvent. 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 which extracts analyte. We investigated into influence of these parameters on the extraction efficiency by three phase HF-LPME. 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. The extracted sample were analyzed by HPLC system.

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## Determination of carotenoids in vegetables using HF-LPME and GC-FID

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 method for the determination of carotenoids in vegetables using hollow fiber-liquid phase microextraction (HF-LPME) and gas chromatograph - flame ionization detector (GC-FID) has been established. 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 carotenoids from sample were established. The established HF-LPME method can be used for the determination of carotenoids in vegetable.

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## **The reaction monitoring of crosslinking reaction of TDI with acrylic acid using MALID and FTIR**

**김지석 김성호**

순천향대 화학과

아크릴 산과 TDI(toluene di isocyanate)의 반응은 아크릴계 PSA(preassure sensitive adhesives) 의 경화반응에 대한 기본이 되는 반응이다. MALDI 와 FTIR 을 이용하여 점착제 경화반응의 반응성, 응용성, 물성에 미치는 영향등에 관하여 연구하였다.

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## Affinity Chromatography-ICPMS를 이용한 셀레노 단백질의 분리

분석

박용남 김경미<sup>1</sup> 김은주

한국교원대 화학교육과 <sup>1</sup>한국교원대 화학교육

인체에서 셀렌의 역할은 필수미량원소로서 매우 중요하며 셀렌은 여러 질병이나 항산화제등과 깊은 연관을 가지고 있다. 셀렌의 총량을 분석하는것도 쉽지않고 중요하지만 더욱 중요한 것은 셀렌이 어떤 형태로 존재하는지에 대한 연구가 꼭 필요하다. 특히, 셀렌이 인체내에 어떤 형태로 존재하는지에 대한 연구는 의학, 건강과 직접연관이 있으므로 수행되어야 한다. 혈청속의 셀레노 단백질중 가장 중요한 것들인 glutathione peroxidase(GPx), selenoprotein P(selP) 및 selenoalbumin(SeAlb)을 분리정량하였다. Heparin Sepharose(HEP)과 Blue Sepharose 를 사용하고 두 개의 6-way 밸브를 사용하여 연속적으로 시료들을 분석할 수 있었다. 또한, 혈청시료내의 여러 음이온들 Cl 과 Br 은 각각 Se77 과 Se81 에 간섭을 심하게 끼친다. 따라서 이 들을 음이온 교환 SPE 를 사용하여 제거한 뒤, SPE-AF-ICPMS 방법으로

혈청내의 셀레노 단백질들을 정량분석하였다. 정량법은 후컬럼동위원소희석법(post column Isotope dilution)을 사용하였으며 표준시료인 BCR-637(Se  $81 \pm 7$  ppb) 에 대하여 비교해본 결과, 85.4 ppb 로서 매우 정확한 결과를 얻을 수 있었다. 만일 음이온들을 제거하지 않으면 주로 GPx 에서 약 15% 이상의 오차가 발생하게 된다. 한국인의 혈청에 대하여 조사해 본 결과 각 셀레노 단백질별 농도는 GPx, SelP, 및 SeAlb 가 각각 11.3, 54.2, 20.0 ppb 로서 총량은 85.4 ppb 로 나타났다. SPE-AF-ICPMS 를 이용한 post column ID 방법은 혈청내의 셀레노 단백질들을 분리하고 정확하게 정량분석할 수 있는 매우 좋은 방법이다.



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## Graphene oxide based enzyme platform for drug screening

**장홍제 유수윤 민달희<sup>1</sup>**

KAIST 화학과 <sup>1</sup>서울대 화학과

Helicases are a class of essential enzymes that unwind double stranded into single stranded nucleic acid. The unwinding of DNA is a key reaction for all single stranded DNA required processes such as cell proliferation and viral replication. Due to their critical role in viral process, helicases have been targeted for therapy in many virus diseases. Therefore, it is important to develop a simple, fast and cost-effective platform for helicase unwinding activity assay for diagnostic and drug discovery. We developed graphene oxide (GO) based helicase activity assay using fluorescence on-off platform. The strategy relies on preferential binding of GO to single stranded DNA over double stranded DNA, thereby quenching fluorescence of dye labeled single stranded DNA. Our GO based strategy enabled real-time monitoring, quantitative and high-throughput assay of DNA unwinding activity. We found SARS and HCV helicase inhibiting hit compounds by using our GO based helicase assay platform.



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## **microRNA detection platform inside living cells based on nanomaterials**

**유수윤 나희경 민달희<sup>1</sup>**

KAIST 화학과 <sup>1</sup>서울대 화학과

As biomolecules inside cells including proteins, nucleic acids, and small molecules show a variety of expression level and pattern, localization or distribution, they are considered as the critical parameters that reflect the state of organism including cellular behaviors, function, proliferation, development, physiological and pathological states. In that point of view, the build-up of the biomolecule detection method is one of the important issues in the biomedical field for the treatment process of all sorts of diseases. 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 oxide and detection probe antisense oligonucleotide for this study. We evaluated that 1) the probe-

nanographene complex can work as microRNA sensing platform with efficient fluorescence quenching and recovery ability, 2) nanographene oxide sheets can serve as a delivery carrier of detection probe into live cells for real-time monitoring and quantitative analysis of microRNA and 3) the nanographene oxide sheets provide the stable loading platform in the complex biological solutions and samples.



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## Ground organic monolith particles as a stationary phase of HPLC

최지호 이진욱 양송희 정원조

인하대 화학과

Ground organic monolith particles were prepared and packed in a glass-lined stainless steel microcolumn. The monomer methacrylic acid, crosslinker EDMA, and initiator AIBN were dissolved in a mixed solvent composed of toluene and iso-octane, and a special porogen component polyethylene glycol (PEG) was added to the reaction mixture. By subtle control of the composition of the reaction mixture, the resultant polymer monolith had proper softness/hardness to be easily smashed into particles of proper properties such as particle size distribution and porosity. Especially, the content of PEG was very critical to control the porosity. The image and elemental analysis of organic monolith was taken using SEM/EDX. In this study, the contents of PEG such as 24mg, 36mg, 48mg were examined and the content of 36mg/ mL solvent was found the optimum value for separation efficiency. This is the very first study to report ground organic monolith particles as a stationary phase of HPLC to give somewhat useful separation efficiency.

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## Speciation analysis of selenium in human serum by HPLC-ICP MS

김은주 김경미<sup>1</sup> 박용남

한국교원대 화학교육과 <sup>1</sup>한국교원대 화학교육

생활수준의 향상으로 인해 건강에 관한 관심이 높아짐에 따라 식품 및 의약 분야에서 미량성분에 대한 빠르고 정확한 분석이 요구되고 있다. 셀레늄(Se)은 생체 내 필수미량원소로서 부족하거나 과잉으로 섭취할 경우 질병을 유발할 수 있어 많은 관심의 대상이 되고 있는 원소 중 하나이다. 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 혈청 시료 중 셀레늄 화학종을 분리하였다. 분광학적 동중간섭을 제거하기 위해 ORC의 reaction gas로 H<sub>2</sub> gas를 사용하였으며, ICP MS와 HPLC를 연결했을 때 탄소흡착에 의한 sampler cone, torch injector 막힘 등의 문제를 해결하기 위해 make up gas로 Ar과 O<sub>2</sub>를 혼합하여(Ar 80%, O<sub>2</sub> 20%) 사용하여 탄소를 산화시켰다. 분리를 위해서는 먼저 5가지 셀레늄 화학종 표준시료(SeIV, SeVI, Selenocystine, Selenomethylcysteine, Selenomethionine)를 이용하여 각각 C<sub>8</sub> column과 C<sub>18</sub> column, anion-exchange column, cation-exchange column을 사용할 때

이동상의 조성(MeOH 농도, ion pairing reagent 농도, pH) 등 분리조건을 찾고, 분리결과를 비교하였다. 이를 바탕으로 혈청시료 중의 셀레늄 화학종을 분리하였다.



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## Simultaneous determination of alkaloids in Corydalis Tuber using ultra-performance liquid chromatography and chaotropic mobile phase additives

김정현 양동혁 한상범

중앙대 약학대학

A new ultra-performance liquid chromatography (UPLC) method using chaotropic mobile phase additives was established to separate and determine tertiary and quaternary isoquinoline alkaloids in Corydalis Tuber. Chaotropic agents employed mostly in reversed-phase liquid chromatography are small inorganic salts (e.g.  $\text{NaBF}_4$ ,  $\text{NaClO}_4$  and  $\text{NaPF}_6$ ). Primarily with anions in the chaotrope, they can bring out beneficial effects on the chromatographic separation of basic compounds. Analytical target compounds were eight isoquinoline alkaloids, including four tertiary alkaloids (glaucine, protopine, tetrahydropalmatine and corydaline) and four quaternary alkaloids (coptisine, palmatine, berberine and dehydrocorydaline). The optimal column for UPLC method was Waters Acquity UPLC BEH C18 column (2.1 mm  $\times$  100 mm, 1.7  $\mu\text{m}$ ) and the optimal mobile phase was consisted of 10 mM potassium dihydrogen phosphate in 30 mM  $\text{NaPF}_6$  (sodium hexafluorophosphate) and acetonitrile. The column

temperature was set at 25°C and the detection wavelength was 280 nm. The developed UPLC method was successfully validated in terms of linearity, precision, accuracy, limit of quantitation (LOQ) and recovery. This UPLC method was applied to determine eight isoquinoline alkaloids in 30 *Corydalis* Tuber samples and multivariate analysis was performed using principal component analysis to differentiate the 30 samples. These analytical methods could be valuable for the quality control of *Corydalis* Tuber and its pharmaceutical preparations.



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## **Ground silica monolith particles prepared by a new simplified and cost-effective process**

**Faiz Ali 정원조**

인하대 화학과

We have been studying silica monolith particles for raw material of chromatographic stationary phases. In this study, the manufacturing process for silica monolith particles becomes much simpler by removing the sieving and washing steps in comparison with the previous methods, causing great reduction of production cost. In addition, silica monolith particles with reduced average particle size and increased average pore size are obtained in this method. Thus the stationary phases comprising the silica monolith particles of this study result in high separation performance in liquid chromatography. The manufacturing process of silica monolithic particles of this study includes three steps: the step for formation of bulk monolith (step 1), the step for powdering the silica monolith (step 2), and the step for calcination of the powdered silica monolith (step 3). The average particle sizes and pore sizes were affected by variation of reaction conditions such as formulation of reaction mixture, combination of heating steps, and, process temperature, etc.



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## Development of Uricase-CdTe nanoparticles for optical sensing of uric acid

서민호 B.T.Huy 임재민 이용일

창원대 화학과

Simple and controllable synthetic procedure for CdTe nanoparticles was developed directly in the aqueous phase. The CdTe nanoparticles are advantageous as the emission can be tuned by changing reaction time and pH values. The interaction between CdTe nanoparticles and hydrogen peroxide was investigated by using fluorescence spectroscopy. Effect of different stabilizers has been studied. The results showed that the fluorescence quenching effect demonstrated excellent sensitivity to H<sub>2</sub>O<sub>2</sub>. The convenient optical detection methodology of uric acid was developed based on the fluorescence quenching of CdTe nanoparticles by H<sub>2</sub>O<sub>2</sub> which was produced from the enzymatic reaction of uricase. The detection conditions, reaction time, the concentration of uricase were optimized. The results show that CdTe nanoparticles can be potentially 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 H<sub>2</sub>O<sub>2</sub>-dependent enzymes due to many enzymatic reactions can produce hydrogen peroxide.

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## Controllable synthesis of CdTe QD nanoparticles and application for optical sensing of TETA

B.T.Huy 서민호 임재민 이용일

창원대 화학과

Semiconductor nanoparticles based on II-VI materials are challenging to develop chemical sensor materials for biomedical and environmental applications. Highly luminescence CdTe nanoparticles were synthesized in a coprecipitation route using aqueous salt solutions and with different thiols as stabilizers. The synthetic procedure is simple, efficient, and stable. It could also allow for controlling the particle size by varying the experimental conditions such as reaction time and pH values. Strong luminescence of the nanoparticles was observed under UV-excitation and emission colors could be adjusted. Triethylenetetramine (TETA) is a candidate treatment for diabetic cardiovascular complication because of TETA's ability to remove excessive extracellular copper. TETA is a selective copper chelator that has been used in the treatment of Wilson's disease; it can reverse diabetic heart failure in diabetes. The interaction between CdTe nanoparticles and TETA was investigated by fluorescence spectroscopy. Based on the quenching effect of CdTe by TETA, a simple assay system for triethylenetetramine was developed.

The preliminary results show that CdTe QDs can be used for the quantitative analysis of TETA in urine samples.



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## Separation and Analysis of Peptide by Capillary Electrophoresis Directly Coupled to Desorption Electrospray Ionization Mass Spectrometry

안지용 이용일 임재민

창원대 화학과

Capillary electrophoresis (CE) separation technique is more efficiency than usual high-performance liquid chromatography (HPLC). The CE coupled to conventional electrospray ionization mass spectrometer (ESI-MS) offer the ability to separate, chemically identify, and provide structural information on analytes in small sample volumes. It is usually carried out using electrospray ionization. However, the salts and detergents used in the mobile phase for CE separations suppress ionization efficiencies and contaminate the inlet of the mass spectrometer. This study describes a new method that uses a CE directly coupled to desorption electrospray ionization (DESI) to overcome these limitations. Collected sample from CE is deposited on a DESI plate that is heated with electric heating coil. As the surface moves, surface-deposited analytes are ionized by DESI and then detected by MS. And several important experimental

parameters influencing CE-DESI-MS were optimized by that uses angiotensin II. At no distant date, CE-DESI-MS will be able to analyse several complex glycoproteins, such as fetuin.



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## **Application of proteomic analysis using trypsin coated magnetic nanofiber in rigorous conditions**

**박현주 이상원**

고려대 화학과

Developments of stabilization of proteases such as trypsin are needed for efficient protein digestion in proteomic analysis. In the present work, trypsin was stabilized in the form of enzyme coating on magnetic nanofiber (EC-TR/NP-NF), which crosslinks additional trypsin molecules onto covalently attached trypsin on magnetic nanofiber (CA-TR/NP-NF). EC-TR/NP-NF showed better stability than CA-TR/NP as well as free trypsin in rigorous conditions, such as at high temperatures of 40 and 50 °C, in the presence of organic co-solvents, various pH's, and super acoustic condition in digesting a model protein, enolase. Covalent linkages among trypsin molecules improved the stability of EC-TR/NP-NF and inhibits the denaturation, autolysis, and leaching of trypsin. Magnetic nanofiber which has magnetic property can be applied in reuses of protease for protein digestion. In rapid proteolytic digestion using super acoustic technology, EC-TR/NP-NF showed better performance and stable repeated digestion under 5 times reuses. The enzyme coating approach will be successfully employed not only for high throughput protein

digestion in proteomic analysis but also for various other fields such as food processing and peptide synthesis.



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## Automated Multidimensional and Multifunctional Ultra-High-Pressure Liquid Chromatography/ Tandem Mass Spectrometry

이정화 이상원

고려대 화학과

Automated multidimensional and multifunctional ultra-high-pressure liquid chromatography (UPLC) system/tandem mass spectrometry that allows 1-dimensional, 2-dimensional separation (strong cation exchange/reverse phase liquid chromatography), and online phosphopeptides enrichment by using a single binary nano-flow pump is developed. With the switching of a multi-channel valve, which is linked with a SCX column and TiO<sub>2</sub> (titanium dioxide) column, an automated selection of three different experiment modes is achieved. Because the system uses the same solvent flow paths, the same SPE (solid phase extraction) column, and the same separation column for reverse-phase separation in 1D, 2D, and phosphopeptides enrichment experiments, the reproducibility of elution time obtained from the these experiments is in great agreement. Furthermore, fast online digestion was attempted using pepsin in a modified high pressure LC system. The system was possible to generate the high pressure condition (~10,000 psi) to accelerate enzyme digestion and reduced sample digestion time from hours to minutes.



This first attempted development of the automated multidimensional and multifunctional ultra-high-pressure LC system is proven to be substantially reproducible, convenient and efficient compared with existing LC system. It also demonstrates potential to effectively evolve into a fully automated UPLC system suitable for high throughput proteomics analysis.



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## Specific Proteins Extraction by Antibody Conjugated Nanoparticles and Its Application to Biomarker Validation

백승훈 이광렬 이상원

고려대 화학과

The detection of diseases in their early stages is important to the success of therapeutic treatment. And it has been assisted by the discovery of altered tissue and fluid protein markers. However, current technologies have limited the analysis of the human proteome; especially, discovery of tumor-derived biomarkers directly is challenging because the abundant proteins impede detection of lower abundance tumor antigens. Here, to overcome that obstacle, specific extraction of target protein was described by using magnetic nanoparticles (NPs). NPs have been developed for an increasing number of applications in biological analysis. Compared with conventional micron-sized bead techniques, the NPs give the advantages such as higher surface-to-volume ratio, higher specificity, higher miscibility and faster binding time. In this study, for advanced target-specific interaction with C-reactive protein (CRP), CRP antibody loaded NPs were used. First, N-Succinimidyl 3-(2-pyridyldithio) propionate (SPDP) functionalized superparamagnetic Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> NPs (ca. 27 nm diameter) were synthesized.

Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> NPs were coated 3-(Trihydroxysilyl) propylmethylphosphonate (THPMP) and 3-Aminopropyltriethoxysilane (APTS). Then, SPDP was modified on the surface of the Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> NPs coated with THPMP and APTS. Cysteine-tagged protein G was loaded SPDP NPs through disulfide bonding. Using the specific interaction with CRP antibody, protein G-SPDP NPs were modified to specific enrichment of CRP from complex samples. Also, protein G-Dynabeads were used to compare the efficiency between NPs and micron-sized beads. The specific extraction of CRP was confirmed by both SDS-PAGE and LC-MS/MS experiments.



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**Discovery of Novel Bladder cancer biomarkers by extensive label-free  
quantitation based on master accurate mass and time tag (AMT)  
database**

**김수진 문동기 이상원**

고려대 화학과

Bladder cancer is a common urothelial cancer and one of the most common malignancies worldwide. This cancer estimated 70,530 newly diagnosed cases per year in the United States, and approximately 14,700 patients die each year of the disease in 2010. One of an easily accessible diagnostic method of the bladder cancer, urine cytology is a non-invasive procedure that is easily accessible, convenient, and no painful procedure to most of patients, but an accurate diagnosis fails in case of low grade (or early stage) tumors. Therefore, many low grade tumors would be missed and then bladder cancer has been reported high recurrence rate. The necessity of repeated screening for reappearance demonstrates the need for novel biomarkers as alternatives to invasive or non-invasive standard diagnostic procedures. Toward this goal, we performed proteomic study using mass spectrometry through “the Master AMT DB” (Master accurate mass time tag database) to extensive proteome profile and “MAD4QUANT” (Master AMT tag

Database approach for label-free QUANTitation). As a result this study, we created a bladder cancer proteome compendium of 31,442 unique peptides covering 4,937 proteins across 11 bladder cancer patient samples (11 normal and 11 tumor tissues). Especially, 25,475 peptides (4,421 proteins) participated in label-free quantitation. Among the 1,163 proteins, differentially expressed proteins (DEPs) were identified as the present proteins with a pair-wise statistical test P-value less than 0.01. Using this approach, we have analyzed 912 up-regulated proteins and 251 down-regulated proteins against tumor and selected candidate biomarkers of bladder cancer. Major changes of DEPs were observed for cell adhesion, cytoskeleton organization, and cell migration, but also inflammatory response and response to oxidative stress were affected in cancer. This study demonstrates that label-free quantification using mass spectrometry can be identified disease dependent protein alterations from bladder tissue biopsies. Thus, this technique might be allowed better disease characterization and may be a valuable tool in potential clinical biomarker studies.



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## Comprehensive analysis of lipid raft proteome of MCF-7 and MCF-7/ADR cells

문동기 김수진 이상원

고려대 화학과

There have been reports that detergent-resistant lipid rafts play important roles in multidrug resistance (MDR). In this work, comprehensive analysis of lipid rafts proteome isolated from MCF-7 and MCF-7/ADR cells are described. Ultra-high pressure microcapillary liquid chromatography/tandem mass spectrometry based approaches were applied identifying 936 proteins in lipid raft proteomes. High throughput protein quantitation was facilitated by label-free quantitative analysis, discovering 176 differentially expressed proteins with p-value of less than 0.05. Comparison of quantity of peptide feature was done by introducing unique mass class (UMC). Among 176 proteins, polymerase transcription release factor (PTRF)/cavin-1 was observed to be upregulated along with multidrug-resistant P-glycoprotein (P-gp), caveolin-1 and serum deprivation protein response (SDPR)/cavin-2 in the lipid rafts of MCF-7/ADR cells. Extracted ion chromatogram as well as results of RT-PCR and immunoblotting supports their highly upregulation in MCF-7/ADR cell. Subsequent experiment such as measuring

fluidity of PTRF knockdown cells indicates the necessity of PTRF for the regulation of MDR in MCF-7/ADR cells.



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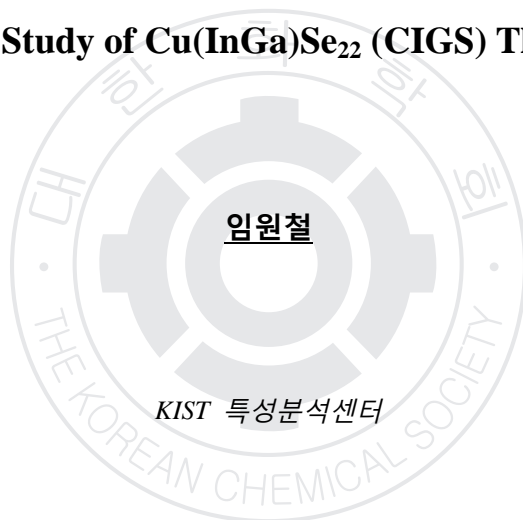
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## A SIMS Study of Cu(InGa)Se<sub>22</sub> (CIGS) Thin Films



In these days, interesting novel applications in photovoltaics are focused on thin and flexible solar modules, especially in the fields of space, aeronautics, and mobile applications. Within the past years, many researchers have been studied the development of flexible and lightweight CIGS modules and especially the role of Na in CIGS films was frequently studied. However, CIGS thin films contain a little amount of Na like 0.1 %, so that depth profiles of Na in CIGS are so difficult to obtain by general analytical techniques. Dynamic SIMS has been widely used in an elemental analysis and a depth-profiling for a trace materials existed on the surface because it is highly sensitive enough to detect small amount of ions like ppm or ppb. There are many experimental conditions and factors to affect the SIMS depth profiling, such as primary ion, beam energy, surface roughness, position in the sample stage, and homogeneity of chemical composition of the sample, etc. Therefore, we evaluated Dynamic SIMS where it is a suitable quantitative analysis technique for thin layer mixed with homogeneous bulk material such as CIGS.



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## Metal-Peptide Framework Compounds That Extend in One and Two Dimensions

이향렬 Neil Marsh<sup>1</sup>

충주대 생명공학과 <sup>1</sup>The University of Michigan, Ann Arbor

Abstract\_Peptides are attractive ligands for the design of metal organic frameworks, with the potential to confer chirality and biological activity on these materials. However, very few such materials have been reported. Here we describe the X-ray structures of four extended molecular framework compounds formed by the complexation of di- and tripeptides with cadmium ions. The tripeptide complex of cadmium with glycine,  $\text{Cd}(\text{Gly}_3)_2 \cdot \text{H}_2\text{O}$ , forms a two-dimensional complex in which the carboxylate group of the peptide bridges between Cd ions. In contrast, the tripeptide complex of cadmium with alanine,  $\text{Cd}(\text{L-Ala}_3)_2$ , forms a onedimensional extended molecular chain comprised of an infinite series of rings linked together through the Cd ions. The dipeptide complexes  $\text{Cd}(\text{L-Ala}_2)_2$  and  $\text{Cd}(\text{L-Ala}, \text{L-Thr})_2 \cdot 4\text{H}_2\text{O}$  form covalently linked two-dimensional square lattices. Hydrogen bonding between peptide amide groups and hydrophobic interactions between side chains are seen to play important roles in defining these extended structures. Most interestingly, substitution of the more hydrophilic threonine side

chain in place of alanine introduces a layer of water molecules into the crystal lattice. These results suggest that it may be possible to engineer the properties of these extended networks through judicious choice of amino acid side chains.



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## **Targeted lipidomic analysis of phosphoinositides of PTEN expression in mammalian cells**

김영준

건국대 응용생화학과

The targets of this study were identification of the molecular species of phosphoinositides and their quantitative analysis upon expression of PTEN protein in HeLa cell and HEK 293 cell line. For PTEN protein expression, transfection was performed by using mutant type (C124S) and wild type plasmid in HeLa cell and HEK 293 cell line. To identify the expression of PTEN protein, western blot was carried out by using appropriate antibodies. For mass spectrometric analysis phosphoinositides were extracted through 2 step extraction process using HCl. In the present experiment it was found that increased number of PIP3 with different fatty acid specificity were identified in the mutant type PTEN expressing cells compared to wild type PTEN expressing cells. In contrast increased number of PIP2 with different fatty acid specificity were identified in the wild type PTEN expressing cells compared to mutant type PTEN expressing cells. Quantitative study also showed that PIP3's were quantitatively increased in mutant type PTEN expressing cells in both cell types compared to the wild type expressing cells. These results suggest

that PTEN act as a suppressor of PIP3 level in cell and thus this may have significant implications for the many cellular processes in cancer cell.



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## Microscopy data analysis using Pipeline Pilot

이창준 최승훈<sup>1</sup>

(주)인실리코텍 ABU<sup>1</sup>(주)인실리코텍

Microscopy is one of the foundational tools of biology, and researchers have for centuries relied on their own visual systems to interpret what they see. Although examining tens of thousands of samples by eye is tedious, researchers are often highly motivated to invest the effort in order to discover samples of interest or annotate large sets of chemically or genetically perturbed samples. Pipeline Pilot is useful tools for microscopy data analysis. It enables researchers to rapidly explore, visualize and report research results. It aggregates and provides immediate access to the volumes of disparate research data locked in silos and automates the scientific analysis of that data. Collections are set of components grouped by category of science or function. Workflows for data retrieval, filtering, analysis, and reporting are developed by graphically combining components. also it enable to deal both simple data formats (text and numeric data) as well as complex scientific data types (image, chemical structures, and biological sequences). So we show various calculation for microscopy data analysis using Pipeline Pilot.

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## Preparation of PAMAM derivatives conjugated with biodegradable oligopeptides for gene delivery system

손상재 유광식<sup>1</sup> 이영화<sup>1</sup> 최준식<sup>2</sup>

분석과학기술대학원(GRAST) <sup>1</sup>충남대 생화학과 <sup>2</sup>충남대 생화학과, 분석과학기술대학원

In gene delivery system, PAMAM dendrimer generation 4 (PAMAM G4) has been widely used as a polymeric nonviral vector. Therefore, we adopted PAMAM G4 as a template polymer and conjugated amino acids on its surface. First, GABA and Arg were conjugated to enhance hydrophobicity/flexibility and transfection efficiency, respectively. Second, oligopeptide of GFLG sequence was used as an enzyme-cleavable linker which should be degraded in lysosome/endosome compartment. Each synthesis step was performed using HOBt/HBTU and DIPEA. The synthesized cationic polymer was evaluated to confirm the formation with plasmid DNA by agarose gel retardation and picogreen reagent assay. The mean size of PAMAM G4 derivatives with plasmid DNA was analyzed by dynamic light scattering. To identify cytotoxicity, we performed MTT assay, and measured absorbance at 570nm. Transfection efficiency of the synthesized products were carried out by protein assay and luciferase assay. As results, we can confirm that PAMAM G4 conjugated with GABA and Arg showed lower cytotoxicity than PEI

25kDa. Particularly, PAMAM G4-GABA-R displayed higher transfection efficiency than other polymers. On the other hand, PAMAM G4 conjugated with GFLG sequence showed lower transfection efficiency and relatively higher cytotoxicity than other polymers.



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## Synthesis of PEG-PEI-dexamethasone conjugate for gene delivery applications

김태훈 최혜 유광식 박정현 최준식

충남대 생화학과

Gene transfer using non-viral vectors is a promising approach for the safe delivery of therapeutic genes. Among non-viral vectors, PEI-Dexa is a lipopolymer proven to be effective for gene delivery. Also, PEG reduces toxicity, improves the overall solubility, diminishes non-specific interactions with the serum proteins, and improve the transfection efficiency of polycationic polymers. In this study, PEG-Glu-PEI-Dexa was synthesized as a kind of biodegradable polycation for gene delivery. Two copolymer, PEG-Glu<sub>8</sub>-PEI-Dexa and PEG-Glu<sub>10</sub>-PEI-Dexa, were synthesized. Dexamethasone is the potent ligand of the glucocorticoid receptor which facilitates the transfer into nucleus, and it is known to enlarge the nuclear pore complexes. It was found that PEG-Glu<sub>8</sub>-PEI-Dexa and PEG-Glu<sub>10</sub>-PEI-Dexa were completely retarded at or above weight ratio (polymer/DNA) of 14 and 12, respectively. The average particle size of PEG-Glu<sub>8</sub>-PEI-Dexa/pDNA complex was  $132.1 \pm 5.97$  nm, and that of PEG-Glu<sub>10</sub>-PEI-Dexa/pDNA complex was  $98.1 \pm 5.27$  nm. To determine the transfection efficiency of PEG-Glu-PEI-Dexa, luciferase



activity was measured using the plasmid DNA (pCN-Luci) as a reporter gene. Cells were treated with PEI25KD, PEI2000 and PEG-Glu-PEI-Dexa at various concentrations. From the results of the transfection study, PEG-Glu-PEI-Dexa showed much enhanced transfection efficiency compared to native PEI2000. Also, PEG-Glu-PEI-Dexa displayed relatively lower toxicity compared to PEI25kD in various cell lines. These results indicate that with good transfection efficiency, low cytotoxicity and drug effect by dexamethasone, PEG-Glu-PEI-Dexa has a potential to be used as an efficient gene carrier.



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## Surface-Charge-Dependent Cytotoxicity of Nanoparticles

박수진 정민숙 송미령 김준성

(주)바이테리얼즈 부설연구소

We engineered nanoparticles with different surface charges(positive, negative) and studied their uptake efficiency and toxicity in cell lines. The differential surface-charge-dependent uptake efficiency of nanoparticles in cells play a critical role in the nanoparticles's toxicity profile.

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## Novel Diagnosis Method of anthrax protective antigen by Polyvalent Directed Peptide Polymer (PDPP) coupled ZnO nanorods

박혜연 윤문영

한양대 화학과

*Bacillus anthracis* is a causative agent of anthrax. The key virulence factor of anthrax toxin is composed of three proteins: the protective antigen (PA, 83kDa), lethal factor (LF), and edema factor (EF). The PA delivers both LF and EF into cells after binding with its cellular receptor and, as a result, the PA has been found to be most reliable method for the early detection of anthrax infection. The existing methods for detecting anthrax PA utilize antibodies, peptides, or aptamers as capture probes. Specifically, peptides are much smaller molecules compared to whole antibodies, have highly specific interactions with targets, possess greater chemical and physical stabilities, are typically less immunogenic, are nontoxic, and are relatively simple to produce. However, single peptides have limited binding affinities and cross-reactivity compared to those of antibodies. Consequently PDPPs, which consist of multiple peptides on a polymer bound to multiple receptors on a target, are a promising method to improve binding affinity and specificity compared to those of single peptides. Herein, we developed a novel technique for ultra-

sensitive detection of PA using an array of zinc oxide (ZnO) nanorod in conjunction with a FITC-labeled PDPP. Furthermore, the use of ZnO as fluorescence enhancing substrates with PDPP permitted a lower limit detection range (ag mL<sup>-1</sup> level) of PA. Therefore, the design of a novel and ultrasensitive PDPP suggests many important possibilities for the development of new probes for future anthrax PA diagnostic methods.



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## Development of Eco friendly Citrus canker prevention agent using oligo-nucleotide

**BAIG IRSHAD AHMED 윤문영**

한양대 화학과

Citrus canker caused by *Xanthomonas axonopodis* pv. *citri* is by far the most widespread and severe form of the disease. *Xanthomonas axonopodis* infection causes lesions on the leaves, stems, and fruit of citrus trees, including lime, oranges, grapefruit, and mandarins. We set FtsZ, a cell division protein, as a target. Since, it has recently shown to be an important target for antibiotics. FtsZ polymerizes into tubulin-like protofilaments by head-to-tail association of individual subunits. As FtsZ plays critical roles in bacteria, FtsZ inhibitor prevents bacterial growth. In this study, we performed FtsZ gene cloning to generate recombinant FtsZ protein. A 1.2 Kbp FtsZ coding gene was amplified by polymerase chain reaction with specific primer and amplified gene was ligated into pET 28a vector plasmid. Recombinant FtsZ was purified with Ni<sup>2+</sup> affinity chromatography column. Furthermore, we looked for characterization and in vitro activity of recombinant FtsZ protein. Through inhibitor screening using SELEX with recombinant FtsZ protein, we will look obtain the oligo-nucleotide which binds specifically to protein.

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**Structure-function relationship of the insect antimicrobial peptide,  
Papiliocin and its analogs isolated from the swallowtail butterfly,**

*Papilio xuthus*

김진경 김양미

건국대 생명공학과

Papiliocin is a novel 37-residue cecropin-like peptide, isolated from the swallowtail butterfly, *Papilio xuthus*. With the aim of identifying a potent antimicrobial peptide, we tested papiliocin in a variety of biological and biophysical assays, demonstrating that the peptide possesses very low cytotoxicity against mammalian cells and high bacterial cell selectivity, particularly against Gram-negative bacteria as well as high anti-inflammatory activity. Dye leakage experiments showed that papiliocin targets the bacterial cell membrane. The three-dimensional structure of papiliocin shows that papiliocin in 300 mM DPC micelle has  $\alpha$ -helical structures from Lys<sup>3</sup> to Lys<sup>21</sup> and from Ala<sup>25</sup> to Val<sup>36</sup> and a hinge structure in between. In order to investigate structure-activity relationships, we designed and synthesized papiliocin analogs. We found a 22mer analog showing outstanding biological activity without toxicity against mammalian cells. Interactions between peptide and LPS studied using tryptophan blue-shift and STD-NMR experiments

revealed that Trp<sup>2</sup> and Phe<sup>5</sup> at the N-terminal helix play an important role in attracting papiliocin to the cell membrane of Gram-negative bacteria. Therefore, study of the structure-activity relationships of papiliocin would be helpful in designing antimicrobial peptides with potent antibacterial activities without cytotoxicity.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Retinoyl-Peptide Derivatives for Enhancement of Type- I Collagen Synthesis and Reducing Cytotoxicity

양진경 곽선영 이윤식

서울대 화학생명공학부

Retinoic acid has a lot of biological activities such as cell differentiation and growth, anti-tumor activities, and cell-cell signaling and enhancing collagen synthesis. It has been intensively studied in the pharmaceutical and cosmetic industries. Analogues of retinoic acid such as retinol, retinyl ester, retinaldehyde, and retinoyl-amino acid derivatives have also been developed as alternatives due to its strong cytotoxicity. We conjugated various peptides to retinoic acid by solid-phase method for reducing cytotoxicity and enhancing type- I collagen expression. As expected, most of the resulting retinoyl-peptides reduced cytotoxicity and increased collagen synthesis compared to retinoic acid, peptide, and a mixture of retinoic acid and peptide. Some retinoyl-peptides increased type- I collagen expression without cytotoxicity.



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## **Combination of Epstein-Barr virus-based plasmid and polyamidoamine dendrimer derivatives for the enhanced and sustained gene expression**

**최혜 최준식**

충남대 생화학과

Epstein-Barr Virus (EBV)-based plasmids contain EBV nuclear antigen (EBNA-1) and origin of replication (oriP) for sustained gene expression and stable episomal maintenance. The plasmids are efficient vectors for nonviral gene therapy through combining with various nonviral gene delivery systems such as cationic polymers and liposomes. In this work, we prepared Epstein-Barr Virus (EBV)-based plasmids and applied to gene transfection study using PAMAM-based dendrimer/EBV-based plasmid complexes in vitro. We constructed pCEP4-Luc and pCEP4-GFP plasmids using pCEP4 vector which contains EBNA-1, EBV oriP gene and hygromycin resistant gene. We measured dynamic light scattering (DLS) and zeta potentials of PAMAM-based dendrimer/EBV-based plasmid complexes (polyplexes). The polyplexes were transfected in HEK 293 cell lines and monitored luciferase activity and

green fluorescence protein (GFP) expression. We observed results of the enhanced and sustained gene expression in our PAMAM-based cationic polymer/EBV-based plasmid complexes system.



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## Synthesis of basic amino acid-conjugated polydiacetylene liposomes for non-viral vector system

배선주 최혜 박정현 최준식

충남대 생화학과

Diacetylene lipid monomers could form vesicles and polydiacetylenes(PDA) could be made by photopolymerization of self-assembled diacetylene monomers. Among the various diacetylene lipids, 10,12-pentacosadiynoic acid (PCDA) is one of the most extensively studied target materials for the preparation of various polydiacetylene structures and the platform application technology of detecting biomolecules as well as diverse environmental stimuli. Visible color change from blue to red occurs in response to a variety of environmental perturbations. 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 introduced cationic amino acids at the surface of PCDA liposome using SPPS ( solid phase peptide synthesis ) methods and prepared liposome solutions at

various molar ratios. When the liposomes were transfected at several mammalian cells, high transfection efficiency and low toxicity was observed.



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## Optimized Expression, Purification, and Structural Characterization of hMC4R-TM2

박유근 김용애

한국외국어대 화학과

Human melanocortin-4 receptor (hMC4R) has a critical role in part of energy homeostasis, and their heterozygous mutations related in genetic cause of severe human obesity. In order to study the structure and function of these human trans-membrane proteins, it is important to prepare reasonable amounts of proteins. However, the preparation of human MC4R transmembrane peptide is seriously difficult and time-consuming. Overexpression and purification of membrane proteins were reported to be difficult due to their innate insoluble and toxic properties. Among the many difficulties, the most important is the difficulty in obtaining sufficient quantities of purified protein. Recently, we succeed to produce large amounts of the second transmembrane domain from the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). The purified protein contains a few amounts of KSI fragment somehow. Therefore, we spend a lot of time to optimize the purification schemes like Fast Protein Liquid Chromatography, dialysis, and CNBr cleavage. In here, we demonstrate the optimization procedures to express and purify wild type-

hMC4R TM2 and mutant-hMC4R TM2 peptides and NMR structural studies in different detergents to get high-resolution spectra. We will also explain the structural difference between wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2) in membrane-like environments.



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## Targeted Genome Editing using Single Chain Zinc Finger Dimeric Nuclease

Muhammad Mustafa

연세대 화학과

The ability to achieve site-specific gene manipulation of the genome has widespread implications for basic and applied research. Gene targeting is a process in which site specific mutations are created which lead to gene knockout or an exogenous DNA molecule is incorporated into target site by replacing the corresponding chromosomal segment via homologous recombination to introduce a desired phenotype. Zinc finger genome engineering is based on the introduction of DSB created at a specific locus to activate the cell's endogenous homologous recombination mechanism with simultaneous supply of exogenous donor DNA to introduce a desired genetic modification. An engineered zinc finger Nucleases (ZFNs) have fusions between the DNA cleavage domain of FokI and a custom-designed ZF binding domain. Two independent ZFNs needs to be organized across the target site on the DNA to create a functional dimeric zinc finger nuclease. Several attempts were made to design rapid assembly methods for the synthesis of custom designed DNA binding domain and to improve the architecture of nuclease for better activity. We developed a Hierarchical Assembly Method for Multi-Zinc Finger Array (HAMZF) to synthesize up to

eight zinc finger domains providing 24bp recognition to zinc finger nuclease. The strategy is based on position specific primer design which enables each zinc finger encoding DNA sequence to be arranged according to their relative position. Further the catalytic domains of FokI were linked via flexible (10× GGGGS) amino acids linker and custom designed zinc finger binding domain to synthesize the single chain zinc finger nuclease.





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## Hypo-pigmenting Activity of Milk-derived Peptides

공새롬 곽선영 이윤식

서울대 화학생물공학부

Recently, several milk-derived peptides were reported as antioxidant. However, their biological roles on melanogenesis have not been thoroughly investigated. Here, we studied hypo-pigmenting activity of milk-derived peptides. Milk-derived peptides and their shorter fragments were prepared by solid-phase method and their antioxidant and tyrosinase inhibitory activities were studied. We found that several peptides revealed good tyrosinase inhibitory activity and studied their structure and activity relationships. Furthermore, we demonstrated that some milk-derived peptides sufficiently reduced melanin synthesis in Mel-A3 and B16 cells, without cytotoxicity.

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## Integrin Targeted PAMAM Dendrimers as Tumor Specific Non-viral Gene Delivery Carriers

유광식 최준식

충남대 생화학과

Targeting moiety of the delivery carrier is essential for the target specific delivery of cargo materials. In this study, we introduced tumor specific RGD (Arginine-Glycine-Aspartic acid) sequence to the 4th generation of PAMAM dendrimer. RGD sequence has been applied in many researches that aiming tumor specific gene or drug delivery carrier system. Tumor specific  $\alpha\beta_3$  integrin selectively interacts with RGD sequence, thus the target specific delivery could be expected. Synthesis of PAMAM G4-R-DGR was performed using HOBt/HBTU coupling method, and the conjugation yield was more than 90%. Synthesized PAMAM G4-R-DGR was effectively condensed pDNA with a relatively low charge ratio (2:1, polymer/pDNA) and the transfection efficiency was examined in HepG2 cell line.

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## Structure of Ferritin and Apoferritin in solution: Assembly and Disassembly Behaviors

김미희 노예철 안병철 정성민 정정운 김경태 권원상 고용기 권경호 김영용<sup>1</sup> 이진석

송성진 이문호

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학

We investigated the structures of apoferritin and the ferritin core in a neutral solution by X-ray scattering measurements. Under neutral conditions, apoferritin assumed an intact hollow spherical structure that was identical to the structure determined in the crystalline state. The structure included 24 homologous subunits (to form a 24-mer). The intact hollow spherical of apoferritin was stable over the pH range 3.40-10.0. The apoferritin shell thickness was 2.3 nm, and the hollow core volume was 233.2 nm<sup>3</sup>. Below pH 3.40, apoferritin became unstable and underwent stepwise disassembly through several structural intermediates: a hollow spherical structure with two holes, a headset-shaped structure, and, ultimately, rodlike oligomers (mainly trimers) or monomers. Below pH 0.80, the disassembled subunits aggregated, which was attributed to denaturation. Structural recovery of the intermediates during the pH-induced

reassembly process depended on the history of the disassembly process: (i) Structural recovery of the rodlike oligomers was limited to the headset-shaped oligomers. (ii) Structural recovery of the headset-shaped oligomers was limited to the hollow spherical structures with two hole defects (20-mer). (iii) The hollow sphere with two hole defects never recovered back to the originally intact hollow sphere. The ferrihydrite core of ferritin under neutral conditions assumed a compact globular structure. The ferrihydrite core was estimated to have a volume of  $142.0 \text{ nm}^3$ , which corresponds to  $\sim 60.9\%$  of the hollow core volume of apoferritin. The ferritin core was stable over the pH range 2.10-10.0. Below pH 2.10, the ferritin core underwent aggregation as a result of the disassembly of the ferritin shell under such strongly acidic conditions.



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## Structure Analysis of Fullerene Attached i-motif DNA with Complementary DNA using Small-angle X-ray Scattering

이진석 노예철 안병철 김미희 정정운 김경태 정성민 권경호 김영용<sup>1</sup> 송성진 위동우<sup>1</sup>

김용완 김종현 이문호

포항공과대 화학과 <sup>1</sup>포항공과대 첨단재료과학

The Structure of fullerene attached i-motif DNA with its complementary sequence were investigated by analyzing the X-ray scattering pattern of fullerene-free and fullerene-bound i-motif DNA in solutions of varying pH. To facilitate a direct structural comparison between the i-motif and duplex structures in response to pH stimulus, we developed atomic scale structural models for the duplex and i-motif DNA structures, and for the fullerene/i-motif DNA hybrid associated with the cDNA strand, assuming that the DNA strands are present in an ideal right-handed helical conformation. We found that fullerene shifted the pH-induced conformational transition between the i-motif and the duplex structure, possibly due to the hydrophobic interactions between the terminal fullerenes and an internal TAA loops in the DNA strand. The hybrid structure showed a dramatic reduction in cyclic hysteresis.

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## Screening of medicinal stuff to improve a cognitive ability

오영희 채용병 남향 박혜정 김경안 홍성국 김문무

동의대 화학과

The aim of this study is to screen a therapeutic agent to develop a medicine with cognitive function. The inhibitory effects of *Curcuma longa*, *Acorus gramineus* and *Polygalae radix* extracts on angiotension converting enzyme and acetylcholine esterase derived from rabbit lung and brain cells (PC12), respectively, as well as antioxidant effects were investigated in this study. First of all, to assess their cytotoxicity, MTT assay was carried out in PC12 cells. They showed no toxicity against these cells below 0.1%. In addition, it was observed that *Acorus gramineus* extract exhibited an excellent reducing power compared to other groups. Especially, *Polygalae Radix* extract showed a remarkable scavenging effect on DPPH radical. *Curcuma longa* extract inhibited production of hydroxyl radical by fenton reaction and increased nitric oxide promoting blood circulation in endothelial cells (EA.hy926). All extracts showed a protective effect on DNA oxidation produced by hydroxyl radical. Furthermore, these extracts at 0.1% exerted inhibitory effects on activities of both angiotension converting enzyme and acetylcholine esterase.

These results suggest that combination of above extracts could have a potential possibility as therapeutic agents for improvement of brain cognitive ability related to oxidative stress.



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## Self-assembly of enzymatically cleavable oligopeptide micelles as a gene delivery carriers

송수정<sup>1</sup> 손상재<sup>1</sup> 유광식<sup>2</sup> 이제일<sup>3</sup> 최준식<sup>2</sup>

충남대 분석과학기술대학원<sup>1</sup> 충남대<sup>2</sup> 충남대 생화학과<sup>3</sup> 충남대 분석과학기술학과

Gene delivery system using peptide micelles has received a considerable amount of attention. Peptide micelle system generally presents relatively low cytotoxicity and transfection efficiency compared to other polymeric gene carrier system. In this report, we propose a micelle model overcoming poor transfection efficiency. The micelle introduces GFLG sequence, Arginine and histidine for improving transfection efficiency. GFLG (Gly-Phe-Leu-Gly) sequence help escape from endosome-lysosome compartment because of enzymatically cleavable characterization. The sequence is known to be cleaved by proteolytic enzyme Cathesin-B. Arginine is a key element for the cell-penetrating peptide (CPP) and histidine displays enhanced the proton sponge effect. To form stable micelle, we make amphiphilic units composed of peptides having different property. The GFLG sequence is a hydrophobic core. The Hn-R segment is hydrophilic and cationic head group. In results, micelles/pDNA complex formation was



analyzed by agarose gel retardation and Pico-Green reagent. Furthermore, the transfection efficiency and cytotoxicity were measured by luciferase assay and MTT assay in HEK 293 cell.



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## ssDNA Aptamer Specifically Binding to Influenza Non-structural 1 (NS1) Protein

우혜민 정용주<sup>1</sup>

국민대 화학과<sup>1</sup> 국민대 생명나노화학과

Influenza is a contagious respiratory viral illness of global important. Influenza A virus belongs to the orthomyxoviridae and contains 8 segments of (-) ssRNA that encode 11 known proteins. NS1, one of the viral proteins of Influenza virus, was known for multifunctional protein. NS1 protein was known for blocking the IFN- $\beta$  pathway. Using a SELEX (systematic evolution of ligand by exponential enrichment) procedure, we selected a high-affinity DNA aptamer capable of binding to NS1 protein with a dissociation constant of 18.91 nM. We investigated the interaction between NS1 protein and aptamer by sandwich ELISA and western blot. We also elucidated the interaction between NS1 protein and RIG-I protein. We measured activation of the INF- $\beta$  promoter in 293T cells as a reporter gene for IFN induction. The aptamer that was isolated in this study are expected to be new molecular drug candidate as well as therapeutics for the design of Influenza diagnosis and treatment.

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## Genotyping of DNA Double Strand Break Repair Gene in Colorectal Cancer

문명진 안영창 조민호 윤일규 김경하 장원철<sup>1</sup>

단국대 화학과 <sup>1</sup>단국대 첨단과학대학

Colorectal cancer is major cause of morbidity and mortality in worldwide. According to ethiological study, colorectal cancers have been attribute to environmental factors. Inherited deficiencies of DNA repair gene, may alter repair capacity lead to increase risk of cancer. The repair gene Ku80 is important protein of non-homologous end-joining repair pathway, is thought to play an important role in the repair pathway of DNA double strand breaks. Here, we investigated to SNP of Ku80 (rs828907) in colorectal cancer tissues and control samples. Genotyping assay is PCR-RFLP followed by Denaturing HPLC (DHPLC).

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## ***SUMO4* gene Polymorphisms in Koreans patientswith Behcet's Patients by DHPLC**

**김경하 안영창 조민호 윤일규 문명진 장원철<sup>1</sup>**

단국대 화학과 <sup>1</sup>단국대 첨단과학대학

We examined the association of Small ubiquitin-like modifier 4 (*SUMO4*) polymorphisms with Behcet's disease (BD) in the Koreans population. *SUMO4* polymorphisms of autoimmune and inflammatory responses through regulation of NF- $\kappa$ B transcriptional activity is associated with autoimmune diseases BD. Moreover, a recent study suggested that *SUMO4* may be a general autoimmunity gene. Therefore, we investigated its association with BD in a well defined group of Koreans patients. Genotyping for *SUMO4* polymorphisms at G-847A, A-504G, A+163G, and C+438T loci was performed on 100 BD patients and 100 controls using denaturing high-performance liquid chromatography(DHPLC). As a results, we were able to identified the haplotype and polymorphisms in *SUMO4* gene by DHPLC of highly sensitivity, specificity and rapid technique.

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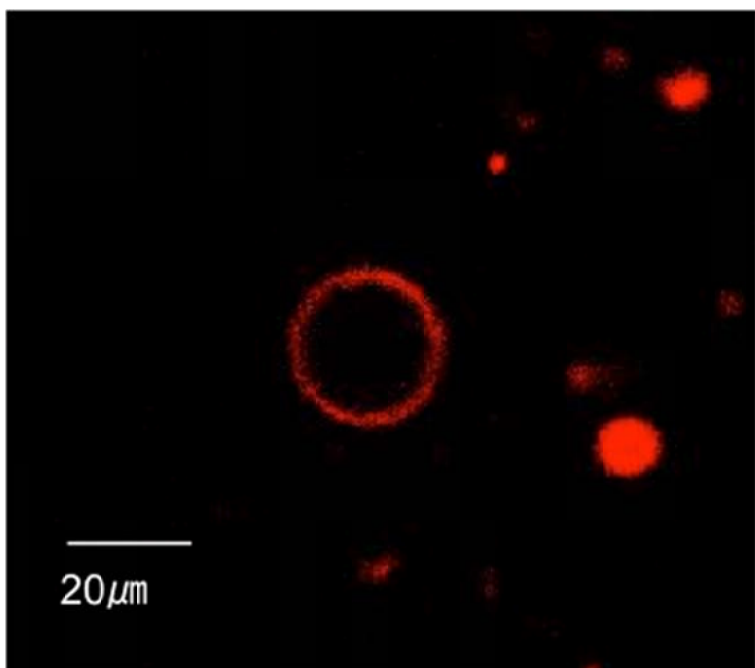
발표종류: 포스터, 발표일시: 수 18:00~21:00

**Direct influence of Plants regulation of Energy-dependent quenching  
caused by protein complex structural change and protein-lipids  
interaction**

**이길용 안태규**

성균관대 에너지과학과

The photosynthesis in plants is designed to perform two seemingly opposing tasks. First to efficiently harvest sunlight but also to rapidly dissipate excessively absorbed light energy harmlessly as heat to avoid deleterious photo damage. Under excessive light, up to 90% of the absorbed light can be dissipated via the non-chemical quenching pathway. This pathway consists of at least four different mechanisms. The fastest component is energy dependent quenching(qE) which due to the formation of the pH gradient. The mechanism of qE is still under debate. In this study, We reconstitute plant membrane protein which is Light-harvesting complex into giant unilamellar vesicle and using this sample we observe that direct influence of Plants regulation of Energy-dependent quenching caused by protein complex structural change and protein-lipids interaction using by fluorescence spectroscopy.



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## Antioxidant Activity Study of Caffeoyl Dipeptides

곽선영 양진경 이윤식

서울대 화학생물공학부

Caffeoyl dipeptides were prepared to develop novel antioxidant containing sufficient stability and strong antioxidant activity. When  $\beta$ -alanyl-L-histidine (carnosine) was conjugated to caffeic acid (CA), they showed excellent antioxidant activity in both hydrophilic and hydrophobic environments. In addition, we found that caffeoyl proline-histidine (CA-Pro-His) showed the excellent antioxidant activity amongst a small library of caffeoyl histidine-containing dipeptides (CA-His-Xaa, CA-Xaa-His) and caffeoyl proline dipeptides (CA-Pro-Xaa). <sup>1</sup>H-NMR study proved that CA-Pro-His existed as s-cis conformation. We assumed that proline provided a structural benefit, and thus, histidine imidazole could stabilize semi-quinone radicals of CA after hydrogen atom abstraction. In addition, CA-Pro-His showed good antioxidant activity in cell systems without cytotoxicity.

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## DNA nanostructures for drug delivery

**김경란 권혁성<sup>1</sup> 안대로<sup>2</sup>**

KIST 테라그노시스연구단 <sup>1</sup>고려대 생명공학과 <sup>2</sup>KIST 생체과학부

DNA cages are nanometer-scale structures formed by self-assembly of synthetic DNA oligonucleotides. It can be potential candidates for carriers in delivery for diagnosis and therapy. In particular, DNA tetrahedron is considered as an attractive tool in delivery technology and biomedical applications since it can be simply prepared with high yield and structural stability and encapsulate other molecules. Herein, we present a study on chemically modified DNA tetrahedron and demonstrate its utilities in drug delivery.



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## **An aptamer-based probe for diagnosis of cancer cells**

**김다래 안대로<sup>1</sup>**

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Nucleolin at the surface of cancer cells has been reported to be overexpressed in rapidly dividing cells. AS1411 aptamer is known to target nucleolin displayed at the surface of cancer cells. Hence, detection of surface nucleolin will be useful to distinguish malignant cells from normal cells. In this context, we studied the aptamer-conjugated DNA probe with signal amplification for diagnosis of cancer cells.

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## Preparation and Characterization of QD-anchored Silica Nanospheres with Silicate Coating

유지혜 이상화

경원대 화학생명공학과

최근에 양자점은 분자에 덮여있는 형광물질 때문에 바이오라벨링(biolabeling)에서 사용이 증가하고 있다. 쉬운 bioapplication 을 위해서는, 양자점은 친수성과 buffer 에서 안정성을 가져야 한다. 본 연구에서는 생체 시스템에서 양자점의 생체적합성과 지속성을 향상시키기 위해 양자점을 붙인 실리카에 sodium silicate 를 덮어 씌웠다. 실리카 표면은 기능화를 포함하며, 무독성이고, 산화로부터 나노입자를 보호한다. 본 연구에서 실리카 나노입자는  $\text{NH}_4\text{OH}$  를 첨가하여 교반 후, TEOS(tetraethyl orthosilicate)를 주입하여 졸-겔 반응을 통해 합성된다. 나노입자의 크기와 형태는  $\text{NH}_4\text{OH}$  와 TEOS 의 주입 양에 따라 달라 지는 것을 관찰 할 수 있다. 실리카 입자의 표면은 말단이 아민기(amine group)인 APTMS silane 에 의해 기능화 되고, 그 후 EDC coupling agent 를 사용하여 표면이 카르복실기(carboxylic group)인 양자점을 고정한다. 나노입자는 PL 분석을 통하여 양자점의 결합을 확인, 분석하였고,

DLS 를 통해 나노입자의 크기를 분석하였으며, SEM 및 TEM 을 통해 외각에 형성된 양자점이나 실리케이트의 형상 및 광학적 특성을 고찰하였다.



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## Fibril Formation of Collagen Confined in Lipid Vesicles

박수진 신관우<sup>1</sup>

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

섬유 단백질들은 대부분의 세포 안과 밖을 구성하고 있는 물질로서 세포의 모양과 세포벽의 단단한 정도와 같은 물리적인 성질에 큰 영향을 미치는 단백질이다. 그러므로 우리는 세포의 물리적인 성질을 측정하기에 앞서, 섬유 단백질을 제어하는 방법에 일차적인 목표를 두기로 하였다. 섬유 단백질로는 흔하고 비교적 다루기 편리한 콜라겐을 선택하였다. 콜라겐을 인공세포의 내부 또는 외부 막에 형성 시키기 위해서, 온도나 pH, 콜라겐의 농도 등을 변수로하여 섬유 형성 과정을 조절하기 위한 실험을 진행하고 있다. 후에는 콜라겐 섬유 뿐만 아니라 세포골격과 같은 섬유들로 단백질의 종류를 넓혀갈 것이다. 더 나아가 단순한 단백질 섬유의 생성 뿐만 아니라, 섬유 단백질의 형성 모양과 구조 등을 제어할 수 있도록 할 것이다.

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## **Substrate Preparation for a multi-cellular co-culture ; A targeted seeding and study of intercellular effects**

**박혜연 신관우<sup>1</sup>**

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

The purpose of this study is to demonstrate the making multi-cellular co-culture. We coated surface with hydrophobic and hydrophilic compounds which can lead a targeted seeding. Silanized glass surface is widely used for targeted patterning. We patterned surface with silane and PEG expecting classified cells attachment which show the selective attachment of cells against the surface. Moreover we can control separated multi-cellular co-culture by using pattern surface. We admire to make the single-single cell culture through minimized pattern size.

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## Screening of ssDNA aptamers using Cell-SELEX against *Salmonella typhymurium*

이상춘 윤문영

한양대 화학과

Food poisoning typically caused by pathogenic bacteria and their accumulated/released toxins. In the review of literature, the *Salmonella* spp. and *Escherichia* spp. are the major/wide spread pathogenic bacteria found the cause for food poisoning in Korea. The emergence of rapid diagnostic systems to detect these pathogenic bacteria was attracted much attention due to the findings of increased food poisoning occurrence from the imported food and public restaurants. Aptamers, generated from Systematic Evolution of Ligands by Exponential Enrichment (SELEX) are promising as diagnostic probes because of their high binding affinity against wide range of targets. Several SELEX methods were reported to date, generally depend on the targets used. Cell-SELEX is one among which has several advantages on aptamer selection. In this study, we performed Cell-SELEX to identify ssDNA aptamers against *S. typhymurium*. The stringent conditions including, salt concentrations, cell number and ssDNA pool concentrations were applied as Cell-SELEX rounds progress to obtain high affinity/specific binding

aptamers. After 10 rounds of Cell-SELEX the pools were cloned and sequenced. A total of 10 aptamer sequences were generated from the 10th round product of Cell-SELEX. Finally, 3 aptamers against *S. typhimurium* which binds with high affinity were synthesized with fluorescence labeling as a signal probe. Each aptamer binding affinity and specificity were characterized, respectively. Further studies of modification and conjugation of aptamers with nano-materials would expect the development of a sensitive detection system against *S. typhimurium*.



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## **Aspiration Setup for the measurements of Mechanical Properties of Artificial Lipid Vesicles : Area dilation and Lysis properites of Mitochondria-mimick vesicles**

**이두호 신관우<sup>1</sup>**

서강대 화학과 <sup>1</sup>서강대 화학과 및 바이오융합과정

Exocytosis 나 cell migration 과 같이 실제 세포에서 일어나는 biological process 는 이 biomembrane 의 mechanical property 에 지배적인 영향을 받는다. 따라서, 세포를 구조적으로 기능적으로 모사하는 작업에 있어서, membrane 의 physical character 를 이해하는 것은 매우 중요하다고 하겠다. 우리는 GUV(Giant unilamellar vesicle)를 membrane model 로 사용하여, cell membrane 의 가장 기본적인 physical property 인 area dilation modulus 를 측정해보았다. 이 측정을 위해서 cell manipulator, pressure sensor, capillary 를 결합하여 micropipette aspiration 장치를 완성하였다. 이번 실험에서는 우리가 setup 한 aspiration 장치를 이용하여, vesicle 의 lipid 조성이 membrane 의 mechanical property 에 어떤 영향을 주는지 알아보았다. 특히, inner mitochondrial membrane 에 특이적으로 많이 존재하는 cardiolipin 의 조성을 달리하여 그



변화를 관찰해보았다. 더불어, 기존 논문에 나와 있는 data 와 비교해 봄으로써 setup 된 장치를 더욱 정교하게 만들고자했다.



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## FACS based Imuunoassay for multiple analytes by using *E.coli* with autodisplayed Z-domains

박민 변재철<sup>1</sup>

연세대 신소재공학과 <sup>1</sup>연세대 신소재공학부

Microsphere-based flow cytometric assay is commonly used immune assay for the analysis of mixed analytes in solution. It is based on antibodies conjugated fluorescence micro beads and uses the flow cytometer for detection. In this study, we developed a new flow cytometric assay by using fluorescence and autodisplaying proteins co-expressing *E.coli*. The autodisplay technology is one of the surface display methods for proteins or peptides at the *E.coli* outer membrane. In the autodisplay technology, proteins are expressed as recombinant proteins in a poly protein precursor for the autotransporter secretion pathway and automatically aligned on the outer membrane surface. These aligned proteins can be used a affinity layer for capturing the analyte. The autotransporter vector and fluorescence protein expressing vector were transfected into the UT5600(DE3) *E.coli*. For the fluorescence proteins, eGFP and tdTomato were used and Z-domains were autodisplayed on the surface of *E.coli*. APC conjugated antibodies were treated to measure the activity of autodisplayed Z-domains and the activity Z-domain and expressed fluorescence

proteins was measured by using a fluorescence photometer and a flow cytometer. the result of fluorescence photometer shows that intracellular expressed eGFP and tdTomato have a excitation/emission wavelength of 488/507 and 554/581 nm. The flow cytometer result shows a clear increasement of fluorescence intensity after APC conjugated antibodies treatment.



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## Tailored preparation of *E.coli* outer membrane with autodisplayed proteins for immunoassays

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The autodisplay technology is one of the surface display methods for proteins or peptides at the *E.coli* outer membrane. In the autodisplay technology, proteins or peptides are expressed as recombinant proteins in a poly protein precursor for the autotransporter secretion pathway and automatically aligned on the outer membrane surface. These aligned proteins or peptides can be used as a molecular recognition layer or a affinity layer for immunoassay. For the preparation of outer membrane from autodisplayed *E.coli*, lysozyme was treated to hydrolyze the peptidoglycan layer and triton X-100 was used for dissolving the cell membrane. After the outer membrane isolation, marker proteins from outer membrane, periplasm, inner membrane and cytoplasm were selected and analyzed by western blot and the enzymatic assay. OmpF,  $\beta$ -lactamase, secA and  $\beta$ -galactosidase were used for western blot and KDO,  $\beta$ -lactamase, NADH oxidase and  $\beta$ -galactosidase were analyzed by enzymatic assay. Isolated outer membrane were layered on the surface of 96 well microplate by using hydrophobic interaction and

layered outer membrane were analyzed by enzymatic assay. The purity of isolated outer membrane and its layer was calculated and the Z-domains, have a binding affinity to Fc region of IgG, autodisplaying outer membrane layer was used for the immunoassay to improve the sensitivity.



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## Langmuir Monolayer Study of Mitochondrial Inner Membrane Lipids

Phan Dinh Minh 신관우<sup>1</sup>

서강대 화학과 <sup>1</sup>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  $\pi$ -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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## **protein immobilization with parylene family**



**고혁 이가연 변재철**

연세대 신소재공학과

A new covalent immobilization method for small proteins and short peptides is presented by using parylene-H film which, is a polymer of p-xylene having formyl groups. The covalent coupling of proteins to the parylene-H film is produced by only one step of incubation of proteins or peptides without additional coupling reagents. In this work, the parylene-H film is coated on a 96-well microplate for immunoassays. The immobilization efficiency to the parylene-H film was compared with the conventional physical adsorption by using human chorionic gonadotrophin protein and a small peptide called circulated citrullinated peptide as model molecules. Additionally, the applicability of this immobilization method for short peptides is demonstrated by detecting autoantibodies in rheumatoid arthritis patient serum.



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## Monitoring of in vitro DNA recombination using impedimetry

조현호 이성환 송시명 반창일

포항공과대 화학과

DNA recombination is essential for every living organism. DNA recombination can be divided into two mechanisms depending on the cell cycle: homologous recombination (HR) and nonhomologous end joining (NHEJ) recombination. In particular, many investigations have focused on the HR system due to its generality. Because the correct operation of the HR system is crucial for preventing diseases, the detection of recombination is of valuable significance for research. In this work, the electrochemical method was used to detect DNA recombination process. The 5'-thiol-modified strand (0.5  $\mu\text{M}$ ) was immobilized on the gold electrode with 1-pentanethiol (0.5  $\mu\text{M}$ ), which improves the interaction between DNA strands and the protein by providing sufficient room for binding. The progression of the reaction at each step was monitored by measuring the changes in  $R_{ct}$  on Nyquist plots. All measurements were carried out in PBS buffer (pH 7.4) with 5 mM  $[\text{Fe}(\text{CN})_6]^{3-/4-}$ . The normal DNA recombination reaction successfully reduces the amount of DNA on the electrode by cutting the strand. Therefore, successful DNA recombination detection was verified by impedance spectroscopy.

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## Development and characterization of ssDNA aptamers against *Plasmodium* lactate dehydrogenase, a biomarker for malaria

이성환 조현호 송시명 반창일

포항공과대 화학과

*Plasmodium* lactate dehydrogenase (pLDH) have been widely used in the diagnosis of malaria as a target protein because of its high expression level in all human malaria species. Herein, pLDH-specific ssDNA aptamers were developed by Systematic Evolution of Ligands by EXponential enrichment (SELEX) using magnetic beads. Both the pL1 and pL2 aptamers selectively bound not only to *Plasmodium vivax* LDH, but also to *Plasmodium falciparum* with high sensitivity ( $K_d = 16.8 \pm 0.6 \sim 49.6 \pm 1.4$  nM). The thermal stability was characterized to investigate its availability in hot conditions. The melting curves of the pLDH aptamers showed high  $T_m$  values (51.3 ~ 53.1 °C), and as the temperature increased (from 25 °C to 60 °C), inflection points at 260 nm were not shifted in CD spectra. In addition, three common portions of the pLDH aptamers were analyzed using a mutational study based on secondary structure predictions. The loop 1 and loop 2 sequences are essential for binding to pLDH proteins, and the G-C rich stem is necessary to maintain the structural stability of the pLDH aptamers. On the other hand, the

enzyme activity with the aptamers was measured to investigate whether the pLDH aptamers work as an antagonist or an agonist. Although the pLDH aptamers did not affect the enzyme activity in this simple system, it is worthwhile to investigate the applications of the aptamers as drugs or as drug delivery tools. In conclusion, the pLDH aptamers have potential for detection of pLDH proteins in various conditions due to their high affinity to targets and high thermal stability. Thus, the pLDH aptamers will be utilized in the effective diagnosis, monitoring, and surveillance of malaria.



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## Streptavidin-based multivalent peptide inhibitors

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KIST 의공학연구소 <sup>1</sup>KIST 생체과학부

Hypoxia-inducible factor (HIF)-1 $\alpha$  is a transcription factor subject to oxygen-dependent ubiquitination and then degradation under normoxia. The activity of HIF-1 $\alpha$  is related with interaction between Pro564-hydroxylated HIF-1 $\alpha$  and von Hippel?Lindau protein-Elongin B?Elongin C (VBC) or HIF-1 $\alpha$ /p300 complexation. This oxygen-dependent activity of HIF-1 $\alpha$  plays an important role for angiogenesis. Thus, control agent for the HIF-1 $\alpha$  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 HIF-1 $\alpha$  activity. We have also evaluated potency of the multivalent peptide inhibitors at the cellular level as well as in vitro.

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## Development of aptamers for sulfadimethoxine

송시명 조현호 이성환 반창일

포항공과대 화학과

Sulfadimethoxine is a widely used antibacterial agent of the sulfonamide class and is employed almost exclusively for the treatment of coccidiosis in many species. In this work, the single-stranded DNA (ssDNA) aptamers, which were specific bio-probes for sulfadimethoxine, were discovered by a systematic evolution of ligands by exponential enrichment (SELEX) method. Among several SELEX techniques such as affinity chromatography, capillary electrophoresis, and magnetic beads-based method, the magnetic beads-based strategy was used because of its simplicity. Sulfadimethoxine was immobilized on the magnetic bead via nucleophilic substitution reaction between the amine functional group of sulfadimethoxine and the tosyl-activated magnetic beads. Through several rounds of SELEX, two aptamers were successfully selected and determined. In order to detect sulfadimethoxine, the aptamers modified by fluorescein amidite (FAM) and a fluorescence quencher were utilized. By detecting the changes of fluorescence, sulfadimethoxine was selectively and sensitively detected.

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## Magnetic bead based immunoassay by using *E.coli* cells with autodisplayed Z-domains

유구 박민 변재철

연세대 신소재공학과

Recently, Z-domain was expressed as a fusion protein at the outer membrane of *E.coli* by using autodisplay technology. Because of the binding activity towards the Fc region of IgG, the Z-domain has been used for the orientation control of the antibodies in order to improve the sensitivity of immunoassays. By immobilizing detection antibodies, the *E.coli* cell with autodisplayed Z-domains could be applied for “direct immunoassay” and this type of immunoassays could achieve hyper sensitive results. For the direct immunoassay, however, the *E.coli* should be centrifuged repeatedly for washing steps and reagent chaging steps. In this work, magnetic beads were used as a solid support of the *E.coli* cells with autodisplayed Z-domains in order to perform the direct immunoassay without centrifugation steps. By using super-paramagnetic beads, the centrifugation step was simply replaced to the separation step by using an external magnet. For the immobilization of *E.coli* cells to the magnetic beads, the surface of magnetic beads was modified with poly-L-lysine to bind the negatively charged *E.coli* cells. In this work,

the changes in surface charge and diameter of the magnetic beads were analyzed during the modification steps to confirm the construction of *E.coli*-magnetic bead complex. The formation of *E.coli*-magnetic bead complex was also analyzed by using SEM images. For the feasibility test of magnetic bead based immunoassay, horseradish peroxidase (HRP) was used as a model analyte and a biomarker for inflammatory diseases called C-reactive protein (CRP) was used for demonstration of an application to medical diagnosis.



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## Modular Aptasensor System Using Cucurbit[7]uril-Ferrocene Derivative As a Supramolecular Linker

이돈욱 공보경 류성호<sup>1</sup> 김기문

포항공과대 지능초분자연구단, WCU 첨단재료과학부, 화학과 <sup>1</sup>포항공과대 분자생명과학부

Aptamers are artificial single-stranded nucleotide sequences that fold into secondary and tertiary structures making them bind to certain targets with extremely high specificity. Several advantages of aptamers over antibodies including high stability and easily modifiable structure make them promising sensing element for biosensor. However, only a few methods for immobilizing the aptamers on a sensor chip have been developed including the ones using the streptavidin-biotin pair, which has yet several demerits such as tedious immobilizing steps and limited stability under harsh conditions. Here we present our efforts to develop a surface plasmon resonance (SPR) sensor for specific protein detection using aptamer as a sensing unit and cucurbit[7]uril-ferrocene derivative (CB[7]-AFc) pair as a novel synthetic non-covalent linker for immobilizing aptamers. The 37 kDa protein thrombin and 15-mer oligonucleotide thrombin binding aptamer (TBA) were chosen as a model target protein and aptamer, respectively, to demonstrate the sensing ability of the system. The monolayer of synthetic receptor CB[7] on a gold



surface produced by spontaneous adsorption successfully immobilized AFc-labeled TBA by ultrastable host-guest interaction between CB[7] and AFc. The immobilized TBA selectively sensed the injected thrombin in the concentration range  $10^{-9} \sim 10^{-7}$  M. The simple and modular method for surface immobilization using the synthetic receptor-ligand pair may broaden the applications of aptamer-based sensor.



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## SPR biosensor based on immobilized *E.coli* cells with autodisplayed Z-domains

이은행 유구 박민 변재철

연세대 신소재공학과

The Z-domains of protein A was expressed as a fusion protein at the outer membrane of *E.coli* by using the autodisplay technology. Because of the specific affinity towards the Fc region of immunoglobulins (IgG's), the Z-domains have been used for the orientation control of antibodies in order to improve the sensitivity of immunoassays. In this work the *E.coli* with autodisplayed Z-domains was immobilized as a monolayer to the SPR biosensor by the charge interaction. The surface modification was carried out by sequential layering of parylene-H film with formyl groups and poly-L-lysine, and then the *E.coli* cells were immobilized by the charge interaction. The effectiveness of this layer for the immobilization of *E.coli* was estimated by counting the number of *E.coli* cells in comparison with bare gold surface and poly-L-lysine coated gold surface. For the test of feasibility of the immobilized *E.coli* cells to SPR biosensor, the stability of immobilized *E.coli* cells was estimated by treatment of concentrated salt solution to the immobilized *E.coli* cells which were bound through the charge interaction. From this test,

the *E.coli* cells immobilized to the parylene-H film with poly-L-lysine coating were determined to be stable under the salt concentration of human serum. Then, the applicability of the immobilized *E.coli* cells with autodisplayed Z-domains was demonstrated by detection of C-reactive protein (CRP). The effect of orientation control by autodisplayed Z-domains was estimated by comparing the sensitivities by immobilization through the physical adsorption and charge interaction to poly-L-lysine coated layer.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Non-labeled immunoassay based on zeta-potential analysis



이은행 변재철

연세대 신소재공학과

Immunoassay has been widely used for the detection of target analytes in complex mixtures such as blood by using highly specific antigen-antibody interactions. In this work, antibodies against a target analyte was immobilized to magnetic beads and the change of surface charge of a magnetic bead was measured after the binding of a target protein by using a zeta potential analyzer. For the feasibility test of the zeta potential analysis for immunoassays, horseradish peroxidase (HRP) was used as a model target analyte. The application to medical diagnosis was demonstrated by detection of C-reactive protein (CRP) which is known to be a biomarker for inflammatory diseases

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## DNA-coated micelles and their application in immunoassays

**Hoang Thi Hoa 안대로<sup>1</sup>**

과학기술연합대학원대 Nanomaterial&Science<sup>1</sup>KIST 생체과학부

Immunoassay is a representative technique for detect the disease biomarkers and pathogenic biological agents which often present a ultra-low levels in sample. To improve sensitivity of the immunoassay, we here described that the nano-sized micelles coated with ss-DNA can be employed to amplify the detectable signal in oligonucleotide-linked immunosorbent assay (OLISA). The OLISA based on the micelles was evaluated for quantification of a liver cancer maker and showed lower limit of detection than ELISA and normal OLISA.

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## Structure-Activity relationships of coprisin isolated from the dung beetle, *Copris tripartitus*

이은정 김진경 이주호 정기웅 김양미

건국대 생명공학과

The novel 43-residue defensin-like peptide, coprisin isolated recently from the Dung Beetle, *Copris tripartitus* exhibits antimicrobial activities against standard bacterial strains as well as drug-resistant bacterial strains. To study structure-activity relationships, we determined the three-dimensional structure of coprisin in aqueous solution by NMR spectroscopy, showing that coprisin has an amphipathic alpha-helical structure from Ala<sup>19</sup> to Arg<sup>28</sup> and beta-sheet from Gly<sup>31</sup> to Gln<sup>35</sup> and Val<sup>38</sup> to Arg<sup>42</sup>. Coprisin has a highly electropositive regions positioned at the end of the helix (Arg<sup>28</sup>), turns between the helix and the first strand of the sheet (Lys<sup>29</sup>, Lys<sup>30</sup>), and C-terminus (Arg<sup>42</sup>). We studied anti-inflammatory activity of coprisin, examining the effect of coprisin on lipopolysaccharide (LPS)-induced inflammatory response by measuring nitric oxide (NO) release and inflammatory cytokines. As coprisin was treated in LPS-stimulated mouse macrophage cells, the process of gene transcriptions for inflammatory cytokines was inhibited. We have demonstrated that coprisin shows profound antibacterial activities since coprisin has

an amphipathic helix and electropositive surface which may play important role in its structure stability and effective interaction with bacterial lipid membrane. Furthermore, coprisin is a potent anti-inflammatory peptide with antibacterial activities, and this work may help to understand its mechanism of action in near future.



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## Antibacterial and anti-inflammatory activities of enantiomeric 9-mer peptide analogs derived from protaetiamycine

이은정 김진경 정기웅 김양미

건국대 생명공학과

Protaetiamycine is an insect defensin, derived from the larvae of the beetle *Protaetia brevitarsis*. We designed four 9-mer peptide analogues based on the sequence of RLWLAIGRG-NH<sub>2</sub>, in which Gly or Ile was substituted with Arg, Lys, or Trp to optimize the balance between the hydrophobicity and cationicity of the peptides and to increase bacterial cell selectivity. We investigated their toxicities to bacteria and mammalian cells as well as inflammatory activities. The results suggest that the bactericidal action of our potent antibacterial peptides, namely 9Pbw2 (RLWLAIKRR-NH<sub>2</sub>) and 9Pbw4 (RLWLAWKRR-NH<sub>2</sub>), may be attributed to the inhibition of the functions of intracellular components after penetration of the bacterial cell membrane. However, the results of anti-inflammatory activities showed that only 9Pbw3 (RLWLAIWRR-NH<sub>2</sub>) has strong inhibition of NO production, implying that Trp<sup>7</sup> as well as optimum level of hydrophobicity may play key roles in the anti-inflammatory activity of 9Pbw3. Furthermore enantiomeric 9Pbw3-D which is the all-D-amino acid analog of 9Pbw3, showed considerably stronger



inhibition of NO production and inflammation-induced cytokine production in LPS-stimulated RAW264.7 cells than 9Pbw3. 9Pbw3-D can be a potent non-cytotoxic antibiotic candidate. The results suggest that our peptides having anti-bacterial and anti-inflammatory activities may be contributed to the potent short antibiotics without cytotoxicity.



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## **Acceleration of Neuritogenesis on Nanostructured Substrates; A Comparative Study on Various Nanotopographies**

강경태

KAIST 화학과

Nervous system is composed of microstructured scaffolds, which have three-dimensionally designed textures and give biophysical cues to overlying cells in many ways. Since little is known about how nanotopography manipulates neuronal development in vivo, it would provide us a new insight into the developmental processes of brain to elucidate unexplored topographical effects on neurite development. To this end, we introduced 3 types of nanostructures as model surfaces for a comparative study; anodized aluminum oxide (AAO), packed glass beads surfaces (GBeads), and vertically grown silicon nanowires (SiNWs). Various GBeads composed of 100 nm to 660 nm-glass beads, and AAO substrates were used to generate precisely tuned nanotopographies, and we have observed that the acceleration of neurite development occurred on the substrates only with bigger than 200 nm-pitched nanostructures, whose size was comparable with the thickness of filopodia at the tip of the growth cones. For the investigation on biological mechanism of the acceleration, we used SiNWs as an extreme of nanotopography at the

effective size range. On SiNWs, we found inhibited formation of F-actin structures (filopodia and lamellipodia). This inhibition would be the major factor to accelerate neurite development, because it might break the F-actin/microtubule balance, causing abnormal proceed of the microtubules.



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## DIFO-based probes react with free thiol-containing molecules

김은주

대구대 과학교육학부/화학교육과

One of the most commonly employed bioorthogonal reactions with azides is copper (I)-catalyzed cycloaddition with terminal alkyne probes (click chemistry). More recently copper-free click chemistry has been developed, in which alkyne is sufficiently strained to promote rapid cycloaddition with azide to form a stable triazole conjugate. However, a carbon-carbon triple bond in a strained ring system such as DIFO-based derivatives can also be coupled with a free thiol-containing molecule to give a covalent adduct. This implies that the blocking of the free-thiol group should be preceded when highly reactive cyclooctyne is used as a capturing agent for azide-labeled molecules.

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## 갈조류 감태에서 분리된 폴리페놀 화합물의 알츠하이머병 발병인

### 자 개선 효과

김현주 임진아<sup>1</sup> 이봉호<sup>2</sup>

한밭대 응용화학 생명공학과 <sup>1</sup>한밭대 생명공학과 <sup>2</sup>한밭대 응용화학생명공학부

제주 연안에 주로 분포하는 갈조류 감태에는 다양한 폴리페놀 화합물이 포함되어 있고 이들의 다양한 항산화 효과는 이미 널리 알려져 있다. 본 연구에서는 감태에서 분리된 eckol, bieckol, 6,6'-bieckol, 8,8'-bieckol, PFF, 7-phloroeckol 이 여섯가지의 폴리페놀 화합물을 활용하여 알츠하이머병의 원인이 되는 산화적 손상과 cholinesterase,  $\beta$ -secretase, GSK-3 $\beta$  등의 효소에 대한 억제 활성을 알아보았다.

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## Preparation of Fluorescent Polymer Based Multifunctional Nanoparticles for Bioapplication

이창수

한국생명공학연구원 바이오테크놀로지 연구단

The advance in biomedical imaging rely on the development of naoprobes with low toxicity with high sensitivity, resolution, and photostability. Fluorescence polymers have received a great deal of interest due to their unique physical properties such as conductivity, electroluminescence. Preparation and characterization of fluorescence polymer/Fe<sub>3</sub>O<sub>4</sub> hybrid nanoparticles coated by silica shell were exhibited in this study. Fe<sub>3</sub>O<sub>4</sub> nanoparticles are extensively inquired for in vivo and in vitro biomedical applications, such as magnetic resonance imaging (MRI). Silica-based fluorescent and magnetic multifunctional nanocomposites have been widely researched in the last few years, because they have a great potential in biomedical applications as optical and magnetic imaging agents. The integration of newly synthesized fluorescent polymer, which is poly[di(2-methoxy-5-(2-3ethylhexyloxy))-2,7-(9,9-dioctylfluorene)](PDDF) and Fe<sub>3</sub>O<sub>4</sub> formed the uniform core/shell nanoparticles coated with silica by reverse micelle method. The bioapplication of core/shell nanoparticles was investigated by the various

evaluations such as optical property, and fluorescent and MRI imaging in HeLa cells. As well as they showed an excellent photostability compared to quantum dots or organic dyes, as good permeability and low toxicity in the cells.[1] Qing Zhang, Yongai Zhai, Fenggi Liu, Meng Yang, Ge Hao, European Polymer Journal 44 (2008), 3957-3962.[2] Jinyoung Jeong, Miyoung Cho, Yong Taik Lim, Nam Woong Song, and Bong Hyun Chung, Angew. Chem. Int. Ed. 48 (2009), 5296-5299.



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## Enhancing cysteine selectivity over glutathione in thiol-sensing

강철훈 한지혜<sup>1</sup> 허경준 김진영<sup>2</sup>

경희대 동서의학대학원 <sup>1</sup>경희대 동서의학대학원 의과학전공 <sup>2</sup>경희대 동서의학대학원/의과학  
과

A series of the position isomers its benzoic acid moiety of a coumarine structure (1) to enhance cysteine selectivity in thiol-sensing is currently under characterization. 1 can react with some biological thiols (Cys, and GSH) to emit fluorescence at 513nm with 480nm excitation, which is used for characterization of its thiol reactivity. At pH 7.4 in an aqueous solution, The order of the rate constant is Cys >> GSH, and the ratio of the rate constant for Cys to that for GSH is found to be highest for the ortho isomer. The associative equilibrium constants for the reaction of the ortho isomer to Cys is much higher than that to GSH. The order of them along with its isomeric position for both is para > meta > ortho. These data indicate that, to achieve the best enhancement of Cys selectivity, the position for the carboxylic group in 1 is the ortho position. Such preference for the ortho position may be caused by repulsive electrostatic interaction between the carboxylate and the additional negative charge on GSH compared to Cys.



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## Development of nano-structured rough surfaces for promoting bone differentiation of osteoblast-like cells

이승윤 김효섭 김재호

아주대 분자과학기술학과

연구의 목적은 나노 표면 구조가 골세포 분화 시 끼치는 영향에 관하여 연구하고자 한다. 우리는 60, 300, 700 nm 의 각각의 실리카 나노 입자를 물과 공기 간의 계면 상에서 monolayer 를 형성하고 그것을 유리 기판 위에 옮기는 방식인 Langmuir-Blodgett technique (LB tech.)를 이용하여 나노 표면 구조를 형성하였다. Human osteosarcoma cell line (MG 63)은 tumor cell line 이지만 1,25-(OH)<sub>2</sub>D<sub>3</sub>-responsive alkaline phosphatase activity 가 높은 골 분화특징을 가지며 또한 collagen type I 과 osteocalcin (OCN)와 같은 골 형성 세포의 합성이 가능하다. 그래서 나노 표면 구조와 유리 기판에서 MG 63 을 7 일동안 배양하였다. 표면의 특징은 Atomic Force Microscopy (AFM) 이용하여 측정하였고 표면 구조와 세포 간의 상호작용은 위상차현미경, 형광 현미경으로 세포의 형상, adhesion 을 관찰하였다. 또한 유전자 발현량, alkaline phosphatase activity 를 정량화함으로서 측정된 결과를 수치화하였다. 나노 기판 중 60 nm 기판에서 활착 속도가 가장 느렸으며 스트레스 섬유가 다른 기판과 비교 시 발생율이

높았다. 골세포 분화 능력 측정을 위한 유전자 발현 값에서도 60 nm 실리카 나노 기관에서 alkaline phosphatase(ALP), osteocalcin (OCN)의 수치가 다른 나노 구조체와 비교 시 상대적으로 높게 나타났다. real-time PCR 을 이용한 결과에서도 60 nm 실리카 나노 기관에서 각각의 두 값의 수치가 높게 나왔다. 이는 세포 외 기질과 60 nm 의 나노 구조를 다른 기관과 비교 시 골 분화 관점에서 효과적인 것을 알 수 있다. 특히 세포 외 기질을 이루는 fibril 은 collagen I 으로 구성되는데 그 사이의 간격은 68 nm, 깊이는 35 nm 이다. 그 안을 구성하고 있는 hydroxyapatite 의 크기 또한 50 X 25 X 4 nm<sup>3</sup> 이다. 결과적으로 60 nm 실리카 나노 구조와 세포 외기질의 크기가 유사하여 골 분화가 유도됨을 알 수 있다. 본 연구는 나노 표면 구조의 규칙성을 재현 가능한 LB tech. 을 이용하여 실리카 나노 입자를 크기 별로 제작하여 MG 63 의 골분화 유도 가능성을 보였다.



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## Fluorescent labeled nanoparticles enable to detect the stem-cell-derived hepatocytes

신진섭

한양대 생명공학과

Hepatic cirrhosis characterized by permanent scarring which restricts its own function and makes it difficult to get cured. Stem cell transplantation is emerging as a possible new treatment for liver cirrhosis, and recent animal studies have documented benefits of stem cell therapy for hepatic fibrosis model. However, the underlying mechanism of stem cell therapy is still unclear. Among the proposed mechanism, the cell replacement mechanism is the oldest and most important one ? permanently damaged tissue can be replaced by normal ones to restore a function. In the present study, c5.5 labeled superparamagnetic iron oxide (SPIO) were used to label human mesenchymal stem cells. Uptaken fluoresce labeled nanoparticle enables to detect and monitor the transplanted stem cells, therefore we can confirm the direct incorporation and differentiation into hepatocyte-like cells of transplanted stem cell.

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## In silico identification and analysis of dog kinome

**임선영 소재원**

인하대 화학과

Protein kinases have been extensively studied and shown to play various distinct roles in multitudes of cellular processes. In this study, we report in silico identification, prediction, and classification of protein kinases in domestic dog (*Canis familiaris*). We found at least 521 putative protein kinases in dog. We classified these kinases into groups, families, and subfamilies based on orthology with human kinases. We also reported a dataset of the modeled three-dimensional structures of the ePK domains of these kinases along with the information about other conserved domains found in these kinases. We aligned these modeled structures and clustered the proteins in a two-dimensional MDS plot. We next compared the dog kinome with the kinomes of previously reported higher and lower eukaryotes including human, mouse, rat, fruitfly, sea urchin, nematode, and yeast. We found at least six novel protein kinases in dog namely, ARGL, BSK146L, Erk1L, JAK1L, TIF1gL, and PDHK1L which are not present in human, mouse, and rat. In addition, we found at least three retro-transposed genes in dog, namely CDK4-rt, Erk1-rt, and G11-rt, which are the retro-transposed copies of CDK4, Erk1, and G11 respectively. Our

evolutionary rate studies of the dog and human protein kinase orthologs between the disease and non-disease associated subsets reveal that a relatively uniform selective pressure was applied to these two subsets of protein kinase genes.



일시: 2012년 4월 25~27일(수~금) 3일간

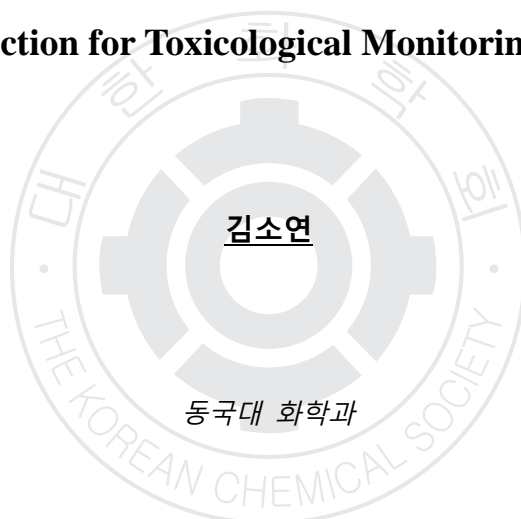
장소: 일산KINTEX

발표코드: BIO.P-705

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Real Time Detection for Toxicological Monitoring using aptamer



Polychlorinated biphenyls (PCBs), 1,1,1-trichloro-2,2-bis-(p-chlorophenyl) ethane (DDT), chloramphenicol, bisphenol and nonylphenol are widely used as pesticide, antibiotics, antioxidant, plasticizers, surfactant and detergent in modern industry. For years, these compounds are proven to be carcinogens or have potentially dangerous effects in animals and humans. As they are a big threat to human health and have even shown serious consequences on environmental and ecological system, it's necessary to do toxicological detection and monitoring. However, traditional detection technology needs sample extraction (GC/MS and HPLC) or critical condition for assay (immunoenzyme assay). They are not able to give specific and fast detection. In our study, a biofriendly detection method using aptamer technology is introduced. High affinity and specific aptamers against water pollutant target were isolated from a random library using an in vitro selection process referred to as SELEX (Systematic Evolution of Ligands by EXponential enrichment). Two subgroups were identified, and consensus sequences are highlighted in brown color. This region was characterized by four G-triplets (GTTYG3TG3AG3CG3C)

and a stem-loop structure. Secondary structure was predicted by mfold program based on free energy minimization algorithm. Selected aptamer candidates were screened and  $K_d$  was measured by OCTET machine. Hopefully, using alkylphenol aptamers, in combination with sol-gel materials, an aptamer-based biosensor will be developed for specific detection of water pollutants, and a sol-gel based detection sensor system could be applied to the universal detection of water pollutant with high sensitivity.



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장소: 일산KINTEX

발표코드: **BIO.P-706**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of DNA aptamers for diagnosing Non-Hodgkin lymphoma

김소연

동국대 화학과

Non-Hodgkin lymphomas (NHL) are a heterogeneous group of malignancies that arise from lymphoid tissue. NHL is fifth most common cancer in the United States. The past decade has seen enormous changes in our understanding of lymphomas, including the identification of better prognostic factors. However, results from efforts to identify good diagnostic factors have been disappointing. Lactate dehydrogenase has been used as an NHL marker, but its accuracy in diagnosis has been unsatisfactory. In this study, we intend to introduce novel NHL diagnosis through ssDNA aptamers. Aptamers are short, single-stranded oligonucleotides with the ability to specifically recognize and bind to target molecules with high affinity. Aptamers offer the utility for biotechnological and therapeutic applications since they have molecular recognition properties which rival commonly used biomolecules such as, antibodies. An aptamer is an ideal material which can reduce the cost and increase the sensitivity of a sensor compared



with other materials. We report the selection of ssDNA aptamers that bind to NHL marker which is hypoxanthine.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO.P-707

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Site-specific labeling of cell surface proteins with fluorescent probes through Npu\_DnaE intein based protein trans-splicing

민경미 정덕호 권영은

동국대 의생명공학과

Here we describe a highly specific, robust and rapid new method for labeling of cell surface proteins with fluorescent probes. The method uses the trans-splicing reaction of Nostoc punctiforme (Npu) DnaE split-intein. Split-intein based protein trans-splicing reaction has been used for site-specific labeling of proteins in vitro for various applications. The trans-splicing reaction is self-processing reaction and can be used for introduction of various synthetic probes to target proteins without a large linker proteins. In this report, we have utilized split-intein based protein trans-splicing reaction for site specific labeling of cell surface proteins. We have prepared a model cell surface protein fused to N-terminal fragment of Npu DnaE Intein and C-terminal fragment of Npu DnaE Intein fused to a fluorescent probe. The model protein was expressed on the cell surface and the proteins were labeled with synthetic fluorescent probes through specific interaction between N- and C-fragment of inteins. This labeling reaction was performed within 30 mins using low concentration of fluorescent molecules (4  $\mu$ M). No external energy was required for

the labeling reaction. This improved labeling method will provide a useful tool for studying functions and mobility of proteins in live cells.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **BIO.P-708**

발표분야: 생명화학

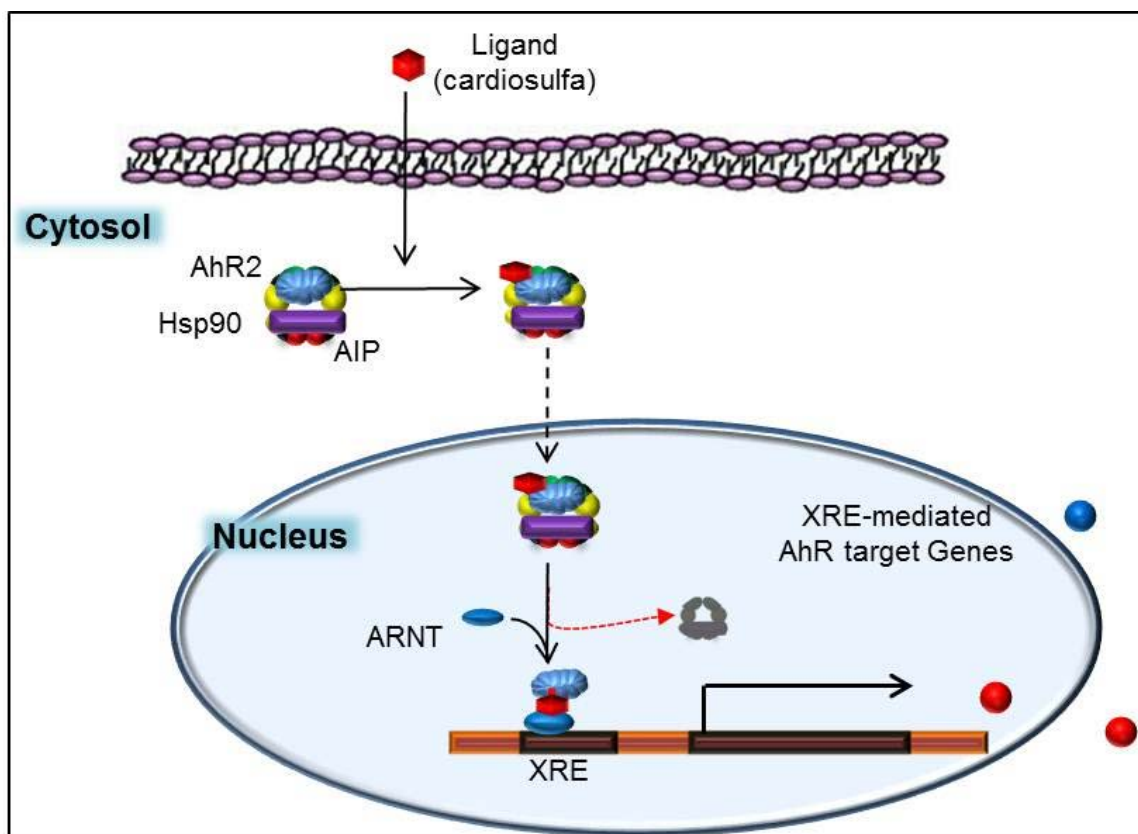
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Abnormal Heart Development Caused by Cardiosulfa is Prevented by Negative Regulators**

고성균 신인재

연세대 화학과

We have previously identified a small molecule cardiosulfa that induces aberrant heart development in zebrafish. In the present study, we show that cardiosulfa-promoted heart deformation is protected by negative regulators (EGCG and CH-223191) for the aryl hydrocarbon receptor (AhR) signaling pathway and the AhR2-morpholino antisense (zfahr2-MO) but is not suppressed by the morpholino antisense of cytochrome P450 1A enzyme (zfcyp1a-MO) which is the most well-characterized target gene of the AhR pathway. These results suggest that cardiosulfa causes aberrant heart development in zebrafish through the AhR-mediated, CYP1A-independent pathway.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **BIO.P-709**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of Anti Cancer Organic Molecule(Apoptozole) Targeted to Hsp70

고성균 신인재

연세대 화학과

The inducible Hsp70 is known to act as anti-apoptotic factor to protect cells from apoptosis induced by various stressful stimuli. This chaperone protein is highly expressed in many cancer cells and its overexpression correlates with tumor development and resistance to chemotherapy. In this study, we present evidence that apoptozole (Az) inhibits Hsp70 activity by binding to its ATPase domain and this binding leads to blocking the interaction of Hsp70 with Apaf-1, thereby inducing apoptosis. However, Az neither suppresses the interaction of Hsp70 with apoptosis inducing factor (AIF) nor influences the expression levels of Hsp70 and other apoptosis-related proteins such as Apaf-1, caspases and AIF. These results suggest that apoptosis induced by Az may take place via caspase activation processes. Interestingly, treatment of cancer cells with combination of apoptozole and doxorubicin enhanced apoptosis in comparison with single treatment with doxorubicin. These findings suggest that apoptozole has a potential of being used as an antitumor agent or combination with other anticancer agents.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: **BIO.P-710**

발표분야: 생명화학

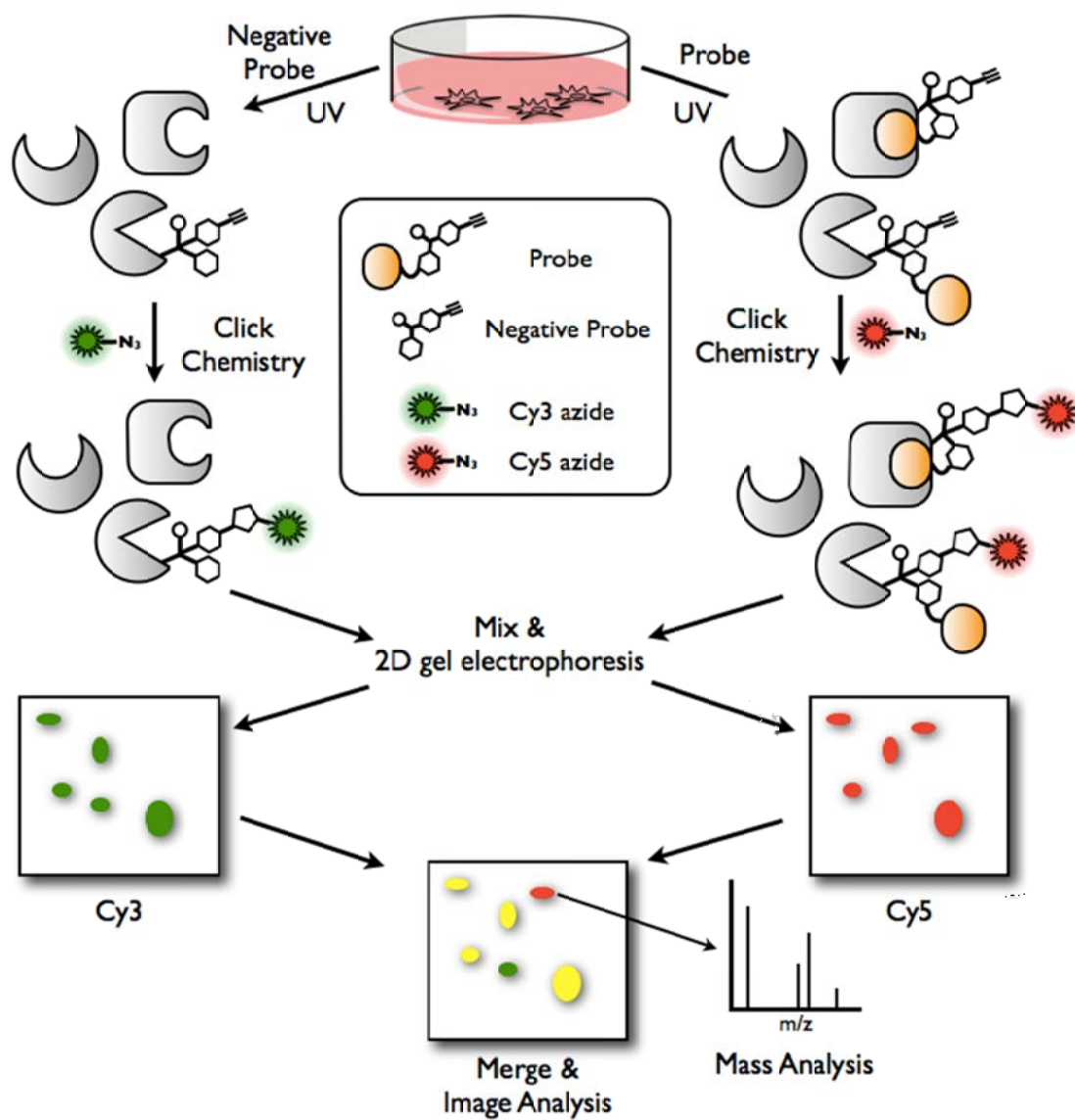
발표종류: 포스터, 발표일시: 수 18:00~21:00

**Discovery of an antiproliferative agent and its target identification in  
live cells using fluorescence difference in two dimensional gel  
electrophoresis**

**박종민 박승범**

서울대 화학부

We developed a new target identification platform, FITGE, which aims to preserve protein-small molecule interactions under the intact cellular environment. After a series of failures using conventional target ID methods, we successfully identified the protein target of anti-proliferative compound 1 with FITGE only under the live cell condition and observed the environment-dependent binding events of a functional small molecule by direct comparison between live cells and cell lysates. Even though it still requires the synthesis of bioactive probes with photo-crosslinker moiety, the FITGE strategy can address the current limitation of conventional target identification methods and significantly enhance the possibility of target ID via covalent capturing of target proteins under the intact cellular environment and the efficient exclusion of nonspecific protein labeling using two-color 2DGE. We believe our FITGE strategy can provide a unique technology platform for target identification in live cells.



LEAN CHEMICAL



일시: 2012년 4월 25~27일(수~금) 3일간

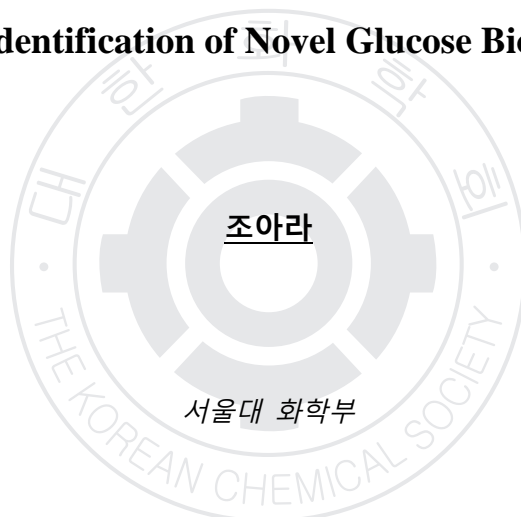
장소: 일산KINTEX

발표코드: **BIO.P-711**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Property Identification of Novel Glucose Bioprobe GB2



We developed a novel fluorescent glucose bioprobe, GB2-Cy3, for the real-time and quantitative monitoring of glucose uptake in living cells. We synthesized a series of fluorescent glucose analogues by adding Cy3 fluorophores to the  $\alpha$ -anomeric position of d-glucose through various linkers. Systematic and quantitative analysis of these Cy3-labeled glucose analogues revealed that GB2-Cy3 was the ideal fluorescent glucose bioprobe. The cellular uptake of this probe competed with the cellular uptake of D-glucose in the media and was mediated by a glucose-specific transport system, and not by passive diffusion. Flow cytometry and fluorescence microscopy analyses revealed that GB2-Cy3 is ten times more sensitive than 2-NBDG, a leading fluorescent glucose bioprobe. GB2-Cy3 can also be utilized for the quantitative flow cytometry monitoring of glucose uptake in metabolically active C2C12 myocytes under various treatment conditions. As opposed to a glucose uptake assay performed by using radioisotope-labeled deoxy-d-glucose and a scintillation counter, GB2-Cy3 allows the real-time monitoring of glucose uptake in living cells under various experimental conditions by using fluorescence

microscopy or confocal laser scanning microscopy (CLSM). Therefore, we believe that GB2-Cy3 can be utilized in high-content screening (HCS) for the discovery of novel therapeutic agents and for making significant advances in biomedical studies and diagnosis of various diseases, especially metabolic diseases.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO.P-712

발표분야: 생명화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Residue mutations in the sweetness loops for the sweet-tasting protein brazzein

조현주 조동현 윤석영 공광훈

중앙대 화학과

Brazzein is a sweet-tasting protein first isolated from the fruit of *Pentadiplandra brazzeana* Baillon found in West Africa. Brazzein is an intensely sweet-tasting protein with good stability, and it is 500-2000 times sweeter than sucrose on a weight basis. To identify critical residues important for sweetness of the sweet protein brazzein, 11 mutants of the residues in three loops of brazzein were constructed by site-directed mutagenesis. We found that mutations of Glu41 to Ala, Lys, or Arg at position 41 in loop40-43 made the molecules significantly sweeter than brazzein, while mutations at two distant residues (changing Arg43 to Lys or Glu) decreased sweetness. A similar pattern occurred at loop30-33, where mutation of the His31 to Arg significantly increased sweetness, while mutations at positions 30 or 33 in the immediate vicinity of this region significantly decreased sweetness. In addition, a Gln17 residue in the loop9-19 was necessary for structural integrity. From these results, we suggest the loops containing His31 and Glu41 to be critical regions of the molecule for eliciting sweetness, and the charge and/or structure of the side chain of these

residues play an important role in the multi-point interactions between brazzein and the sweet-taste receptor.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: BIO.P-713

발표분야: 생명화학

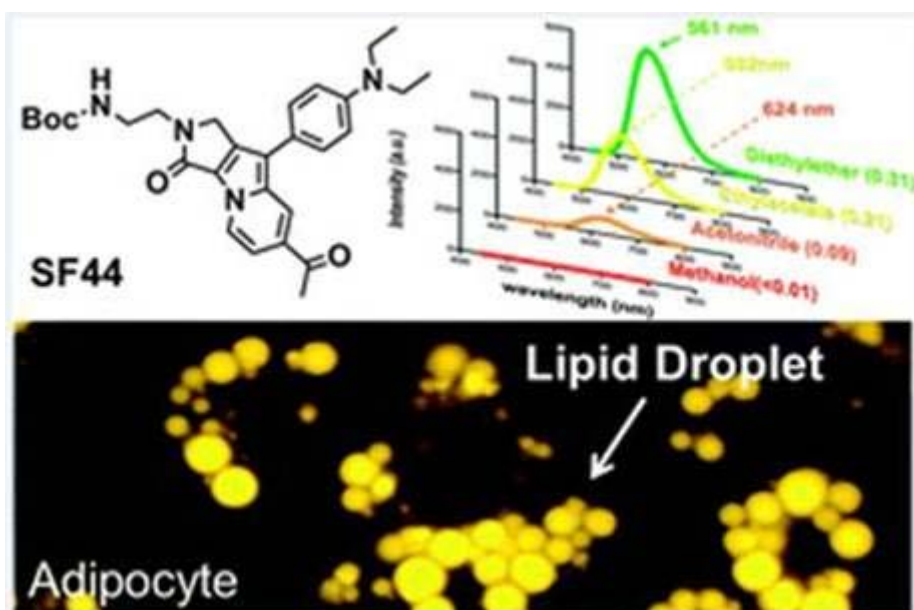
발표종류: 포스터, 발표일시: 수 18:00~21:00

**A Seoul-Fluor-based bioprobe for lipid droplets and its application  
in image-based high throughput screening for discovery of autophagy  
modulator**

이상희

서울대 화학부

We developed a novel fluorescent bioprobe (SF44) that can specifically visualize the cellular lipid droplets in *in vitro* and *in vivo* systems and illustrated the mechanistic rationale of its fluorogenic property. Its application to image-based high throughput screening led us to the identification of a new small-molecule modulator for related signaling pathway, such as autophagy process.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-714

발표분야: 유기화학

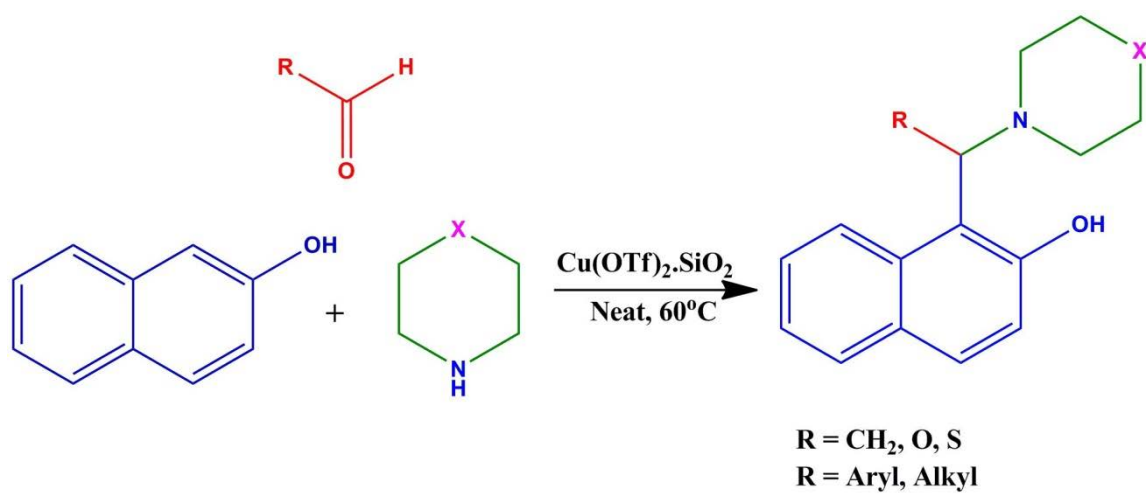
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Supported copper triflate as catalyst for Aminoalkylation of Phenols under solvent free condition

백관 Someshwar 정연태

부경대 이미지시스템공학과

We have developed an efficient silica gel anchored copper triflate heterogeneous catalyst for the multicomponent synthesis of Betti base from secondary amine, aromatic aldehydes, and b-naphthol using Mannich-type reaction under solvent free condition. The catalysts exhibited both Lewis and Brønsted acidities due to the presence of residual moisture within  $\text{Cu}(\text{OTf})_2$ , as well as the surface silanol groups of the silica and the methanol used as solvent in the catalyst preparation. The catalyst was recovered quantitatively by simple filtration and reused several times.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-715

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Lithium triflate (LiOTf) an efficient and recyclable catalyst for the one-pot synthesis of propargylamines under neat condition**

**Someshwar 정연태**

부경대 이미지시스템공학과

An efficient process has been developed for the synthesis of propargylamines via a three-component coupling reaction (A3) of aldehyde, secondary alicyclic amines and alkyne under solvent-free conditions using lithium triflate (LiOTf) as expeditious reusable catalyst. This one-pot transformation generates one C?C and one C?N bond, which was presumably proceeds by lithium acetylide as well as formation of iminium ion in situ. Which undergoes nucleophilic addition to the iminium ion, to give the propargyl amine. The solvent free condition, easy recovery of the catalyst, simple, user-friendly and quantitative yield in short time renders the protocol economic and reasonable.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-716

발표분야: 유기화학

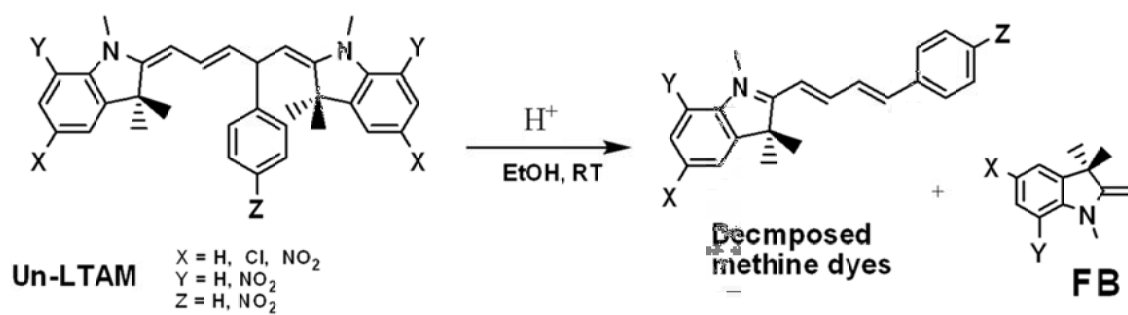
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Unsymmetric leuco-TAM dyes: Acid-catalyzed decomposition

마소영 금삼록<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

Unsymmetric leuco-TAM dyes, (2*E*, 2'*E*)-2,2'-{(*E*)-4-phenylpent-2-ene-1,5-diylidene}bis(1,3,3-trimethylindoline)derivatives, 1-5 were prepared from the reaction of excess 5-substituted Fischer base with substituted cinnamic aldehyde. The X-ray crystal analysis showed that the *EEE* for 4. The prepared molecules were characterized by <sup>1</sup>H, <sup>13</sup>C-NMR, COSY, HETCOR, NOESY spectroscopy. It is known that the LTAM molecules are generally not stable in acidic media. From the acid-catalyzed reaction of unsymmetric leuco-TAM dyes, the decomposed methine dyes were obtained, in addition to substituted Fischer bases. The nature of the leaving group (FB) is expected to profoundly influence the reaction rate for the acid-catalyzed decomposition of the LTAM molecules.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-717

발표분야: 유기화학

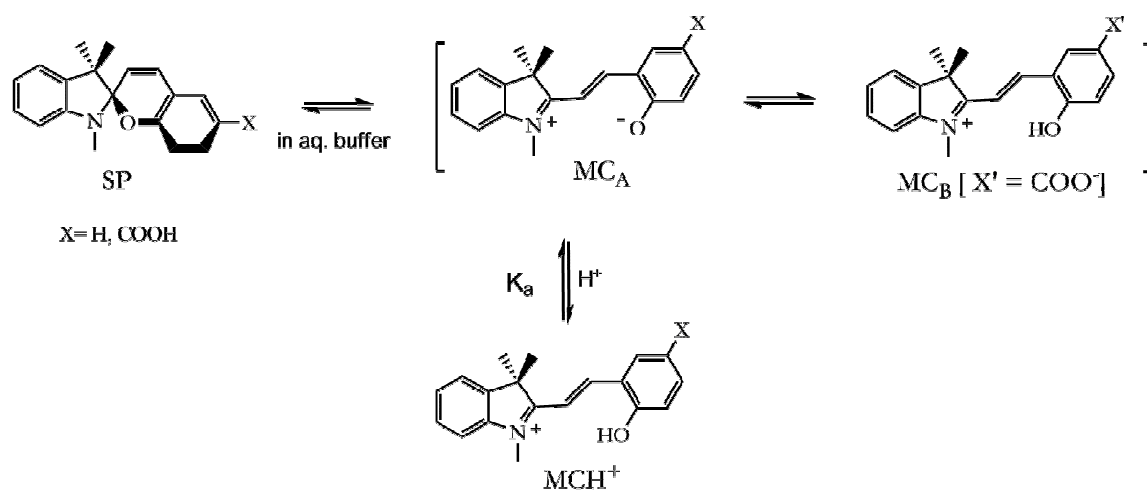
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermal ring-opening reaction of Indolinobenzospiropyran molecules in various pH buffer media

임현우 김도경 금삼록

고려대 소재화학과

The protolytic properties of the indolinobenzospiropyran (SP) molecules have been examined by UV-Vis spectrometry in the aqueous buffer media. The non-activated indolinobenzospiropyran (SP) molecules show generally no chromotropism in organic solvent, but show the reverse photo- and thermochromic behavior in aqueous buffer solution. In aqueous buffer solution, the acid-catalyzed ring-opening reaction, the acid-catalyzed ring-opening reaction is generally expected. However, SP-1 does not show the expected acid-catalyzed ring-opening reaction. The SP-1 undergoes the ring-opening behavior in various buffer solutions (pH 3.0-10), forming the cyclic spiro- (SP,  $\lambda_{\max}$  290nm), merocyanine-A ( $\text{MC}_A$ ,  $\lambda_{\max}$  514nm), merocyanine-B ( $\text{MC}_B$ ,  $\lambda_{\max}$  367nm) and protonated ( $\text{MCH}^+$ ,  $\lambda_{\max}$  414nm) forms of the SP molecule. The key to understanding these various behaviors is the possibility of proton transfer from the carboxylic (-COOH) to the phenoxide ( $\text{O}^-\text{-Ph}$ ) group of the MC isomer. Thus the protolytic equilibria of SP-1 molecules need to be determined in buffer media.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-718

발표분야: 유기화학

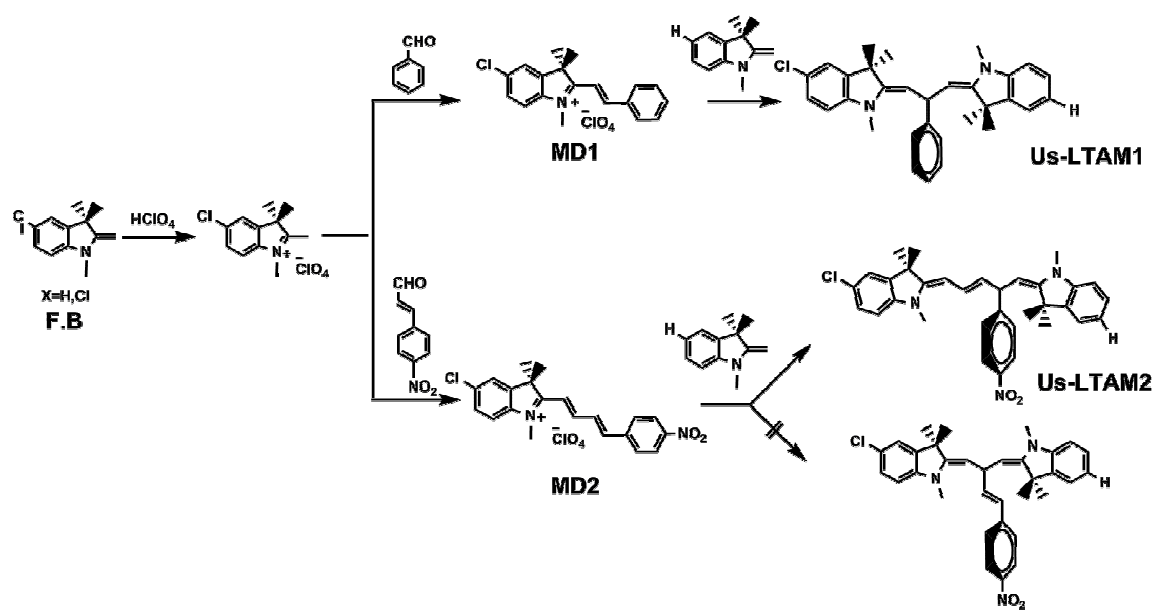
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Novel unsymmetrically substituted leuco-TAM derivatives : synthesis and characterization

김도경 임현우 금삼록

고려대 소재화학과

Novel unsymmetrically substituted LTAM molecules, (2Z, 2E)-2,2-(2-phenyl-propane-1,3-diylidene)bis(1,3,3-trimethylindoline), Us-LTAM1 and LTAM molecules, (2Z,2'E)-2-2'((E)-4-(4-nitrophenyl)pent-2-ene-1,5-diylidene)bis(1,3,3-trimethylindoline), Us-LTAM2 were prepared from the reaction of excess 5-substituted Fischer base (FB) with the conjugated dye molecules MD1 and MD2, respectively. via a Michael-type reaction. Since the conjugated dye molecules are the  $\alpha$ ,  $\beta$  or an extended  $\alpha$ ,  $\beta$ -unsaturated iminium salts, they behave like the corresponding carbonyl compounds toward the Michael type reactions. The compound MD1, MD2 were obtained from the reaction of 1,3,3-trimethyl-2-styrylindolium perchlorate with benzaldehyde and 4-nitrocinnamic aldehyde, respectively. The prepared molecules MD1, MD2, Us-LTAM 1 and 2 were characterized by  $^1\text{H}$ ,  $^{13}\text{C}$  1D, 2D-NMR, COSY, Hetcor, NOESY spectroscopy.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-719

발표분야: 유기화학

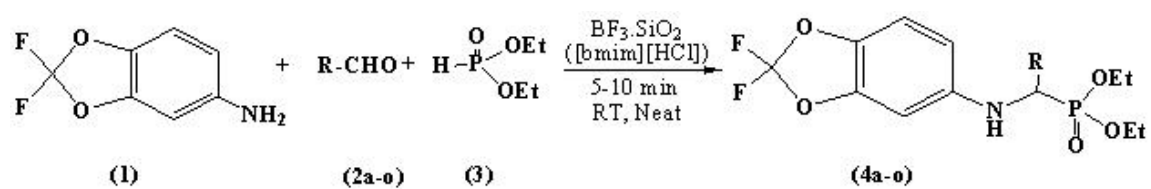
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **BF<sub>3</sub>·SiO<sub>2</sub> -Catalyzed one-pot synthesis of $\alpha$ - aminophosphonates in ionic liquid and neat conditions**

mudumala veerananaraya 정연태

부경대 이미지시스템공학과

$\alpha$  -Aminophosphonates were synthesized in a simple and efficient method from the three-component condensation reaction of 5-amino 2, 2-difluoro- 1, 3-benzodioxole, aromatic aldehydes, and diethyl phosphite by Silica-supported boron trifluoride (BF<sub>3</sub>·SiO<sub>2</sub>) in ionic liquid [bmim][Cl] under solvent-free conditions at room temperature in good to excellent yields and short reaction times. The catalyst can be recovered and reused for several times without any significant loss of activity.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-720

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Fluorescent Fréchet-type Dendrimers via Homo-coupling Reaction

곽승환 이재욱 한승철

동아대 화학과

Palladium-assisted homo-coupling reactions mediated by Pd (0) or Pd (II), are arguably the most mild, efficient, and selective methods for the synthesis of 1,3-diynes. However palladium reagents are expensive, and often required air-sensitive and poisonous ligands. Recently, Zhang's group reported that CuI/NBS/DIPEA as promoting system is found to efficiently promote Glaser-type coupling reaction under very mild conditions. Taking advantage of these facts, herein we will disclose the general and efficient strategy for the convergent synthesis of fluorescent Fréchet-type dendrimers containing via homo-coupling reaction of terminal alkyne.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-721

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Dendrimers based Fluorescence Sensors

최인화 이재욱 한승철

동아대 화학과

The homo-coupling of terminal alkynes is a straightforward method for the synthesis of buta-1,3-diyne, which are important building blocks in the organic synthesis of natural products, pharmaceuticals, organic/inorganic composites, and polymers. Since Rossi's group used a palladium/CuI catalytic system to catalyze the homo-coupling of terminal alkynes, this method has attracted a great deal of interest due to its mildness and wide-ranging substituent tolerance. Taking advantage of these facts, herein we will present the efficient strategy for the convergent synthesis of emissive Fr $\pi$ chet-type dendrimers containing a chromophore from alkyne focal point functionalized Fr $\pi$ chet-type dendrons via homo-coupling reaction of terminal alkyne.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-722

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 2,3-Dihydrobenzo[*b*]oxepines and Benzo[*b*]furan derivatives from Baylis-Hillman Acetates of Methyl (2-formylphenoxy)acetates

안상현 김영근 이기정

한양대 화학공학과

A new synthetic method for dimethyl 2,3-dihydrobenzo[*b*]oxepine-2,4-dicarboxylates and methyl 2-(2-carbomethoxybenzo[*b*]furan-3-yl)propanoates by an  $S_N2'$  or an  $S_N2$  reaction of acetates of Baylis-Hillman adducts of methyl (2-formylphenoxy)acetates has been described.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-723

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Direct SET-Photochemical Route to Novel Lariat-Type Crown Ethers for $\text{Hg}^{+2}$ and $\text{Pb}^{+2}$ Cations

박혜정 김지나 유현지 윤웅찬

부산대 화학과

Our recent studies also showed that SET-promoted photomacrocyclization reactions of trimethylsilylmethoxy-terminated polyethylenoxy-linked bis-phthalimides can serve as highly efficient and chemoselective routes to generate interesting bis-crown ethers. Another Potentially interesting application of SET-promoted photomacrocyclization reactions of trimethylsilyl-terminated polydonor-linked phthalimides and naphthalimides is found in the synthesis of novel metal cation complexing agents related to the well-known crown ethers. Our recent studies found in the preparation of  $\text{Hg}^{+2}$  and  $\text{Pb}^{+2}$  metal cation selective, naphthalene chromophore containing fluorescence sensing, alkylthioether chain containing lariat-type crown ether. The presentation will discuss about synthesis of the naphthalimide based lariat-type thiocrown ethers utilizing SET-promoted photochemical cyclization reaction and strong enhancement of its fluorescence emission (310 nm) and decrease in intramolecular exciplex emission (510 nm) on increased concentration of  $\text{Hg}^{2+}$  in solution.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-724

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Copper-Free Sonogashira Coupling in Water with Immobilized Pd Catalyst on Thermo-Responsive Polymer

홍명찬 이용우 이학준

한양대 응용화학과

We have developed immobilized Pd catalysts (Pd(0), Pd(OAc)<sub>2</sub>, and PdCl<sub>2</sub>) on thermo-responsive poly(*N*-isopropylacrylamide-co-4-vinylpyridine)(PNIPAM-co-4-VP) as a solid-supporter. We present Sonogashira coupling reaction which is conducted with the catalyst(1mmol%) and K<sub>2</sub>CO<sub>3</sub>, Na<sub>2</sub>CO<sub>3</sub>, pyrrolidine, or triethylamine(3 equiv) at 60 °C in water. In case of using triethylamine as base and the immobilized PdCl<sub>2</sub> on the polymer supporter, the coupling reaction gave the best result. We demonstrate the Sonogashira coupling reaction with various haloarenes and arylacetylenes in water.



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장소: 일산KINTEX

발표코드: ORGN.P-725

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Intramolecular Oxidative Diamination and Aminohydroxylation of Olefins under Metal-Free Conditions**

**김현진 장석복**

KAIST 화학과

A metal-free procedure, simple to operate and convenient to handle was developed for the facile intramolecular oxidative diamination of olefins using iodobenzene diacetate oxidant and halide additive to furnish bisindolines at room temperature. The present reaction is featured by mild conditions, broad substrate scope, and excellent functional group tolerance. The same protocol was successfully extended to the aminohydroxylation



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-726

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Which Carbonyl is the Reactive Chromophore in Photochemistry of Ortho-alkylbenzils? : A Mechanistic Study**

**장미 박봉서**

동국대 화학과

For decades there have been disputes over which carbonyl is the reactive one in photochemical cyclization of ortho-alkylbenzils. Depending on which carbonyl participates in the reaction initially, the reaction pathways become clearly altered even though the products are always 2-hydroxyindanones. We recently had a chance to reinvestigate the issue and found a clear cut evidence to support the mechanism where direct delta-hydrogen abstraction is involved, at least in non polar solvents. The details of our experimental results related to the subject will be described and compared with previously known data.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-727

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Electroluminescent Properties of Blue Emitting Materials Based on Binaphthyl Derivatives for OLEDs

나은재 이금희 윤승수

성균관대 화학과

Organic light-emitting diodes (OLEDs) have been extensively studied due to their great potential in flat-panel displays and as a solid-state lighting source. Particularly, Blue light-emitting material is one of the important research subjects. In this paper, five binaphthyl derivatives were synthesized by joint of luminescent chromophores onto 4,4'- positions of binaphthyl moieties and their electroluminescent properties were investigated. The device with the structure of ITO/ NPB(50nm)/ EML(30nm)/ Balq(30nm)/ Liq(2nm) /Al(100nm) were fabricated. Among those, a device shows the maximum luminance of 3280 cd/m<sup>2</sup> at 12 V. The luminous efficiency, power efficiency and quantum efficiency are 4.81 cd/A, 3.78 lm/W and 4.68 %, respectively. The maximum peak wavelength of the electroluminescence is 458 nm with the CIE coordinates of (x=0.15, y=0.11) at 8 V.

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장소: 일산KINTEX

발표코드: ORGN.P-728

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Correlation of the Rates of Solvolysis of Electron-Rich Benzenesulfonyl Chloride Using the Extended Grunwald-Winstein Equation

김수련 최호준<sup>1</sup> 양기열<sup>1</sup> 박종근<sup>1</sup> 구인선<sup>1</sup>

경상대 교육대학원 화학전공 <sup>1</sup>경상대 화학교육과

The specific rates of solvolysis of 2,4-dimethoxybenzenesulfonyl chloride have been determined in binary aqueous solvent mixtures at 25.0 °C. Comparison of the specific rates of solvolyses of 3,4-dimethoxybenzenesulfonyl chloride in terms of linear free energy relationships (LFER) are helpful in mechanistic considerations, as is also treatment in terms of the extended Grunwald-Winstein equation. It is proposed that the solvolyses of 2,4-dimethoxybenzenesulfonyl chloride in binary aqueous solvent mixtures proceed through an dissociative S<sub>N</sub>2 pathway rather than through an addition-elimination pathway.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-729

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Triphenylene Derivatives as emitting materials for efficient Blue Organic Light-Emitting Diodes

장흥수 이금희 윤승수

성균관대 화학과

Full-color displays, it is essential to have the three primary colors, red, green and blue. Each emitters with sufficiently high luminous efficiency and properly balanced color chromaticity, as well as adequate operational stability. We have synthesized new blue light-emitting triphenylene-derivatives, which have been prepared in a one-step procedure via Diels-alder reaction. Organic light-emitting devices (OLED) with the structure ITO/NPB(50nm)/EML(30nm)/Bphen(30nm)/Liq(2nm)/Al(100nm) has been fabricated to investigate their electroluminescent properties. OLED using 1,4-bis[8-(7,10-diphenylfluoranthenyl)]benzene as the emissive layer exhibited a high external quantum efficiency of 1.11% at 20mA/cm<sup>2</sup> with color coordinates of (0.15 , 0.10).

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장소: 일산KINTEX

발표코드: ORGN.P-730

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly efficient blue organic light-emitting diodes based on ambipolar anthracene derivatives containing electron donating and withdrawing moiety

권성민 이금희 윤승수

성균관대 화학과

Organic light-emitting diodes (OLEDs) have drawn great scientific and commercial attention, due to their potential applications in full-color. we have synthesized new blue light-emitting ambipolar anthracene derivatives containing electron donating cabazole moiety and electron withdrawing pryidine moiety at at the C-9 and C-10 positions of the anthracene. The color and the energy levels were modified by the phenyl bridge position between the functionalized moieties and the anthracene core. Organic light-emitting devices (OLED) with the structure ITO(180nm)/NPB(50nm)/EML(30nm)/Bphen(30nm)/Liq(2nm)/Al(100nm) has been fabricated to investigate their electroluminescent properties. A device incorporating 9-[4-(cabazole-9-yl)-phenyl]-10-[4-(pyridine-2-yl)-phenyl]-anthracene as the emissive layer exhibited a high external quantum efficiency of 2.22% at 20mA/cm<sup>2</sup> with color coordinates of (0.15, 0.17)

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장소: 일산KINTEX

발표코드: ORGN.P-731

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Small Molecule Organic Semiconductors Containing Fused Thiophene for Solution Processed Small Molecule Organic Solar Cells with

이재관 <sup>1</sup>이슬 <sup>1</sup>유철휘 <sup>1</sup>조나라 <sup>2</sup>고재중 <sup>2</sup>

조선대 화학교육학과 <sup>1</sup>호서대 일반대학원 그린에너지공학과 <sup>2</sup>고려대 소재화학과

Great achievements in obtaining power conversion efficiencies (PCEs) of above 8% has rendered organic solar cells (OSCs) strong candidates for next generation solar cells, threatening the position of inorganic thin film solar cells as well as dye-sensitized solar cells (DSSCs). Most of these high efficiencies have been reported in OSCs fabricated with bulk heterojunction (BHJ) materials comprised of low-bandgap semiconducting polymers and C61(or 71)-PCBM). Nevertheless, small molecule organic semiconductors seem to be of greater interest than these polymers from the viewpoint of mass production for commercial application, due to the low reproducibility of characteristics as well as the difficulty in purification exhibited by these polymers. Motivated by this, considerable research effort has been focused on developing efficient small molecule materials for improved device performance, with the short-term goal being a PCE comparable to polymer-based solar cells (PSCs). Recently, we have also reported an

efficient organic semiconductor with moderate PCEs for solution processed small molecule OSCs (SMOSCs). This successful approach led us to attempt to develop a higher efficiency small molecule organic semiconductor, considering the correlation of photophysical and photochemical properties with the structures of DSSC organic dyes or NLO chromophores. Herein, we wish to present the synthesis and photovoltaic characteristics of new small molecule organic semiconductor containing fused thiophene conjugation bridges for SMOSCs. This work was supported (funded) by the New IT Project for growth foothold of green-semiconductor industry based on IT of the Chungcheong Leading Industry Office of the Korean Ministry of Knowledge Economy.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-732

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Lewis Acid-Catalyzed Domino Reactions for the Synthesis of Fused Polycyclic Compounds

주진혁 강다영 윤소원

한양대 화학과

We have developed a mild and efficient Lewis acid-catalyzed domino reaction of 2-(2-(alkynyl)benzylidene)malonates with phenols to give the fused polycyclic compounds containing indane and hydrocoumarin moieties. Among a variety of Lewis acids, Sn triflate was the most effective catalyst. In addition, it was found that electron-rich phenols were required as a reactant with enough nucleophilicity for the successful transformation.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-733

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Pd-Catalyzed Intermolecular Heck-Type Reaction between Alkenes and $\beta$ -Aryl Elimination Intermediates**

**김병석 윤소원**

한양대 화학과

We have developed a new Pd-catalyzed reaction of 2-alkenyl 1,3-dicarbonyl compounds with external alkenes, affording to 1-naphthols and Heck-type coupling products via sequential C-C bond cleavage and C-C bond formation processes. In sharp contrast to typical Pd-catalyzed reactions, this protocol showed the first example in which  $\beta$ -aryl elimination of a carbon-metal species occurs predominantly over  $\beta$ -hydride elimination.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-734

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Novel Organic Sensitizers Containing Sulfur-Bridged Bithiophene for Dye-Sensitized Solar Cells

이재관 김혜선<sup>1</sup> 유철휘<sup>1</sup> 한재호<sup>2</sup> 백상현<sup>3</sup> 고재중<sup>3</sup>

조선대 화학교육학과 <sup>1</sup>호서대 일반대학원 그린에너지공학과 <sup>2</sup>(주)포톤와트 연구소 <sup>3</sup>고려대  
소재화학과

Enormous efforts have intensively focused on improving the device performances toward power conversion efficiency (PCE) of dye-sensitized solar cells (DSSCs) through developments of various metal-free organic photosensitizers. The effective sensitizers should absorb the whole visible light and have the long-lived charge-separated state for favorable electron-transfer dynamics, showing an analogy of molecular structure comprising of electron-donating, electron-conducting, and electron-accepting characteristics. Among them, we have focused the introduction of new characteristics of electron-conducting unit. Herein, we wish to present the synthesis of novel organic sensitizers containing sulfur-bridged bithiophene and the photovoltaic characteristics in DSSC. This work (Grant no. s1072673) was supported by Business for Development of Technology Innovation funded Korea Small and Medium Business Administration in 2010.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-735

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Pd-Catalyzed Intramolecular Aromatization for the Synthesis of 1-Naphthol Derivatives

김병석 송형설 윤소원

한양대 화학과

Transition metal catalyzed carbon-carbon bond formations between 1,3-dicarbonyl compounds and alkenes have instigated significant synthetic interests in recent years. We have developed an effective Pd-Catalyzed intramolecular aromatization of alkenyl 1,3-dicarbonyl compounds leading to 1-naphthol derivatives. This process operates through the nucleophilic character of the 1,3-dicarbonyl functionality, building a carbon-carbon bond with the alkene component through  $\pi$ -philic transition-metal activation.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-736

발표분야: 유기화학

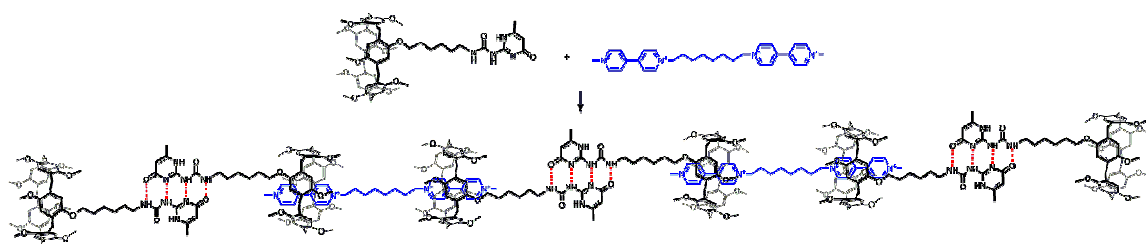
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-assembled linear supramolecular polymers based on copillar[5]arene with ureidopyrimidone unit

황성민 박연실 백경수

충남대 화학과

Pillararenes are new calixarene analogues. The hydroquinone units of this macrocycle are connected by methylene bridges in the para positions of the benzene rings, affording a  $D_5$ -symmetric structure with an overall pillar-like shape. Pillar[5]arene and its derivatives were reported as good hosts for viologens via cation- $\pi$  interactions between the electron-rich cavities inside the pillar[5]arene and the electron-deficient viologens. New self-assembled linear supramolecular polymers were developed using quadruple intermolecular hydrogen bondings of a copillar[5]arene mono-substituted with ureido-4[1H]-pyrimidone moiety. Copillar[5]arene itself forms stable dimers in nonpolar solvent through self-complementary hydrogen bonding. The synthesis and characteristics of these self-assembled supramolecular polymers will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-737

발표분야: 유기화학

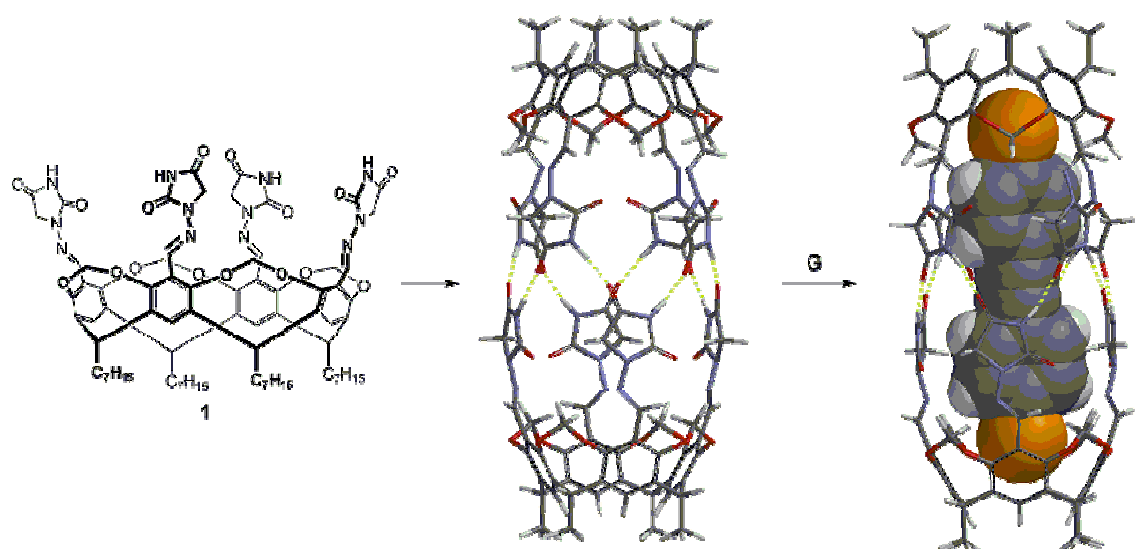
발표종류: 포스터, 발표일시: 수 18:00~21:00

## New Molecular Capsules based on Hydantoinylimino-cavitand

박주완 박연실 백경수

숭실대 화학과

Self-assembly is a smart approach to build nanoscale molecular capsules. The cavitands derived from resorcin[4]arene are the most versatile platforms for self-assembled molecular capsules. An adequate functional group attached on the upper rim of a cavitand could make it an attractive supramolecular building block for molecular capsules. New molecular capsule assembled by hydrogen bonds of hydantoin groups on a imino-cavitand was developed. Hydantoinylimino-cavitand 1 is the product of the condensation between tetraaldehyde cavitand and 1-aminohydantoin hydrochloride. Cavitand 1 forms a cylindrical molecular capsule  $1_2$  in nonpolar solvent through self-complementary hydrogen bonding of imide groups in hydantoin moieties on the upper rim of its imino-cavitand. The synthesis and versatile characteristics of this molecular capsule toward various guests will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-738

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Molecular and Supramolecular Control of the Work Function of an Inorganic Electrode with Self-assembled Umbrella-shaped Fullerene Derivatives**

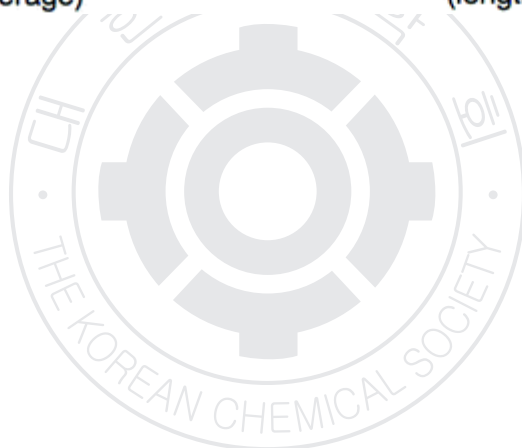
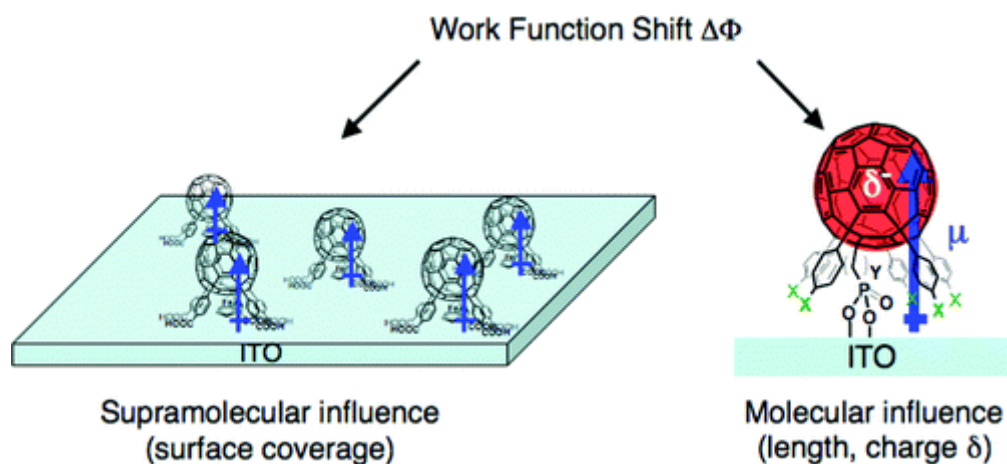
**Lacher Sebastian**

서울대 화학과

The work function control of inorganic electrodes is of major importance for organic electronic devices to reach high performances. Such control is often achieved by the use of self-assembled monolayers (SAMs) of polar compounds. For an understanding of the work function change, the interaction of single molecular dipoles with each other and the substrate is of high importance. Tracing the work function shift to the molecular level of single molecular dipoles has not been possible so far due to difficulties in generating SAMs with well defined molecular orientation and density on a substrate. We designed umbrella-shaped fullerenes for studying the interaction of molecular dipoles with each other and the substrate.<sup>1</sup> With these molecules we were able to generate SAMs with controlled variable density. The special umbrella design fixed the molecule (and thus, the intrinsic dipole) into a perpendicular orientation to the substrate. This allowed us to trace the important macroscopic characteristics of work function and water contact angle down to the molecular level and will open a way for an improved rational design of new compounds in



molecular electronics. We found that polar compounds generate an electric field through intermolecular interaction of the molecular charges, which strongly depends on the surface coverage. This field counteracts the molecular dipoles and reduces the observed work function shift (depolarization effect). We furthermore investigated the differences of work function control for these SAMs on gold and indium-tin oxide and found a high interaction of the compounds with gold responsible for reduced work function shifts. References: [1] Lacher, S.; Matsuo, Y.; Nakamura, E. *J. Am. Chem. Soc.* 2011, 133, 16997



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-739

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

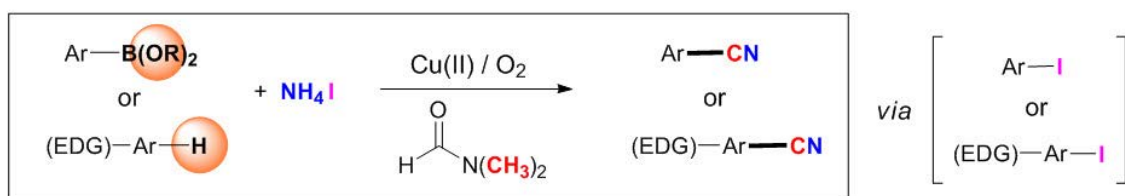
## Copper-Mediated Sequential Cyanation of Aryl C-B and Arene C-H Bonds Using Ammonium Iodide and DMF

최지호

KAIST 화학과

Nitriles are a ubiquitous structural motif frequently found in natural products and synthetic intermediates, and their facile access is important in the manufacture of pharmaceuticals, agrochemicals, and dyes. Cyano unit is a key precursor for diverse functional groups including aldehydes, amines, amidines, tetrazoles or amides. Recently, the synthetic utility of organonitriles has been investigated relying on the catalytic cleavage of carbon-cyano bond. Whereas traditional methods such as Sandmeyer or Rosenmund-von Braun reaction are routinely employed for the preparation of nitriles, metal-mediated approach has also been investigated in the coupling of aryl (pseudo)halides with metal cyano reagents such as MCN (M = K, Na, or Zn), TMS-CN, or  $K_3Fe(CN)_6$ . In those reactions, not only aryl halides but also C-H bonds of (hetero)arenes bearing suitable directing groups can be directly cyanated under various conditions mainly using metal cyanides. We recently reported that aqueous ammonia and N,N-dimethylformamide (DMF) were used in combination to afford “cyano” unit in situ under copper-mediated oxidative conditions, and

this protocol was successfully utilized in the Pd-catalyzed C-H cyanation of 2-phenylpyridines. Labelling experiments revealed that nitrogen and carbon atom of “CN” were originated from ammonia and the N,N-dimethyl moiety of DMF, respectively. Similar approaches of generating the cyano unit by using ammonium salts and DMF (or DMSO) were subsequently applied to the Pd-catalyzed cyanation of indoles and Cu-mediated cyanation of aryl halides. Herein, we present our new cyanation protocol of aryl boronic acids, boronates, and borate salts using ammonium iodide and DMF under Cu-mediated oxidative conditions.



$\text{NH}_4\text{I}$  : **Dual Role** (Supply of **N** and **I**)

**DMF** : Source of **C**



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-740

발표분야: 유기화학

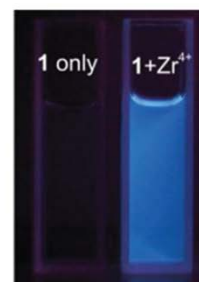
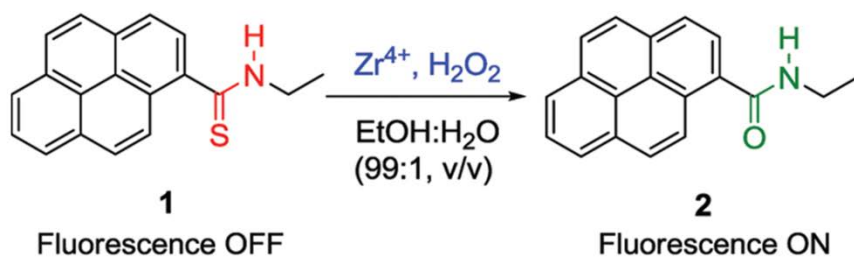
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescence Signaling of $Zr^{4+}$ by Hydrogen Peroxide Assisted Selective Desulfurization of Thioamide

배지희 최명길 장석규

중앙대 화학과

Thioamide derivative with a pyrene fluorophore was smoothly transformed to its corresponding amide by  $Zr^{4+}$  ions in the presence of hydrogen peroxide. The transformation was evidenced by  $^1H$  NMR spectroscopy and the signaling was completed within 10 min after sample preparation. Interference from  $Ag^+$  and  $Hg^{2+}$  ions in  $Zr^{4+}$ -selective fluorescence signaling was readily suppressed with the use of  $Sn^{2+}$  as a reducing additive. Discrimination of  $Zr^{4+}$  from closely related hafnium, which is a frequent contaminant in commercial zirconium, was not possible. Prominent  $Zr^{4+}$ -selective turn-on type fluorescence signaling was possible with a detection limit of  $4.6 \times 10^{-6}$  M in an aqueous 99% ethanol solution.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-741

발표분야: 유기화학

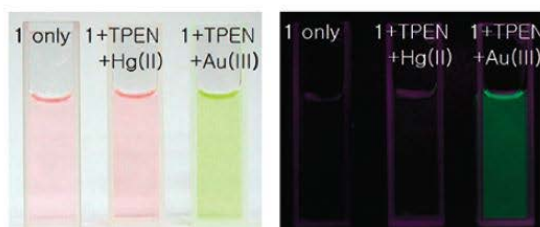
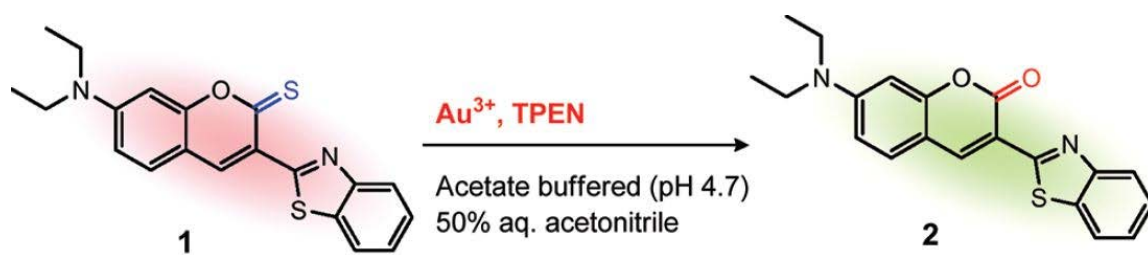
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Colorimetric and Fluorescent Signaling of $\text{Au}^{3+}$ by Desulfurization of Thiocoumarin

최명길 문정옥 장석규

중앙대 화학과

We investigated the chemosignaling of  $\text{Au}^{3+}$  by the selective desulfurization of thiocoumarin. In the presence of a heavy metal ion chelator N,N,N',N'-tetrakis-(2-pyridylmethyl)ethylenediamine, thiocoumarin was selectively converted to its oxo analogue by reaction with  $\text{Au}^{3+}$ , resulting in a pronounced chromogenic and fluorescent signaling. Selective signaling of  $\text{Au}^{3+}$  was possible in the presence of common alkali, alkaline earth, and transition metal ions, as well as  $\text{Au}^+$  in a mixed aqueous environment. The colorimetric determination of  $\text{Au}^{3+}$  was possible by the color change from pink to yellowish green of the designed probe. The detection limit for the determination of  $\text{Au}^{3+}$  in 50% aqueous acetonitrile was  $1.1 \times 10^{-7}$  M.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-742

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

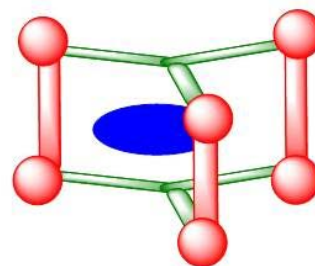
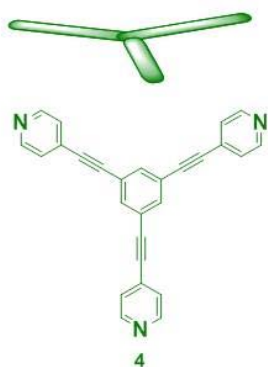
## Host-Guest Chemistry in the Hexanuclear Arene-Ruthenium Metalla Prismatic Cages: Synthesis and Antioxidant Studies

DUBEY ABHISHEK 송영호 지기환

울산대 화학과

Ellagic acid has antiproliferative and antioxidant properties in a number of in vitro and small-animal models. The host-guest properties of (6-8) have been studied with hexanuclear arene-ruthenium metalla prismatic cages and ellagic acid. A large cationic triangular metalla-prism allows encapsulation of ellagic acid as guest molecule which was characterized by NMR and ESI-MS. We have demonstrated antiproliferative and antioxidant studies by using host-guest chemistry.

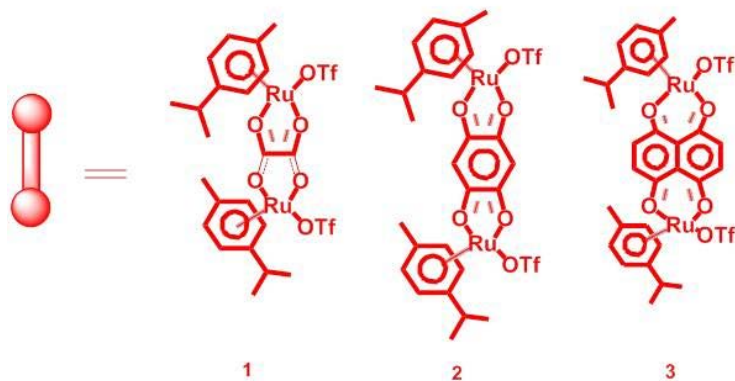




$$1+4+5=6$$

$$2+4+5=7$$

$$3+4+5=8$$



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-743

발표분야: 유기화학

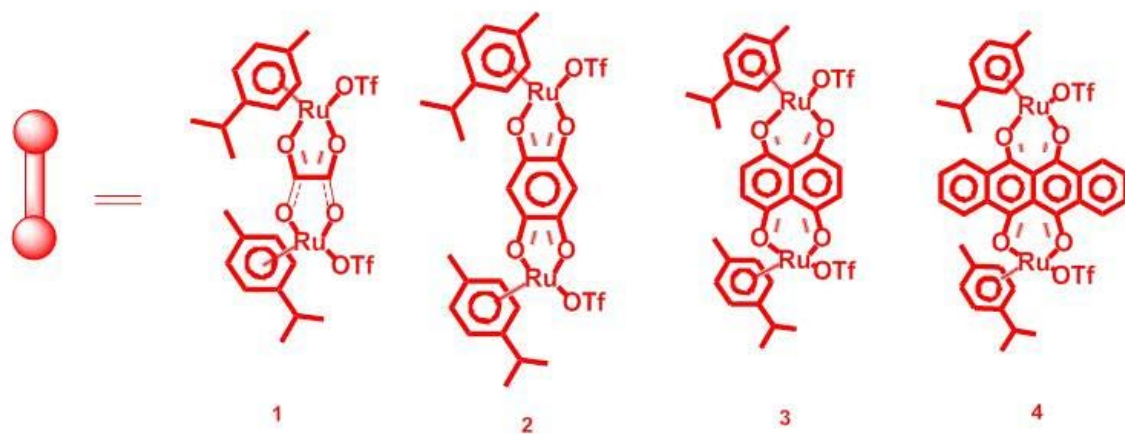
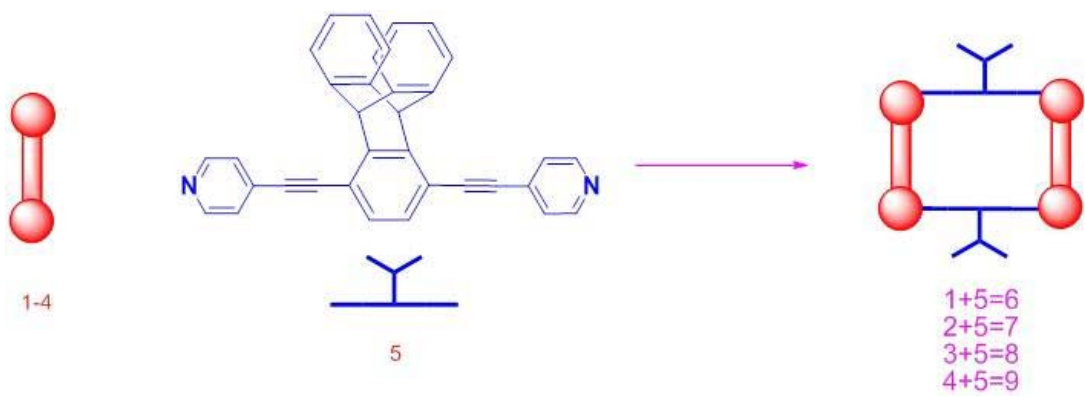
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-Assembly of Arene-Ruthenium Rectangles and Their Application in Fluorescent Detection of Nitro aromatics

DUBEY ABHISHEK 이선미 민진욱 지기환

울산대 화학과

Four new arene-ruthenium [2+2] metalla-rectangles (6-9) have been synthesized by the self-assembly approach using arene-ruthenium acceptors (1-4) and dipyrindyl ethynyl ligand (5) and characterized by NMR and ESI-MS. The luminescent nature of these rectangles, due to the presence of their electron rich ethynyl and anthracene functionalities, prompted photophysical studies, which revealed that electron-deficient nitro aromatics, in particular TNT and picric acid are effective quenchers of the rectangles' emission. Excited-state charge transfer from the rectangles to the nitro aromatic substrates can be used as the basis for the development of selective and discriminatory turn-off fluorescent sensors for nitro aromatics.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-744

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

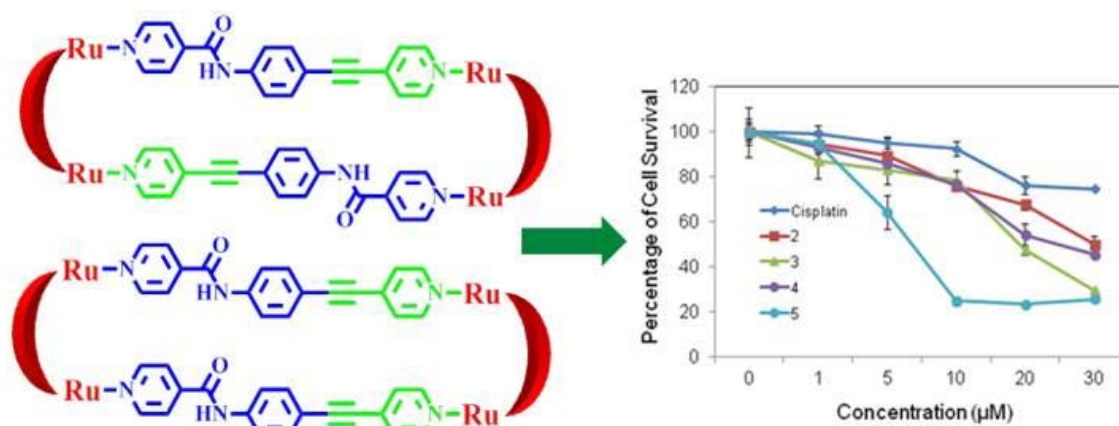
## Self-assembly of molecular rectangles via unsymmetrical amide ligand and areane ruthenium acceptors for anticancer activity

ANURAG MISHRA 송영호 지기환

울산대 화학과

The rational design and synthesis of discrete supramolecular metallacyclic structures with well-defined shape and size have drawn much attention due to their promising applications in molecular recognition, separation, host-guest, catalysis and biology. Ligands that incorporate pyridine-N donors are appealing candidates for coordination-driven self-assembly because of their ability to interact with metal acceptors to generate interesting assemblies. However, recently organometallic half-sandwich complexes based on Ru fragments are being used as potential building blocks to construct metallacycles and cages due to their stability and interesting electronic as well as structural properties. Such organometallic acceptors have mostly been used with nitrogen based organic linkers. Herein, we apply this strategy to the synthesis of new large molecular rectangles using a new unsymmetrical amide ligand with two different lengths of arene-ruthenium building blocks. These complexes have been characterized by various spectroscopic and

X-ray single crystal structure determination. In additions, we used these new rectangles for antitumor activity and found better results than that of reference drug cisplatin.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-745

발표분야: 유기화학

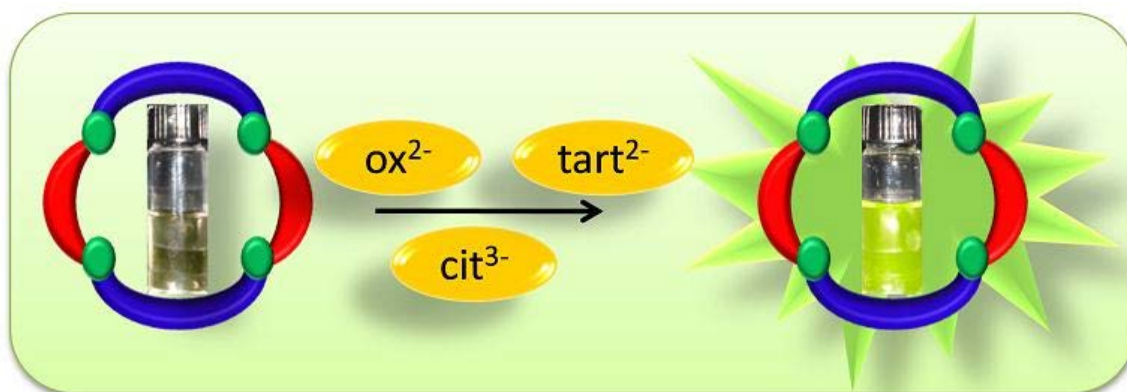
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Self-assembled supramolecular metallacycles for selective anion sensing

ANURAG MISHRA 정현지 이승창 지기환

울산대 화학과

The coordination-driven self-assembly of metallacyclic structures has attracted interest for promising applications in molecular recognition, separation, catalysis, encapsulation of guests and biological systems. The present work demonstrates the coordination behavior of amide ligands with different Ru-arene functionality to synthesized new self-assembled supramolecular metallacycles. These complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. The crystal structures of these complexes show that the metal ion coordinate between two nitrogen containing donor ligands. These self assembled metallacycles were further explored 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 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-746

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Non-Aromatic, Chiral Metallo Schiff-base Macrocycles: Synthesis and Chemical Properties

박은화 이창희

강원대 화학과

The meso-alkylidene porphyrins and expanded analogues are rather recently developed porphyrininoid macrocycles. We have demonstrated unique chemical and spectroscopic properties in terms of their tautomerization and protonation behaviour. In continuous efforts for the development of new meso-alkylidenyl expanded porphyrins, we hereby present a synthesis, characterization and metallation chemistry of the expanded porphyrinoid Schiff-base macrocyhcles that bear inherent chirality. The synthesis of these macrocycles have been accomplished by utilizing a typical '3+1' type aldehyde-amine condensation followed by matalation. The two meso-positions of the macrocycles are resistant to DDQ oxidation and maintain non aromatic characteristic. The synthesized compounds displayed unique spectroscopic behavior upon treatment with acids.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-747

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Anion Binding Behaviour of Pyrenyl-Pyrrole Strapped Calix[4]pyrroles

박건유 이창희

강원대 화학과

The strapped calix[4]pyrroles and their congeners have been actively studied as superior anion-binding receptors compared with other hydrogen bonding receptors. As a part of the continuing efforts for development of new anion receptors, we have demonstrated that the pyrrole-strapped calix[4]pyrrole is a superior fluoride binding receptor. In order to verify the high binding affinities in quantitative way, we tried to introduce a fluorescent reporter group on the position that can directly interact with pi-system. The new pyrrole-strapped calix[4]pyrroles bearing a signaling unit at one of the beta-pyrrolic positions. The identity of the synthesized receptors was fully characterized by spectroscopic means including proton NMR, HRMS and single crystal X-ray crystallography. The binding studies indicate that the receptor could be excellent fluorogenic anion receptors. Current modification showed fluorescence quenching upon anion binding possibly due to more efficient PET process upon anion binding. The anion selectivity and binding affinity of the receptors will be presented in detail.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-748

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Dicationic Calix[4]pyrrole Derivative and its Use for the Selective Recognition and Displacement-based Sensing of Pyrophosphate**

**박경화 이창희**

강원대 화학과

A Series of calix[4]pyrrole-based supramolecular host-guest complexes have been synthesized and studied for selective recognition of anions through fluorescent dye displacement assay (FDDA). The strong fluorescence of the dye, chromenolate anion, was completely quenched upon complexation with calix[4]pyrrole derivatives. Exposure of these supramolecular complexes with anionic analytes, whose binding affinities were greater than the dye with receptor, resulted in complete displacement of the dye with the full restoration of fluorescence. While fluoro-substituted receptor showed greater affinity towards only fluoride anions, the iodo-substituted one exhibited relatively high selectivity for both acetate and fluoride anions. On the other hand, the pyridinium substituted calix[4]pyrrole displayed preferential selectivity for pyrophosphate over phosphate and other anions. We expect that the present work could provide structural foundation for selective sensing of various anions through an ON-OFF-ON

fluorescence mechanism with a visual change in fluorescence intensity by introducing suitable substituent in the receptor.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-749

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 1,3-Dipolar Cycloaddition of meso-Alkylidenyl Porphyrins

박도우 이창희

강원대 화학과

1,3-Dipolar cycloaddition reaction of azomethine ylides has been drawn attention to the chemical modification of porphyrin 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-(m-benzi)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 MALDI-TOF mass spectrometry. The reaction can generate wide variety of new porphyrinoids which can be potentially in various porphyrin-related applications.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-750

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **“Turn-off” Phosphorescent Chemosensor for Selective Hg<sup>2+</sup> Detection Based on Iridium(III) Complex**

**안지혜 현명호**

부산대 화학과

Fluorescent chemosensors can highly sensitively and selectively detect heavy metal ion such as Hg<sup>2+</sup>, Pb<sup>2+</sup>, Cd<sup>2+</sup>, Cu<sup>2+</sup>, Ag<sup>+</sup> and Zn<sup>2+</sup>. Phosphorescent chemosensors are similar. The use of phosphorescent heavy metal complexes as chemosensors has recently attracted considerable interest, because of advantageous photophysical properties of heavy-metal complexes such as relatively long lifetimes and high stability compared with those of pure organic luminophores. Hg<sup>2+</sup> is one of the most serious environmental and health threats originating from natural and industrial sources. When absorbed in the human body, Hg<sup>2+</sup> causes damage to the central nervous, DNA, mitosis, and endocrine system even at very low concentration. Despite a reduction in its industrial use as a result of stricter regulations, high concentrations of mercury is still present in many environmental compartments, and it can still be found in many products of daily life such as paints, electronic equipment and batteries. As a result, developing

new and practical multisignaling chemosensors for  $\text{Hg}^{2+}$  is still a challenge. The new iridium(III) complex can quench for  $\text{Hg}^{2+}$  in aqueous 50% acetonitrile solution with respect to the selective phosphorescent detection of various metal ions including  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\text{Cs}^+$ ,  $\text{Li}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Cr}^{3+}$  and  $\text{Hg}^{2+}$ . The phosphorescence quenching for  $\text{Hg}^{2+}$  increased linearly with increasing concentration of  $\text{Hg}^{2+}$  in the range of  $2\mu\text{M}$ – $30\mu\text{M}$ .



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-751

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Phosphorescent Sensor for Copper(II) Ion based on Iridium(III) Complex

김혜빈 탁경미 현명호

부산대 화학과

Chemosensors had attracted great attention in the field of biology. Of those sensors, phosphorescent chemosensors based on heavy metal complexes have been recently synthesized and applied successfully. New phosphorescent chemosensor based on the Iridium(III) complex incorporating 2-phenylpyridine, 2,2-bipyridyl and 2,2-dipicolylamine chromophores was synthesized and characterized. The photoluminescence (PL) studies of the synthesized sensor with different metal ions showed significant phosphorescence quenching for copper(II) ion than other metal ions such as Ag(I), Ba(II), Ca(II), Cd(II), Cr(II), Cs(III), Fe(II), Hg(I), K(I), Li(I), Na(I), Pb(II), Rb(II), Zn(II). The PL intensity of the iridium(III) complex solution was found to be linearly decreased for copper(II) ion by increasing the concentration from 0 to 2 equivalents. In addition, the PL maximum of the iridium(III) complex in 50% acetonitrile solution was found to be red shifted for the addition of zinc(II) ion, and also the color of the complex solution was observed to change from yellow to orange for the addition of zinc(II) ion.

일시: 2012년 4월 25~27일(수~금) 3일간

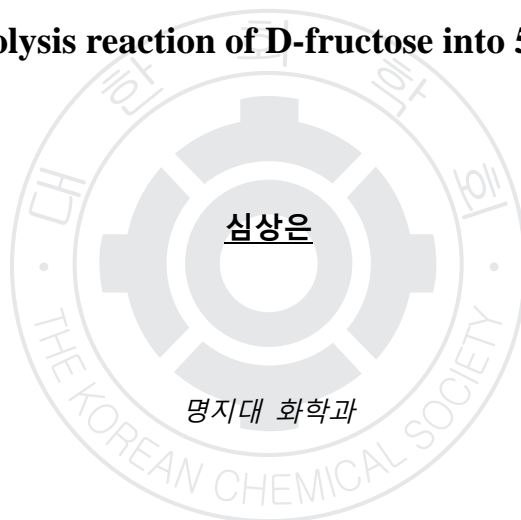
장소: 일산KINTEX

발표코드: ORGN.P-752

발표분야: 유기화학

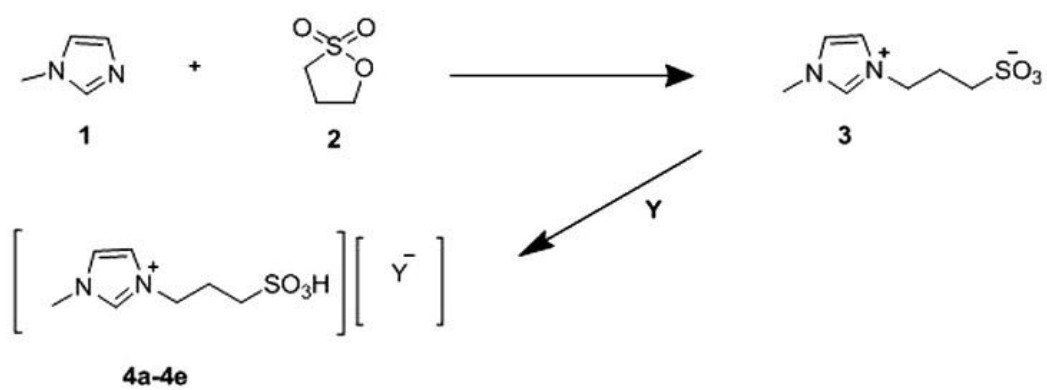
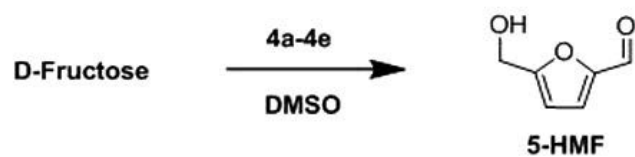
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Hydrolysis reaction of D-fructose into 5-HMF



Conversion of biomass into 5-hydroxymethylfurfural was studied from various scientists. They had known that D-fructose are easily converted to 5-HMF under acidic condition with Ionic Liquids. So we studied this reaction using strong acidic Ionic Liquids. The results showed that sulfonic acids contained Ionic Liquids have high activity for this hydrolysis reaction. For example, a 72% yield of HMF was obtained for 1hr at 100°C with [(SO<sub>3</sub>-p)Mim]<sup>+</sup> [CH<sub>3</sub>SO<sub>3</sub>]<sup>-</sup> (4a). This poster include synthetic methods of Zwitterion (3), various Ionic Liquids (4a-4e) and hydrolysis reaction of D-Fructose using sulfonic acid contained Ionic Liquids.





Y : a- CH3SO3H    b- H2SO4    c- p-TsOH    d- P3CSO3H    e- ClSO3H



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-753

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mn(III)-initiated oxidation and cyclization of $\beta$ -ketoester derivatives

Wang Chao Ju Yeming 구상호<sup>1</sup>

명지대 나노공학과 <sup>1</sup>명지대 화학과

We have devised heterocyclic compounds which could be synthesized from isoprenoid chains via intermolecular Hetero-Diels-Alder reactions that are induced by  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$ . In addition,  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  is developed to form various kinds of furan containing diverse functional groups that may contribute to the synthesis of furan. The best condition for the reaction was achieved by a series of optimizing experiments. As the figure showed, compounds with this particular structure undergo Mn(III)-mediated oxidation through peroxy-radical, decarbonylation and subsequent cyclization to form a variety of furan.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-754

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient method of regioselectivity in the esterification of glycerol

**최보슬 구상호<sup>1</sup>**

명지대 나노공학과 <sup>1</sup>명지대 화학과

Phosphatidylcholine is a important component that is in every cell membranes and tissues of human body. A general phosphatidylcholine is composed of a choline head group and two acyl chains, being fatty acids. Synthesis of phosphatidylcholine using esterification of glycerol is possible. Since glycerol has three hydroxyl groups, it is difficult to synthesize diglycerides regioselectively. We tried to use  $\alpha$ -tocopherol for one fatty group because it is a well known anti-oxidant, which may protect other molecular or cell. And then we tried the regioselective epoxide ring opening by acid nucleophiles. We were able to synthesize various diglycerides, which would be efficiently utilized for the formation of diversely substituted phosphatidylcholine derivatives.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-755

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Synthetic method of Stabilized Carotenoids as Molecular Wires

전선화 김영훈 구상호<sup>1</sup>

명지대 나노공학과 <sup>1</sup>명지대 화학과

The carotenoids are an important class of organic molecules with delocalized  $\pi$ -electrons, which show electric conductance. We have perfectly proved the efficient synthesis of natural carotenoids, which can be extended to the synthesis of unnatural carotenoid wires. The unnatural carotenoids can be disconnected into two parts, the allylic sulfone and the dialdehyde containing aromatic substituents. The unnatural carotenoids can be combined with these two parts, followed by coupling, protecting and the double elimination reaction. 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 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-756

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of efficient units for the carotene wire containing phenyl substituents

임보람 이규상 구상호<sup>1</sup>

명지대 나노공학과 <sup>1</sup>명지대 화학과

Unnatural carotenoids containing various phenyl substituents is expected that it will better than existing carotenoids in terms of stability and Electronics. So It is important things that synthesis of multi-functional carotenoids molecular wire. Allylic sulfone unit is used useful material for synthesis of carotene wire containg phenyl substituents. For the construction of allylic sulfone unit, we will construct Chloro allylic sulfone unit containg substituent X first. This material can make from Acetophenone derivative depending on the location. According to Indium addition and oxonia- cope rearrangement using Lewis acid , we will make Allylic sulfone unit provides regioselectivty. and using this material, We will make carotene wire various phenyl substituents on diverse synthetic route.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-757

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Pyrene end-capped oligothiophene derivatives for organic thin-film transistors and organic solar cells

권종철 이성훈 홍종인

서울대 화학부

The good fluorescent quantum yield and solid state  $\pi$ - $\pi$  stacking properties of pyrene derivatives have been exploited in biological probes, electrogenerated chemiluminescent (ECL) materials, active OTFT materials, and blue light-emitting and electron transporting materials in OLEDs. Recently, Fages et al. reported new active materials for OTFTs, consisting of oligothiophene and pyrene moieties linked with conjugated bonds. The devices fabricated using pyrene-substituted thiophene oligomers as p-type OTFTs exhibited field-effect mobility values in the range of  $10^{-3} \sim 10^{-5} \text{ cm}^2/\text{Vs}$ . Furthermore, only a few pyrene derivatives have been studied as donor materials for OSCs and organic dye materials for dye-sensitized solar cells (DSCs). To the best of our knowledge, pyrene-based organic materials have not so far been simultaneously utilized as both donor materials in OSCs and active materials in OTFTs. We report new organic semiconducting materials (1s and 3s), consisting of oligothiophene and pyrene, as active materials for OTFTs and donor materials for OSCs. A fabricated OTFT device based on 3s

exhibited a field-effect mobility of 0.11 cm<sup>2</sup>/Vs, and a power conversion efficiency of 1.2% was achieved in OSCs.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Correlation of the Rates of Solvolysis of Electron-Rich Benzoyl Chloride Using the Extended Grunwald-Winstein Equation

오현정 최호준<sup>1</sup> 박종근<sup>1</sup> 양기열<sup>1</sup> 구인선<sup>1</sup>

경상대 화학교육<sup>1</sup> 경상대 화학교육과

The specific rates of solvolysis of piperonyl chloride have been determined in binary aqueous solvent mixtures at 25.0 °C. Comparison of the specific rates of solvolyses of piperonyl chloride with those for *p*-methoxybenzoyl chloride in terms of linear free energy relationships (LFER) are helpful in mechanistic considerations, as is also treatment in terms of the extended Grunwald-Winstein equation. It is proposed that the solvolyses of piperonyl chloride in binary aqueous solvent mixtures proceed through an ionization [I] pathway rather than through an S<sub>N</sub>1/S<sub>N</sub>2 and/or ionization/(ionization-elimination)=[I/(I-E)] pathway.



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발표코드: ORGN.P-759

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Oxidation of benzylic alcohols using $\text{CuBr}_2$ and $\text{HNO}_3$ in ionic liquid

임채미 이종찬

중앙대 화학과

The oxidation of primary and secondary benzylic alcohols into corresponding aldehyde or ketones was carried out in homogeneous solution in bmim[BF<sub>4</sub>] ionic liquid at 60 °C in presence of catalytic amounts of nitric acid and copper(II) bromide. The generality of this reaction was shown by the successful oxidation of aromatic alcohols with  $\text{CuBr}_2$  (1.5 equiv.) and  $\text{HNO}_3$  (0.5equiv.) in ionic liquid (1mL) at 60 °C to give corresponding aldehydes or ketones in high yield. Moreover, five- and six-membered cyclic compounds successfully undergo oxidation reactions; 9-fluorenone,  $\alpha$ -tetralone afforded the corresponding ketone compounds in excellent yield (>95%). Electron withdrawing group (p-NO<sub>2</sub>) took longer reaction times compared to the substrate containing electron donating substituents (p-CH<sub>3</sub>). In conclusion, our work is an efficient and eco-friendly protocol for oxidation of benzylic alcohol to corresponding carbonyl compounds with the reagent combination of  $\text{CuBr}_2$  and  $\text{HNO}_3$  in ionic liquid.

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장소: 일산KINTEX

발표코드: ORGN.P-760

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Oxidation of benzylic alcohols with sodium perborate in aqueous polyethylene glycol

한미경 이종찬

중앙대 화학과

The oxidation of alcohols to the corresponding carbonyl compounds is very important transformation in organic chemistry. In general, the oxidation of benzylic alcohols has been achieved using toxic, transition metal containing oxidants. However, in this eco-conscious era, development of green oxidative methodologies has become a prime area of research interest. We wish to describe a new environmentally benign and effective method for the oxidation of benzylic alcohols employing sodium perborate in polyethylene glycol. The generality of this reaction was shown by the successful oxidation of benzylic alcohols with SPB(2.0equiv.), KBr(1.0equiv.), and sulfuric acid(1.0equiv.) in PEG-200/H<sub>2</sub>O(v/v, 4:1) at 80°C for 1.5~2h giving the corresponding aldehydes and ketones in high yields. To investigate the versatility and applicability of this method, the reaction was investigated with various structurally benzylic alcohols. And, we have studied the effect of electron-donating and electron-withdrawing substituents at the aromatic ring. At the result, the reactions proceeded efficiently and electron-donating

substituent was higher isolated yield than the substrate containing electron-withdrawing substituent. Herein, we report an efficient and environmentally friendly protocol for oxidation of benzylic alcohols.



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발표코드: ORGN.P-761

발표분야: 유기화학

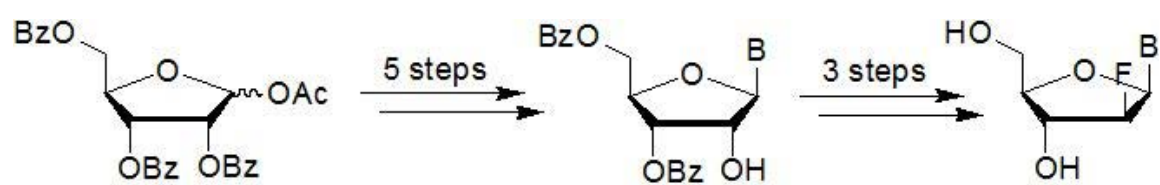
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of 2'-deoxy-2'-fluoro- $\beta$ -D-arabinonucleic acid (FANA)

손의호 황길태

경북대 화학과

항암제 후보물질의 양전자 방출 방사선동위원소 F-18 의 도입 및 생체영상정보를 이용한 암세포 증식 진단 및 제어 연구를 위한 2'-deoxy-2'-fluoro- $\beta$ -D-arabinonucleic acid (FANA)를 합성하였다. FANA 는 진단제 및 치료제로서의 특성을 가지며 다양한 질병에 대한 연구가 진행되고 있다. Sugar ring 의 2' 위치에 상대적으로 긴 반감기를 가지는 F-18 을 표지함으로써 PET 조영제로서 이용이 가능하며, 종양억제 능력을 측정해 봄으로써 선택적인 억제제로서의 가능성에 대해 측정을 할 수 있다. 특히, [18-F]ANA 를 합성함에 있어서 F-18 의 반감기를 고려하여 합성의 가장 마지막 단계에 표지함으로써 F-18 의 반감기 손실을 줄일 수 있는 경로로 합성을 제안하였다. FANA 의 합성은 1-acetyl-2,3,5-tribenzoyl- $\beta$ -D-ribofuranose 를 시작물질로 하여 unnatural base 를 glycosylation 한 후  $S_N2$  반응으로 F 를 2' 위치에 표지한다.



B = unnatural base



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장소: 일산KINTEX

발표코드: ORGN.P-762

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Protecting-Group-Free Synthesis via Unstable Organolithium Intermediates Using a Flow Microreactor

김희진 함정엽 Aiichiro Nagaki<sup>1</sup> Jun-ichi Yoshida<sup>1</sup>

KIST 천연의약센터 <sup>1</sup>Kyoto University, Japan

Protecting-group-free synthesis has received significant recent research interest in the context of ideal synthesis and green sustainable chemistry. In general, organolithium species react with ketones very rapidly, and therefore ketone carbonyl groups should be protected before an organolithium reaction, if they are not involved in the desired transformation. If organolithium chemistry could be free from such a limitation, its power would be greatly enhanced. In this study, we show that a flow microreactor enables such protecting-group-free organolithium reactions by greatly reducing the residence time (0.003 s or less). Aryllithium species bearing ketone carbonyl groups are generated by iodine-lithium exchange reactions of the corresponding aryl iodides with mesityllithium and are reacted with various electrophiles using a flow-microreactor system. The present method has been successfully applied to the formal synthesis of Pauciflorol F.

일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-763

발표분야: 유기화학

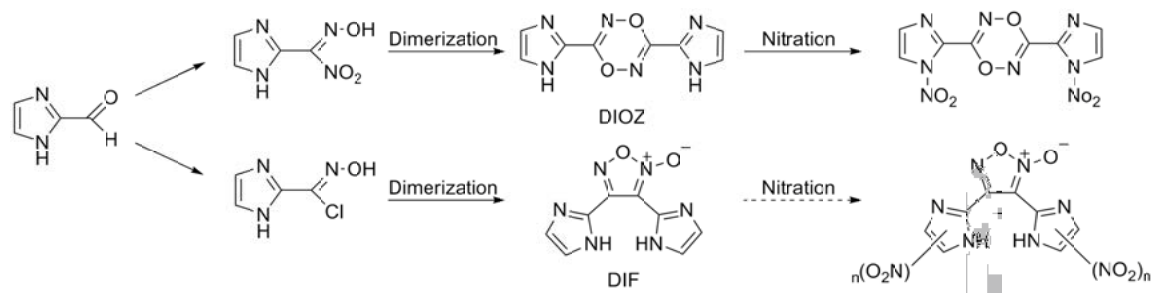
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies on the Dimerization and Nitration of Imidazole Derivatives

최준호 이병우 김태근 정규현

인하대 화학과

In our previous work, we successfully synthesized DIOZ[3,6-di(imidazol-4-yl)-1,4,2,5-dioxadiazine] via 1,3-dipolar cycloaddition of the corresponding nitrile oxide. To synthesize its structural isomer, DIF[3,4-di(imidazol-4-yl)-1,2,5-oxadiazole 2-oxide], we prepared other intermediate as a precursor of the nitrile oxide and successfully synthesized DIF. The subsequent nitrations of DIOZ were examined under various reaction conditions. Due to low stability of the dioxadiazine ring system, anhydrous and mild nitration conditions were favored.





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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Site Selective Coupling Reaction and Decarboxylation for  
the Synthesis of Aryl Alkynyl Carboxylic Acids and Aryl Alkynes from  
Propiolic Acid and Aryl Halides**

**박경호 Thiruvengadam Palani 이선우**

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-765

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Pd-Catalyzed Carbonylative Reaction for the Synthesis of  
Benzoylacetonitriles**

표아영 이선우 김원영

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-766

발표분야: 유기화학

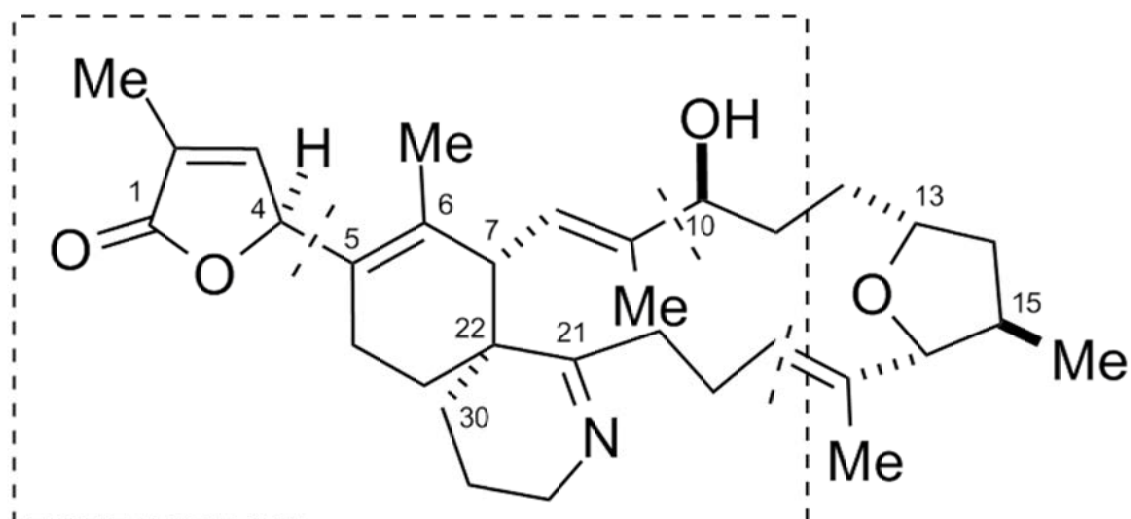
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies on the Synthesis of (-)-Gymnodimine A: the Construction of a Spiroimine System

최소영 최일영<sup>1</sup> 이효원

충북대 화학과 <sup>1</sup>한국화학연구원

(-)-Gymnodimine A is a macrocyclic imine phycotoxin produced by the dinoflagellate *Karenia selliformis*. For the purpose of preparing a spiroimine system, we conducted firstly the Diels-Alder reaction between a modified Danishefsky diene and a dienophile of a chiral oxazolidinone derivative, secondly a cyclization involving alkylation after the Birch reduction of an aromatic ring attached with a chiral auxiliary, and thirdly aldol condensation using proline as an organic catalyst.



**(-)-Gymnodimine A**



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장소: 일산KINTEX

발표코드: ORGN.P-767

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Site Selective Coupling Reaction and Decarboxylation for  
the Synthesis of Aryl Alkynyl Carboxylic Acids and Aryl Alkynes from  
Propiolic Acid and Aryl Halides**

**최주석 이선우**

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-768

발표분야: 유기화학

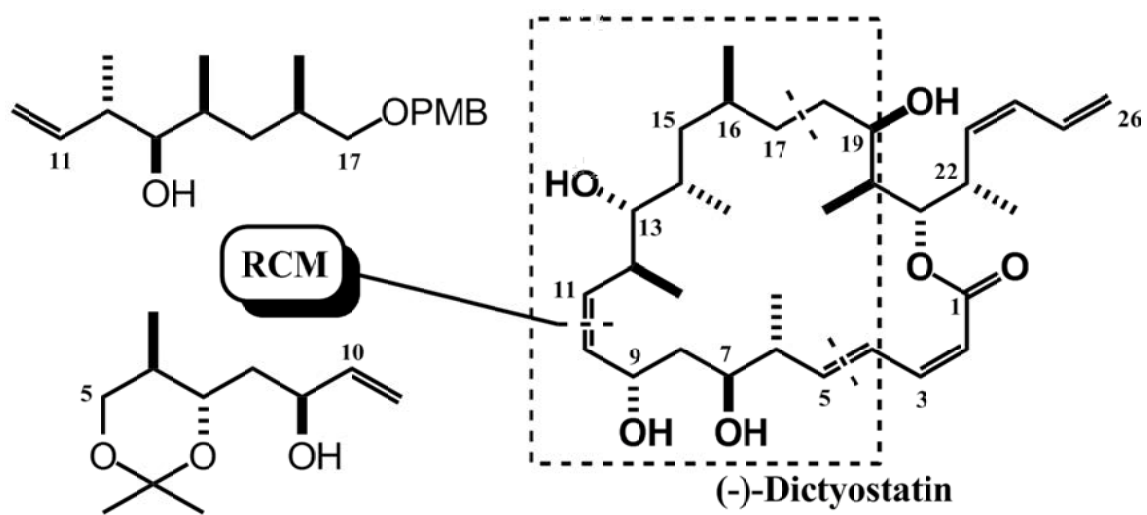
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthetic Studies of C5-C17 Subunits of (-)-Dictyostatin

곽달용 이효원

충북대 화학과

The 22-membered antimitotic macrolide (-)-dictyostatin was first isolated from the marine sponge *Spongia sp.* by Pettit and co-workers in 1994 and is structurally related to discodermolide. Dictyostatin inhibits the growth of human cancer cells by stabilizing tubulins like taxol<sup>7</sup> resistant tumors. We planned the asymmetric synthesis of C5-C17 fragment the northern part of (-)-dictyostatin. This structural unit was prepared using key chemical manipulations such as silicon-tethered ring-closing metathesis (RCM) and the Roush asymmetric allylation. The details will be disclosed.



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발표코드: ORGN.P-769

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Copper-Catalyzed One-Pot Three Component Reaction for  
the Synthesis of Benzothiazoles**

허유미 이선우 변아름

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-770

발표분야: 유기화학

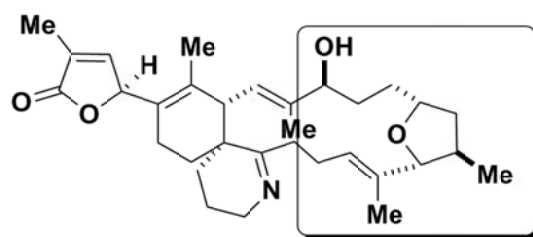
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of the C10-C20 Fragment of Gymnodimine

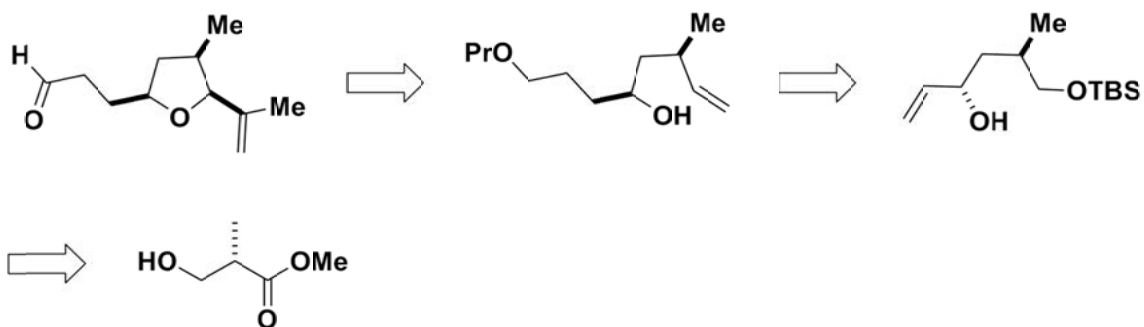
GAOYAQIONG 이효원

충북대 화학과

A new marine toxin gymnodimine was isolated from New Zealand oysters collected at Foveaux Strait in 1994. This macrocyclic imine phycotoxin was produced from dinoflagellate *Karenia selliformis* and *Gymnodinium cf. mikimotoi*. Gymnodimine and its analogues usually include a spirocyclic imine ring system and a trisubstituted tetrahydrofuran embedded within a 16-membered macrocycle. Gymnodimine exerts its toxic effects *via* binding to nicotinic acetylcholine receptors with picomolar affinities with no sign of apparent reversibility in short time frames. An access to the C10-C20 skeleton of gymnodimine incorporates a tetrahydrofuran fragment. The elaboration of the tetrahydrofuranose moiety is based on a stereocontrolled cyclization by using 5-*exo* opening reaction on an epoxide. Further details will be disclosed.



**Gymnodimine**



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발표코드: ORGN.P-771

발표분야: 유기화학

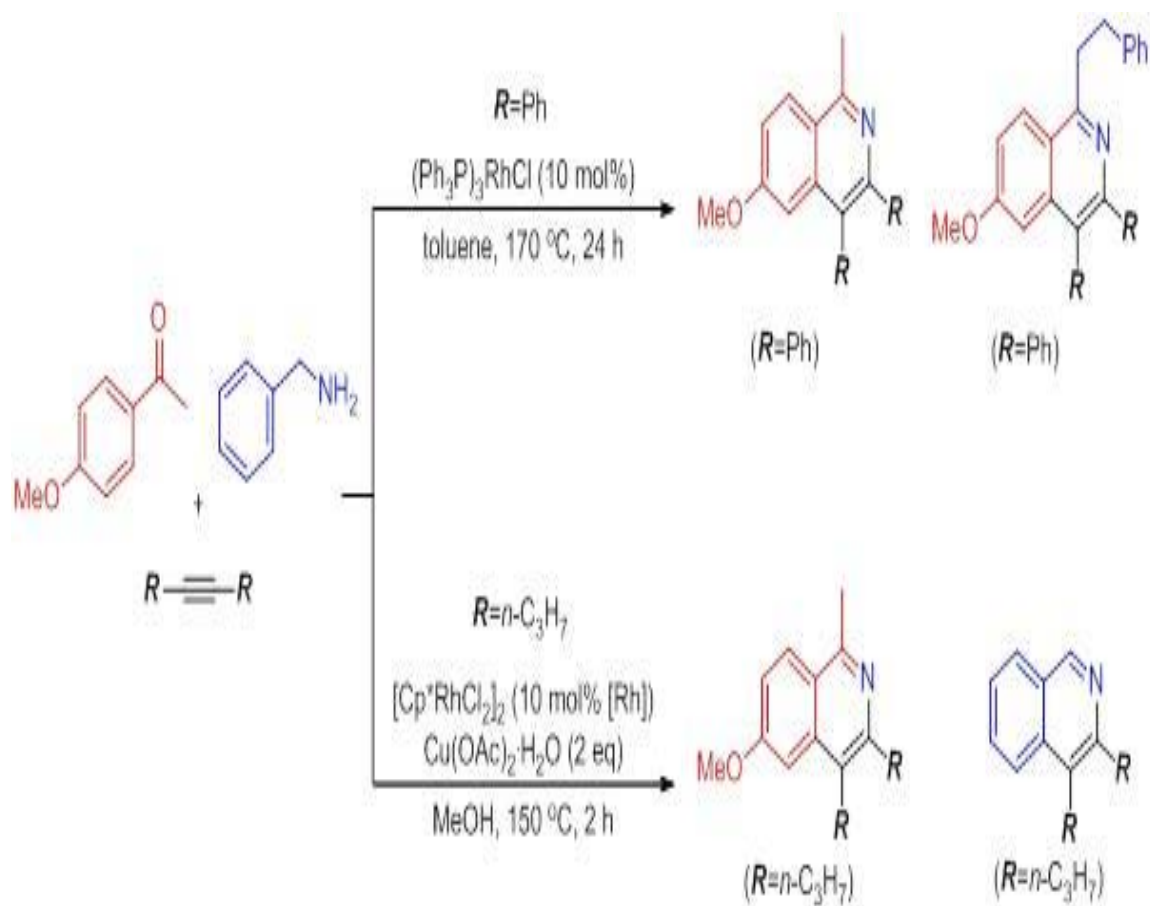
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Funtionalized Mesoporous Materials using Methallylsilane derivatives

김한일 전철호

연세대 화학과

Various functional group-modified SBA-15 mesoporous materials were prepared by co-condensation method using methallylsilane derivatives. Instead of alkoxysilane derivatives, commonly used in the synthesis of SBA-15, stable methallylsilanes were introduced. Not like trialkoxysilane, trimethallylsilane derivatives were conveniently prepared and purified by column chromatography. In the presence of Pluronic P123 as a surfactant, methallylsilane derivatives having organic functional groups are efficiently hydrolyzed to co-condensate with TEOS under acidic condition. In this poster, we describe synthesis of azido, fluorescent dansyl, and pyrenyl group-modified SBA-15 mesoporous materials using corresponding organic functional group-impregnated methallylsilane derivatives as starting materials. SBA-15 materials are prepared with various molar ratios of methallylsilane(x %) and TEOS(100 - x %).



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장소: 일산KINTEX

발표코드: ORGN.P-772

발표분야: 유기화학

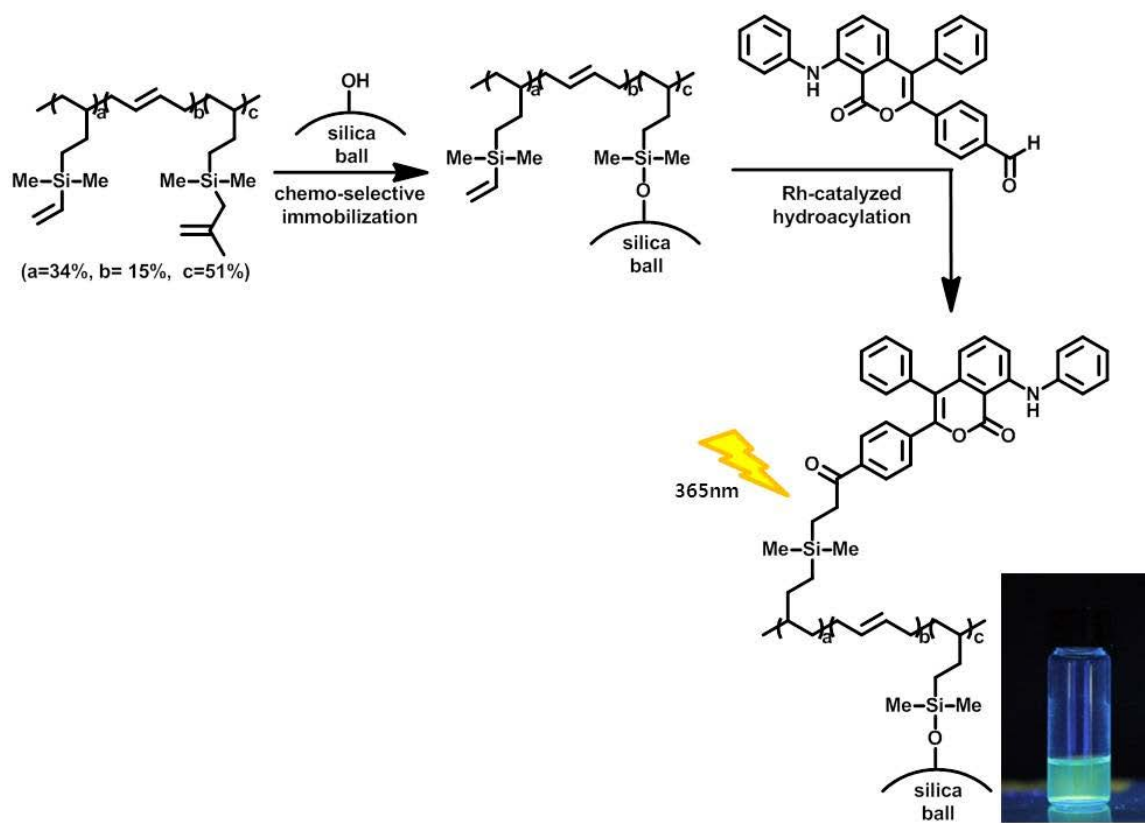
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Catalytic Grafting Reactions of Functionalized Polymers On Solid Surface

이은택 전철호

연세대 화학과

In this research, we describe fabrication of highly robust organic-inorganic hybrid material that can be modified to various functional group by catalytic grafting reactions. Recently, we have developed highly efficient  $\text{Sc}(\text{OTf})_3$ -catalyzed immobilization method using stable methallylsilyl group. Meanwhile, vinylsilyl group has been widely used for catalytic reactions owing to their electrophilic character. Thus, we expected that the molecules impregnating methallylsilyl group and vinylsilyl group would be highly efficient and variously modifiable organic-inorganic hybrid materials. Because polybutadiene has many vinyl groups that can be transformed into many functional groups, bi-functionalized polymer with methallylsilyl and vinylsilyl groups can be used for the preparation of vinyl group-immobilized solid support using methallylsilyl group and further application of synthesis of organic molecule-functionalized material by catalytic grafting reactions using residual vinylsilyl group.



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장소: 일산KINTEX

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발표분야: 유기화학

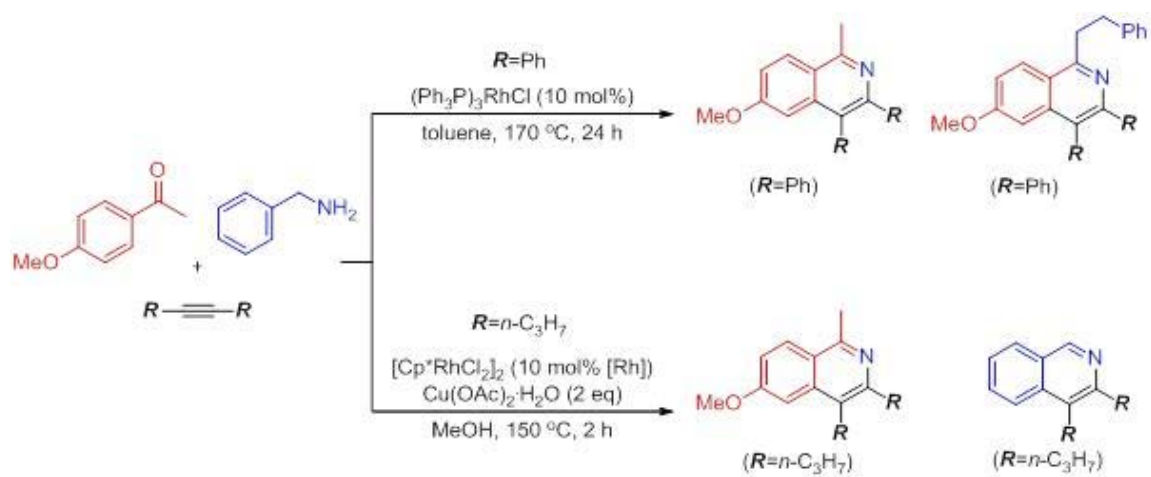
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Rh(III)-Catalyzed Synthesis of Isoquinoline and Pyridine Derivatives from Benzyl or Allyl Amine

김동수 심용균 박정우 전철호

연세대 화학과

Transition metal catalyzed C-H bond activation has been focused on by many organic chemists since it can be applied for wide range of synthetically useful C-C bond formation. In particular, ortho-alkyl or alkenylation provides an efficient synthetic method for preparing ortho-substituted aromatic ketones. In the course of our ongoing studies on ortho-alkylation, we found an efficient single-step synthesis of isoquinoline derivatives by three-component coupling reaction of aromatic ketone with benzylamine and alkyne through the Rh(I)-catalyzed direct ortho-alkenylation. However, the reaction required vigorous reaction conditions such as high temperatures and resulted in product mixtures. Moreover, the reaction took place with only aromatic ketone, not aromatic aldehyde. In this poster, we report a new protocol for the preparation of isoquinolines from benzylamine and alkyne by Rh(III)-catalyst with Cu(II) as an oxidant. Furthermore, pyridine derivatives could be also produced from non-aromatic allylamines.





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장소: 일산KINTEX

발표코드: ORGN.P-774

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescent On-Off Chemosensor for Fluoride Anion with Pyrene Based on Triphenylphosphine Salt Derivative

조재원 전남중 남계춘

전남대 화학과

The supramolecular chemistry of anions provides a means to sense and manipulate anions in their many chemical and biological roles. Anions are ubiquitous and they have major roles in the natural world. In particular, the studies of chemosensors toward  $F^-$  anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, the development of reliable sensors for  $F^-$  is needed for environment and human health care. Fluorescent chemosensors can be effectively used as a tool to analyze and classify such roles of charged chemical species in living system as well as to measure the amount of ions from the sources contaminated with them. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. Pyrene phosphonium ligand was obtained successfully by the reaction of triphenylphosphine with pyrene derivative. The binding properties of

triphenylphosphine derivative investigated with  $^1\text{H}$ -NMR and fluorescence titration methods with various anions.



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-775

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescent On-Off Chemosensor for Fluoride Anion with Pyrene Based on Bipyridine Salt Derivative

전남중 조재원 남계춘

전남대 화학과

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. In particular, the studies of chemosensors toward  $F^-$  anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, the development of reliable sensors for  $F^-$  is needed for environment and human health care. Color changes that can be detected by the naked eye are widely used as signals for events owing to the inexpensive equipment required or no equipment at all. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. Especially, pyrenes are a particularly elegant basis for ratiometric based optical sensors, where the ratio of two emission wavelengths comprise the analytical signal. Pyrenebipyridine ligand was obtained

successfully by the reaction of bipyridine with pyrene derivative. The binding properties of pyrenebipyridine derivative investigated with  $^1\text{H}$ -NMR and fluorescence titration methods with various anions.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-776

발표분야: 유기화학

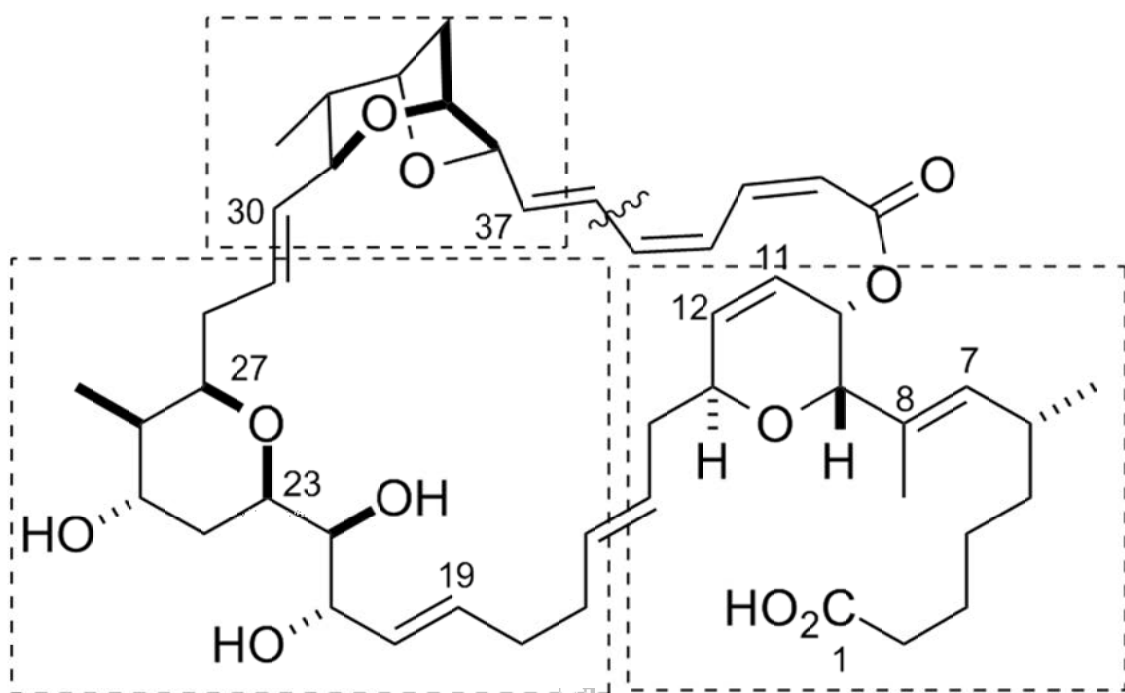
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthetic Study of the C1-C15 Fragment of Sorangicin A

한선영 이효원

충북대 화학과

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 Julia olefination reaction. Herein, we report the synthesis of key fragments of sorangicin by utilization of several reactions such as ring-closing metathesis (RCM) for the preparation of (*Z*)-double bond (C<sub>11</sub>-C<sub>12</sub>), Julia olefination for the (*E*)-double bond (C<sub>7</sub>-C<sub>8</sub>), and the Evans aldol reaction.



(+)-Sorangicin A



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-777

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Organic Sensitizers Based on 3,6-Disubstituted Carbazole and benzothiadiazole for Efficient Dye-sensitized Solar Cells

성지연 홍종인

서울대 화학부

Solar energy is one of the most viable alternative energy to fossil fuel, main cause of global warming. In many kinds of solar cell, dye-sensitized solar cells (DSSCs) have attracted attention due to the advantages of low cost, easy fabrication and relatively high power conversion efficiency. As a key factor in highly efficient solar cells, dyes should possess several properties, for example, optimum absorption overlap with the solar spectrum for efficient light harvesting, appropriate HOMO and LUMO energy level for efficient electron injection and regeneration and hydrophobicity for minimizing charge recombination. In this respect, we reported organic dyes of a D-D- $\pi$ -A structure since the bulky shape is advantageous to reduce the molecular aggregation as well as enhance the blocking effect of the dyes so as to improve the Voc.[1] In this presentation, we report several organic dyes based on 3,6-disubstituted carbazole donor and an electron-withdrawing unit in the bridge group for efficient dye-sensitized solar cells. An electron-deficient unit introduced as the bridge group such as benzothiadiazole or benzoxadiazole, which exhibits

good electron-withdrawing ability as well as a red shift of the absorption region, increases the photo-conversion efficiency. Photophysical and electrochemical properties of the dyes as well as photovoltaic performance of the device were systematically investigated. Details will be discussed in the presentation. Reference [1] Chem. Asian. J. 2012, 7, 343





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-778

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Intermolecular Oxidative C-N Bond Formation under Metal-Free Conditions: Control of Chemoselectivity between Aryl  $sp^2$  and Benzylic  $sp^3$  C-H Bond Imidation**

김지유 김현진 장석복

KAIST 화학과

A new synthetic approach toward intermolecular oxidative C-N bond formation of arenes has been developed under transition-metal-free conditions. Complete control of chemoselectivity between aryl  $sp^2$  and benzylic  $sp^3$  C-H bond imidation was achieved by the choice of nitrogen sources, representatively being phthalimide and dibenzene sulfonimide, respectively.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-779

발표분야: 유기화학

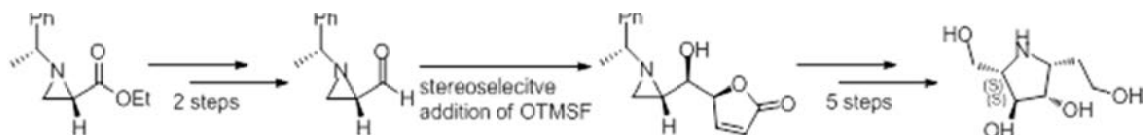
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Enantiomerically Pure 2,5-Imino-2,5,6-trideoxy-D-gulo-heptitol from Chiral Aziridines

이호균 강필준 이원구 하현준<sup>1</sup>

서강대 화학과 <sup>1</sup>한국외국어대 화학과

Heptitols can be found in various natural products and the importance of heptitol derivatives is also found in pharmacologically and biologically active substances. We were interested in the new synthetic strategy for the efficient preparation of 2,5-Imino-2,5,6-trideoxy-D-gulo-heptitol from sequential reactions including a stereoselective addition of (furan-2-yloxy)trimethylsilane in the presence of ZnBr<sub>2</sub> followed by regioselective ring opening with acetic acid and subsequent intramolecular cyclization.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-780

발표분야: 유기화학

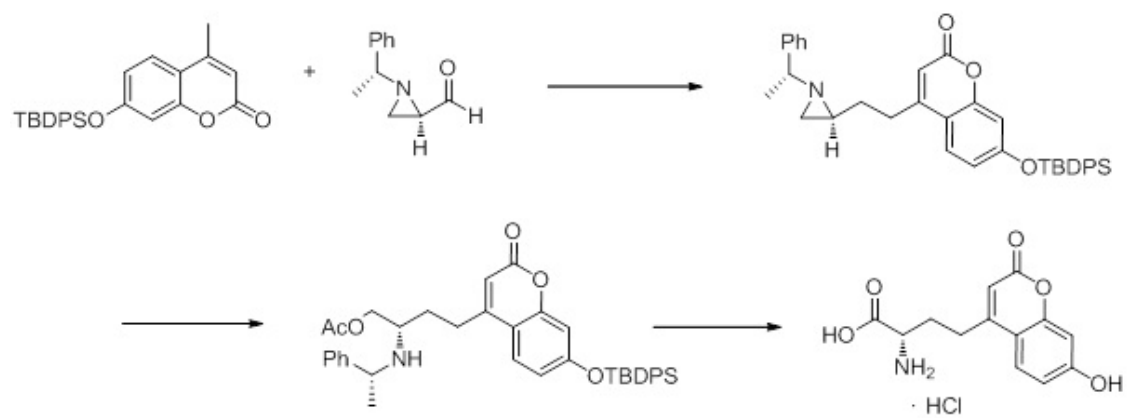
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of a Fluorescent Unnatural Amino Acid from a Chiral Aziridine

심연수 정미진 이원구 하현준<sup>1</sup>

서강대 화학과 <sup>1</sup>한국외국어대 화학과

The site-specific incorporation of fluorescent unnatural amino acids (UAA) becomes more powerful tool when they are combined with fluorescent proteins. Among various kinds of UAAs, we were interested in L-(7-hydroxycoumarin-4-yl)ethylglycine which contains coumarin unit. Coumarin has been reported to have high fluorescence quantum yield and also has sensitive fluorescent ability depends on both pH and solvent polarity. We synthesized enantiomerically pure fluorescent unnatural amino acid L-(7-hydroxycoumarin-4-yl)ethylglycine as hydrochloride salt form starting from commercially available 4-methylumbelliferone sodium salt and a chiral aziridine-2-carboxylate.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-781

발표분야: 유기화학

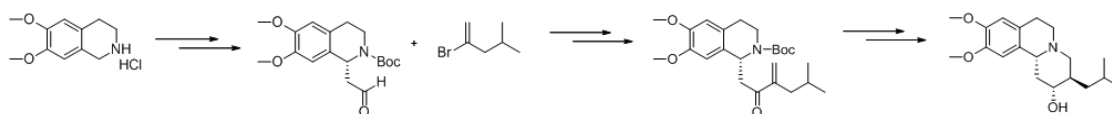
발표종류: 포스터, 발표일시: 수 18:00~21:00

## An Efficient Synthesis of Enantiomerically Pure (+)- Dihydrotetrabenazine from 6,7-Dimethoxy-1,2,3,4- tetrahydroisoquinoline hydrochloride

장만수<sup>1</sup> 현진섭 이원구 하현준<sup>1</sup>

서강대 화학과 <sup>1</sup>한국외국어대 화학과

Recently, it was turned out that (+)-dihydrotetrabenazine (DTBZ) can combine with a vesicular monoamine transporter-2 (VMAT-2) in the brain and the conjunction of DTBZ and VMAT-2 with positron emission tomography (PET) can be used for the diagnosis of the progress of brain diseases at the initial stage. Thus, we were interested in the enantioselective synthesis of DTBZ from a 6,7-Dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-782

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and evaluation of novel lipoic acid-piperazine derivative as cholinesterase inhibitors with selectivity towards butyrylcholinesterase

연고홍 임용배<sup>1</sup> 김재관<sup>2</sup> 김범철<sup>3</sup> 박정호<sup>4</sup>

한밭대 응용화학과 <sup>1</sup>한밭대 응용화학 <sup>2</sup>한밭대 생유기화학실험실 <sup>3</sup>한밭대 생명공학과 <sup>4</sup>한밭대  
응용화학생명공학부

Alzheimer's disease (AD) is a progressive neurodegenerative brain disorder. Even though cholinergic drugs approved by FDA to treat AD are inhibitors for acetylcholinesterase (AChE), they have some severe side effects. BuChE has been recently considered as a potential target because it also plays an important role in regulating acetylcholine level in AD patients. Therefore, the concurrent inhibition of both AChE and BuChE or the selective inhibition of BuChE should provide additional benefits in the treatment of AD. In this work, we synthesized novel lipoic acid-piperazine compounds and evaluated them as acetylcholinesterase and/or butyrylcholinesterase (AChE/BChE) inhibitors.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-783

발표분야: 유기화학

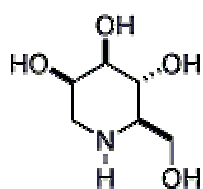
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Stereoselective Synthesis of Polyhydroxypiperidines Using an Aldol-RCM (Ring-closing Metathesis) Strategy

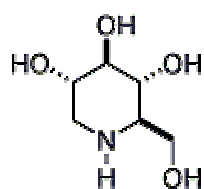
강한영 전기수

충북대 화학과

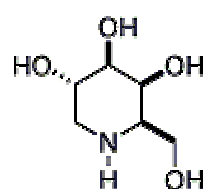
A group of glycoside hydrolase inhibitors known as azasugars, which are nitrogen-containing sugar mimics, has attracted much attention due to their impressive biological activities. We have investigated a general strategy to prepare azasugars, in particular, polyhydroxypiperidines. As an extension of the Crimmins' glycolate aldol-RCM strategy for constructing oxacycles, we have examined a glycine enolate-RCM approach to prepare azasugars, specifically, polyhydroxypiperidines. Our efforts for the synthesis of polyhydroxypiperidines will be presented.



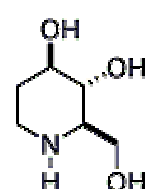
1-Deoxymannojirimycin



1-Deoxynojirimycin



1-deoxygalactonojirimycin



fagomine





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-784

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Stereoselective Nucleophilic Ring Opening of cis-3-Substituted-2-vinylaziridines

강한영 이가은

충북대 화학과

Aziridines have been used as key intermediates in organic synthesis. Their synthetic utility mostly relies on the ring strain. Stereoselective ring-opening reactions of aziridines with broad ranges of nucleophiles have served as important synthetic reactions to offer 1,2-difunctional organic compounds. Stereo- and regioselective opening of cis-3-substituted-2-vinylaziridines was investigated, in particular, under Lewis acidic conditions. With a variety of nucleophiles diverse 1,2-functionalized fragments were successfully obtained.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-785

발표분야: 유기화학

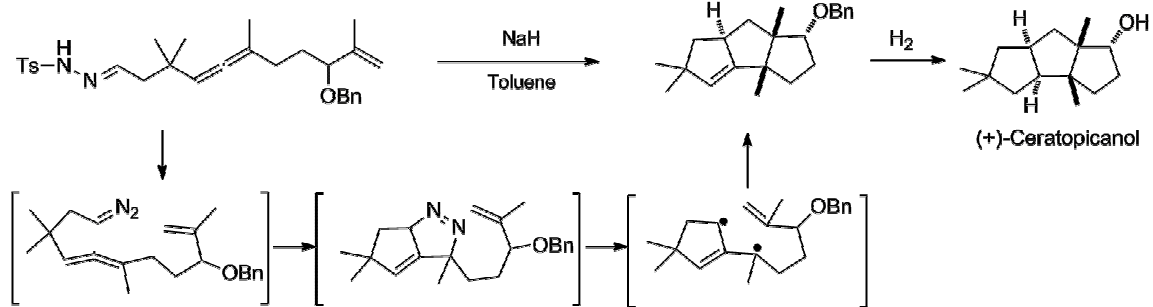
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Asymmetric total synthesis of Ceratopicanol

이상신 이희윤

KAIST 화학과

In 1988, Hanssen and Abraham reported the isolation of a novel triquinane sesquiterpene (+)-Ceratopicanol in agar cultures of the Ascomycete *Ceratosystis piceae* Ha 4/82, and proved to be indirect evidence for the biosynthetic origins of the entire class of cyclic sesquiterpenoid, hirsutene and related natural products via humulene cyclization cascade. The structure of ceratoicanol with two consecutive quaternary carbon centers has been a challenge to synthetic organic chemistry. Recently we developed a novel one pot sequential transformation that a pyrazole obtained through [2+3] cycloaddition reaction of diazoalkane with allene produces TMM diyl for another [2+3] cycloaddition reaction with olefin to form a triquinane structure. Through the tandem reaction sequence, we completed the synthesis of racemic Ceratopicanol in 15 steps, and (+)-Ceratopicanol in 18 steps stereoselectively. The stereochemical outcome was rationalized by theoretical calculation (HF/6-93\*)



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-786

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Naturomimetics Approach를 이용한생리활성 천연물의 유도체화 연

구

김태정 정규혁<sup>1</sup> 함정엽

KIST 천연의약센터 <sup>1</sup>강릉원주대 화학신소재학과

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 morphine, codeine 과 같은 천연물 및 그 유도체는 시중에서 항암제, 진통제등으로 널리 이용되고 있다. 특히, 이러한 천연물은 합성물에 비해 독성에 대한 우려가 적어, 신약개발분야에서 크게 주목받고 있으며 국내를 비롯한 전세계적으로 천연물을 이용한 신약개발의 비중은 크게 증가하는 추세에 있다. 이에 본 연구팀은 자연에서 발견된 생리활성 천연물을 lead compound 로 하여 활성을 나타내는 pharmacophore (약물특이분자단)의 합성과 더불어 다양한 유도체 합성을 통한 신약개발에 주력하고 있다. 또한 보다 효과적인 천연물의 유도체화 연구를 위해 본 연구팀에서 고안한 Naturomimetics

Approach 개념을 도입하여 생리활성 천연물의 활성을 나타내는 pharmacophore 에 해당하는 모체를 합성한 후, 전이 금속을 이용한 C-C, C-N bond coupling 반응을 통해 효율적인 유도체화 연구를 진행중에 있다. 본 포스터 발표에서는 현재까지의 연구결과와 함께 이후의 연구계획에 대해 보고하려 한다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-787

발표분야: 유기화학

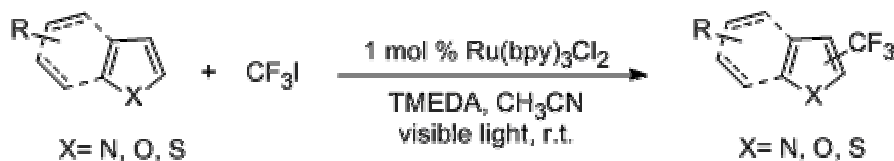
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Trifluoromethylation of heterocycles via visible light photoredox catalysis

Naeem Iqbal 조은진

한양대 응용화학과

A method has been developed for the visible light-induced trifluoromethylation of heterocyclic compounds. A variety of electron-rich heterocycles were transformed into trifluoromethylated products by using  $\text{CF}_3\text{I}$  as the trifluoromethyl radical source and  $\text{Ru}(\text{bpy})_3\text{Cl}_2$  as the photocatalyst under mild reaction conditions. This operationally simple and eco-friendly process can introduce trifluoromethyl groups without prefunctionalization.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-788

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Absolute structure determination and evaluation of herbicidal activities of new chiral isoxazoline derivatives

김명수 남준호<sup>1</sup> 류재욱<sup>1</sup> 고영관<sup>1</sup> 연규환<sup>1</sup> 김문환<sup>1</sup> 김은애<sup>1</sup> 구동완<sup>1</sup> 이동국<sup>2</sup> 조창우

경북대 화학과 <sup>1</sup>한국화학연구원 친환경 신물질 연구그룹 <sup>2</sup>목우연구소

5-(((2,6-difluorobenzyl)oxy)methyl)-5-methyl-3-(o-tolyl)-4,5-dihydroisoxazole(1) demonstrated good grass selectivity and potent herbicidal activity against annual weeds at a dose range of 0.25kg~2kg a.i./ ha under greenhouse conditions. 1 controlled annual weeds rapidly with a good tolerance on transplanted grass seedlings by postemergence and soil application. However, 1 has the racemic configuration. After chiral separation of the intermediate followed by coupling reaction, we could isolate the optical isomers of 1. We could also determine the absolute structures employing X-ray crystallography. Greenhouse experiments for the optical isomers showed that the isomer having S configuration was active and the isomer having R configuration was inactive.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-789

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

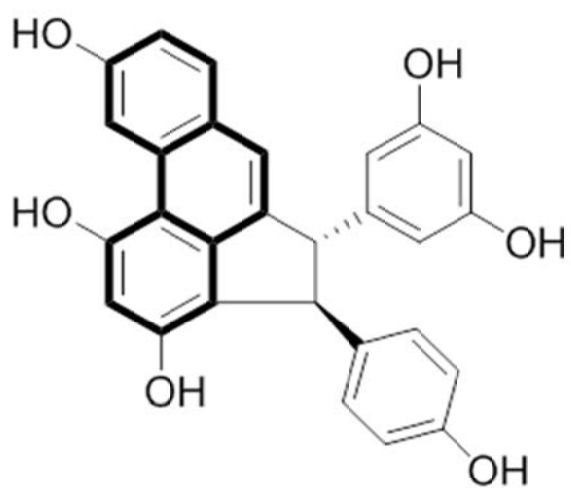
## Total Synthesis of Laetevirenol A via Intramolecular Friedel-Crafts Alkylation

최영록 허정녕<sup>1</sup> 이봉향<sup>1</sup> 임혜선<sup>2</sup> 권재관<sup>1</sup>

고려대 화학과 <sup>1</sup>한국화학연구원 의약화학연구센터 <sup>2</sup>충남대 신약전문대학원

Laetevirenol A belong to a large and important family of naturally occurring polyphenols derived from resveratrol. polyphenols have received considerable attention in the chemical and biological fields, owing to their structural complexity as well as their diverse bioactivities. We will describe a strategy for total synthesis of laetevirenol A via a combination of Suzuki-Miyaura coupling/aldol condensation cascade reaction for the construction of the phenanthrene ring and Friedel-Crafts reactions as an end game tool.





Laetevirenol A



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-790

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 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

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-791

발표분야: 유기화학

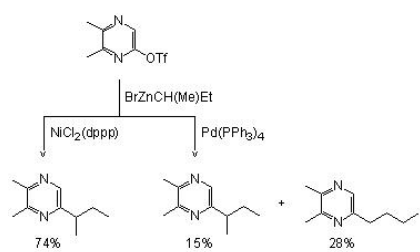
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ni-Catalyzed Negishi Cross-Coupling of Pyrazine Triflate: Regioselective Synthesis of Trialkylpyrazines

A.PITCHAIAH 김미리<sup>1</sup> 황진수<sup>2</sup> 황인택<sup>3</sup> 이기인<sup>2</sup>

한국화학연구원 바이오리파이너리<sup>1</sup> 과학기술연합대학원대 청정화학 및 생물학<sup>2</sup> 한국화학연  
구원 그린화학연구단<sup>3</sup> 한국화학연구원 바이오리파이너리연구센터

The regioselective synthesis of trialkylpyrazines via metal-catalyzed cross-coupling reactions and facile synthesis of 2,3-dimethyl-5-hydroxypyrazine are reported. The 5-substituted 2,3-dimethylpyrazine derivatives, including trail pheromone components of the ant *Eutetramorium mocquersyi*, have been successfully synthesized in good yields by Ni-catalyzed cross-coupling reactions of pyrazine triflate with alkyl and arylzinc halides.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-792

발표분야: 유기화학

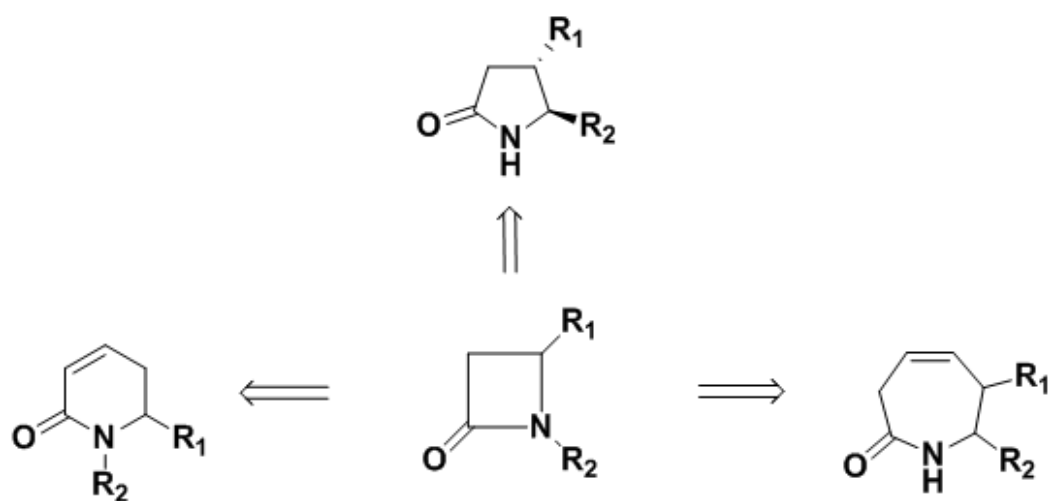
발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Preparation of various Lactam Derivatives via Ring Expansion of $\beta$ -Lactam Derivatives

장지성 안철진

창원대 화학과

The  $\gamma$ -lactam,  $\delta$ -lactam or  $\epsilon$ -lactam derivatives have been prepared stereoselectively via ring expansion from the corresponding  $\beta$ -lactam derivatives. The stereochemistry of  $\gamma$ -lactams with aryl and alkyl substituents on C-3 has been investigated systematically. The regiochemistry of  $\delta$ -lactam over  $\epsilon$ -lactam derivatives with vinyl substituents on C-4 has been investigated too.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-793

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

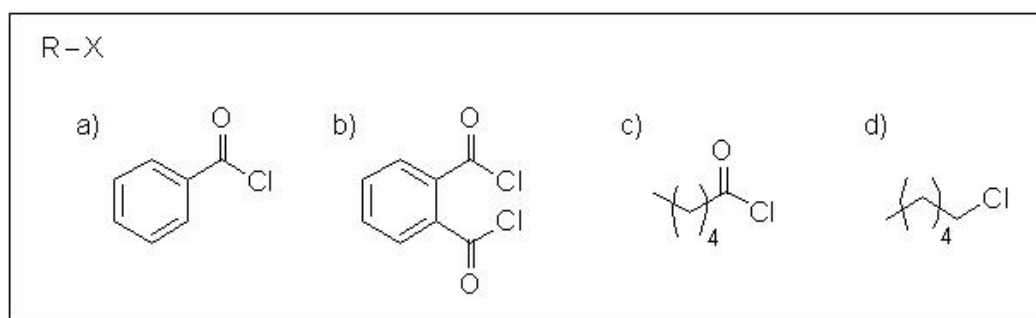
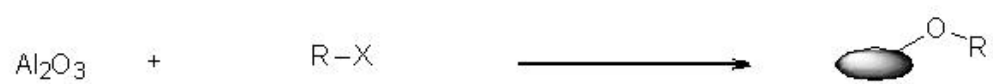
## Functionalization of Porous-Alumina For Luminescence Hybrid Material



김기우 안철진

창원대 화학과

The functionalization of porous alumina with organic ligands is developed by preparing the organic-inorganic hybrid luminescent material. 1) We will discuss about reaction method of hybrid material that used by porous alumina with some of organic ligands. The characterization of organic-inorganic hybrid luminescent material will be discussed.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-794

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of pyrrolo and furo-heterocycles heterogeneous Pd catalyzed annulation with alkynes

김지은 염을균

충남대 화학과

In heterogeneous catalysis, carbon materials have been used for long time because they can be used directly as catalysis, and moreover, they can satisfy most of the properties desired for a suitable support. In this study, we examined heteroannulation with alkynes to synthesize biologically active pyrrolo- and furo heterocycles under carbon supported palladium catalyst compare with heterogeneous and homogeneous palladium catalyst. We also examined recycling and recovery of palladium catalyst for biologically active heterocycles.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-795

발표분야: 유기화학

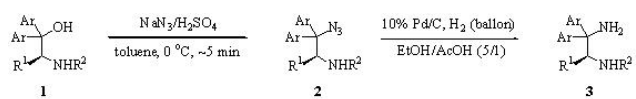
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Direct Azidation of 1,1-Diaryl-2-Aminoethanols Derived from Amino Acids

Rov Harendra Nath 이선아<sup>1</sup> 김형록<sup>2</sup> 황인택<sup>3</sup> 이기인<sup>1</sup>

한국화학연구원 그린화학연구소 <sup>1</sup>한국화학연구원 그린화학연구단 <sup>2</sup>한국화학연구원 그린화학  
연구본부 <sup>3</sup>한국화학연구원 바이오리파이너리연구센터

A direct azidation of tertiary alcohols using sodium azide/sulfuric acid is presented; the present method provides an efficient and practical path for the synthesis of trisubstituted ethylenediamins from 1,1-diaryl-2-aminoethanols derived from amino acids with a minimum use of chemicals.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-796

발표분야: 유기화학

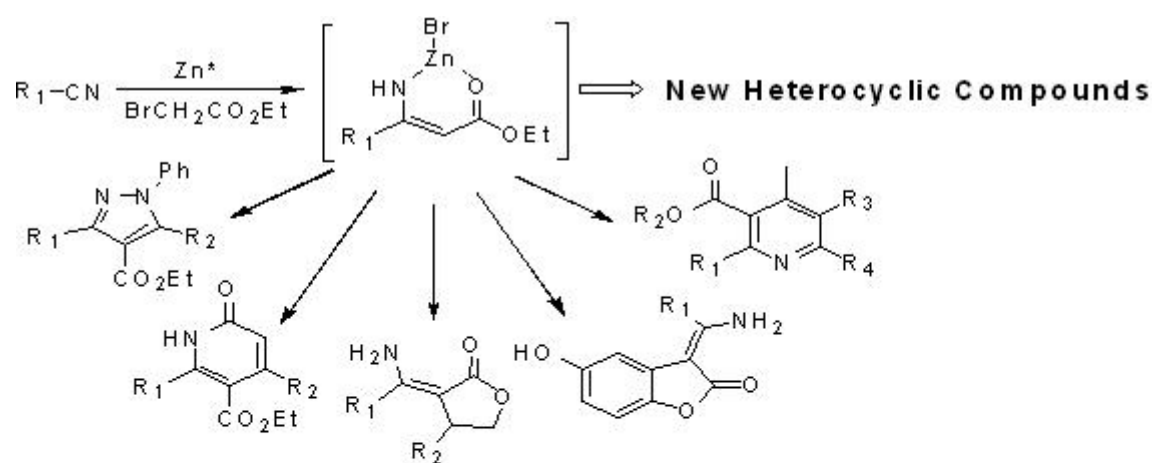
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Tandem Synthesis of Heterocyclic Compounds using the Blaise Reaction intermediate

전유성 최서영 이상기

이화여대 화학/나노과학과

Tandem bond formations are highly attractive in modern synthetic design, as they enable minimize the synthetic steps together with maximization of molecular complexity. Recently, we have demonstrated that the Blaise reaction intermediate, a zinc bromide complex of  $\beta$ -enaminoesters, could react with various electrophiles to afford heterocyclic compounds, which are important component as 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.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-797

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**A facile three-component sequential protocol in the expedient synthesis  
of novel Bis-pyrazolines in the presence of cerium trichloride under  
neat condition**

**RAMACHANDRAN 정연태**

부경대 이미지시스템공학과

A series of bis-pyrazolines have been synthesized by one-pot, three-component sequential reactions of phenylhydrazine, methyl acetoacetate and aromatic aldehydes in the presence of cerium trichloride in good yields under neat condition. This method has the advantage of easy work-up, convenient, relatively short reaction times and the products were isolated with high yields. The synthesized compounds were characterized by spectral and analytical methods

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-798

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Functionalization of Potassium Organotrifluoroborates via Chemoselectively C-N Cross-coupling Reaction

이정현 송중호<sup>1</sup> 최필주<sup>1</sup> 함정엽

KIST 천연의약센터 <sup>1</sup>강릉원주대 화학신소재학과

Recently, organotrifluoroborate salts have been used as important synthetic reagents in the Suzuki-Miyaura cross-coupling reaction. Potassium organotrifluoroborates are easily prepared by the addition of inexpensive  $\text{KHF}_2$  to various organoboron intermediates, and they are stable to air and moisture. Moreover, the inert property of organotrifluoroborates to a number of reaction conditions has allowed the synthesis of more complicated molecules that may not be prepared from boronic acids or boronate esters. For example, the direct functionalization of organotrifluoroborates successfully performed include a variety of epoxidations, *cis*-dihydroxylations, oxidations, olefinations (Wittig reactions), nucleophilic substitution reactions, metal-halogen exchange reactions, 1,3-dipolar cycloadditions, reductive aminations, and condensation reaction, etc. We found that the use of iodoaryltrifluoroborates led to the desired chemoselectively C-N coupled trifluoroborates products in the presence  $\text{Cu(I)}$  catalyst with good yields. Furthermore, these substrates are shown for the C-C bond

formation via Suzuki-Miyaura cross-coupling reaction which allows a convenient entry to open new possibilities for organic synthesis of various pharmaceutically and biologically active natural products.





일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-799

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Aluminum amide mediated synthesis of unsymmetrical terephthaloyl bis-amide

이상협 박혜정<sup>1</sup>

대구가톨릭대 생명화학과 <sup>1</sup>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.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-800

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Combinatorial oriented Solid Phase approach for the synthesis of quinoxaline library

이상협 RAMACHANDRAN<sup>1</sup>

대구가톨릭대 생명화학과 <sup>1</sup>대구가톨릭대 화학과

Quinoxaline derivatives are a very important class of nitrogen containing compounds and have been widely used in dyes, pharmaceuticals and electrical/ photochemical materials. Combinatorial chemistry has emerged as a powerful new technology for chemists to synthesis large number of compounds for biological evaluation. One of the techniques used in combinatorial chemistry is polymer support or solid phase organic synthesis. Our research works is mainly focused on synthesis of various heterocyclic compounds which are useful for the biological and industrial applications. Quinoxaline are one of the heterocyclic compounds of biological, pharmaceutical and industrial interest, our aim is to prepare libraries of quinoxaline derivatives in solid and solution phase by using various azidoanilines and oxa acetate as starting materials. Azidoanilines were subjected to coupling reaction in presence of base followed by alkylation. Then, alkylated products were cyclised to yield corresponding quinoxalines, which can be further derivatized by Lewis acid amidation reaction.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-801

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Three-Component Solution-Phase Synthesis of fused imidazole libraries**



최인희

연세대 화학과

The three-component condensation between a amidine, an aldehyde and an isocyanide catalyzed by perchloric acid was conducted. These small molecules can affect the function of their targets and are useful tools for dynamic cellular processes. Various fused imidazole derivatives show a broad range of bioactivities, such as antiinflammatory agents,calcium channel blockers and antibacterials.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-802

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Supported Multi-function Catalyst for Tandem Catalytic Reaction

신주연 정다정<sup>1</sup> 이상기

이화여대 화학/나노과학과 <sup>1</sup>이화여대 화학나노과학과

Nature created multi-enzymetic systems to accomplish extremely efficient one-pot tandem catalysis. Mimicking of such multienzymetic tandem catalysis made synthetic chemistry more sustainable. Due to the confronted society's bottle-neck problems associated with energy shortages and environmental pollution, the development of tandem catalytic reactions has become especially important and valuable. We developed enzyme-like multi-function catalyst, composed of Lewis acidic lanthanide triflate, palladium, and ionic liquid for the sequential tandem reactions: selective hydrogenation of phenol, oxime formation, and Beckmann rearrangement giving  $\epsilon$ -Caprolactam, which is an industrially important intermediate for nylon 6.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-803

발표분야: 유기화학

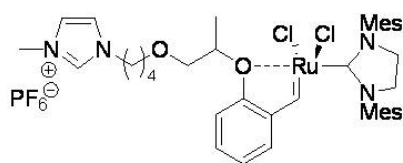
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Recoverable Ru-Catalysts Supported onto Carbon Nanotubes for Ring Closing Metathesis

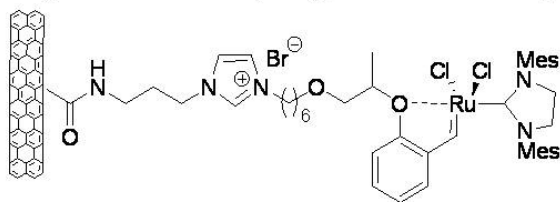
이수진 이상기<sup>1</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학/나노과학과

To solve the problems of homogeneous Ru-carbene catalysts associated with the difficulty in the recovery and reuse of the expensive metal catalysts, as well as the product contamination caused by metal leaching, a number of approaches for the immobilization and heterogenization of the homogeneous catalysts have been developed. In our previous work, novel Hoveyda-type Ru-carbene complexes **1** tethering imidazolium tags at chelating isopropoxy group have been synthesized, and investigated their catalytic activities and recyclabilities in ring-closing metathesis (RCM) in ionic liquids. In present work, in order to increase the recyclability of the catalysts, the Ru-catalysts were incorporated into the CNT surfaces to give the supported Ru-carbene complex **2**. In dichloromethane, this CNT supported Ru-catalyst allowed several times recycling without significant loss of catalytic activity in RCM.



**Figure 1. Novel Hoveyda-type Ru-carbene complexes**



**Figure 2. Recoverable CNT supported Ru-catalyst**



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-804

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Syntheses and Antioxidant Activity Evaluation of Resveratrol Derivatives

김미정 정세훈<sup>1</sup> 전종갑 이정태

한림대 화학과 <sup>1</sup>한림대 화학과, 응용화학연구소, 천연의약연구소

Resveratrol is one of the well-known aromatic compound that has antioxidant activity. Therefore, various resveratrol derivatives have been synthesized to enhance antioxidant activity. These resveratrol derivatives are different in the type and position of the substituents. The antioxidant activity of these resveratrol derivatives has been evaluated by ABTS and DPPH assay. From these antioxidant activity data,  $IC_{50}$  values of these compounds were obtained and the trend in antioxidant activity was revealed.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-805

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of small molecule library on solid support by using multi-component condensation

김태형

연세대 화학과

Small molecules can affect the function of their targets and are useful tools for dynamic cellular processes. Various imidazole and pyridine derivatives show a broad range of bioactivities, such as antineoplastic, immunosuppressive, and anti-inflammatory activities. Thus we synthesized an imidazole and pyridine library to discover bioactive compounds. Furthermore, to identify structure-activity relationship (SAR) of Apoptozole (Az), apoptosis inducing agent discovered from imidazole library, we synthesized Az focused library.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-806

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Study on the reaction of Heteroaromatics containing Nitrogen atoms and Pyranose

이수지 정대일 이도훈 김윤영 이용균 한정태<sup>1</sup>

동아대 화학과 <sup>1</sup>영동대 뷰티케어과

Tropane alkaloids and Pyranose derivatives have received great deal of attention because of their remarkable pharmaceutical significance. There is also considerable interest in the synthesis of non-natural carbohydrate based anti-infective agents. In particular flexible multivalent arrays of receptor carbohydrates are considered of interest, due to their enhanced activity resulting from the cluster effect. Our attention thus focused on the development of a one-pot strategy involving condensation of a series of multivalent amines with unprotected saccharides and tropane rings. As a part of a research program related to the synthetic study of pharmacologically interesting sccharide and tropane compounds, we now report the reactions of Diamine and triamine with 2,5-dimethoxytetrahydra-furan, acetonedicarboxylic acid at 0 °C. Biological tests of new synthetic compounds are currently in progress.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-807

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A Study on the Synthesis of amino acid derivatives containing heterocycles or saccharides**

**양욱모 이용균 이연진 최순규 한정태<sup>1</sup>**

동아대 화학과 <sup>1</sup>영동대 뷰티케어과

Amino acids are important in nutrition and are commonly used in nutrition supplements, fertilizers, food technology. Carbohydrate also play a key role in the process of life. Saccharide derivative also from part of many vital enzyme systems, specifically as coenzymes. They are also responsible for cell recognition and a therefore of great important in immunology. As a part of a research program related to the synthetic study of amino acid derivatives, we now report reactions of amino acids with 2,5-dimethoxytetrahydrofuran, and 1,3-acetonedicarboxylic acid at 0℃ (or reflux). And in order to obtain bioactive new amino acid derivatives, we executed reactions of amino acids and glucose (or mannose).

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-808

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Diazepine and Pyrido[3,4-b]pyrazines by cyclic reagents having acetyl group

이상곤 정대일 이연진 이용균 한정태<sup>1</sup>

동아대 화학과 <sup>1</sup>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. Nowadays, it is important to develop new medicine, such a enoxacin, diazepam and brotizolam, for resolving many disease. In this trend, we tried to synthesize pyrazine and diazepine derivatives which are used pharmaceutical and antibiotics like echinomycin, levomycin and actinoleutin. We now report the reactions of 3,4-diaminopyridine with 1,3-acetonedicarboxylic acid (or acetone and acetoneoxime) in various acidic conditions under Microwave irradiation or reflux. Moreover, we tried the reactions of 3,4-diaminopyridine with cyclic reagents having acetyl group to obtain various pyrido[3,4-b]pyrazine derivatives.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-809

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Convenient One-pot Synthesis of 8-Azabicyclo[3.2.1]octan-8-ylphosphonate and Heteroaromatic compounds

김아영 최순규 이도훈 한정태<sup>1</sup> 송주현

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Nitrogen containing heterocycles, such as pyrroles, indoles and carbazoles have attracted considerable attention due to their numerous applications in pharmaceutical and synthetic chemistry. Especially, a series of tropanes showed anticonvulsant activity against pentylene-tetrazol-induced convulsions in mice and antiarrhythmic activity in rabbit previously treated with ouabain. 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 phosphinic acid(or phosphoramidate) with 2,5-dimethoxytetrahydrofuran and acetone equivalents at room temperature or reflux.

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장소: 일산KINTEX

발표코드: ORGN.P-810

발표분야: 유기화학

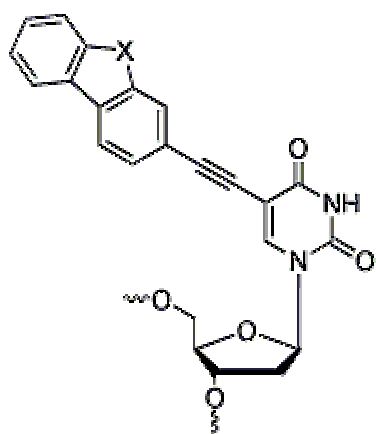
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Dibenzofuran- and Dibenzothiophene-Labeled 2'-Deoxyuridine

조현이 황길태

경북대 화학과

본 연구에서는 기존의 분자 비콘(molecular beacon)이 가지고 있는 제한성을 극복하며 보다 효율적으로 SNP (single nucleotide polymorphism) typing 을 수행할 수 있는 새로운 분자 비콘을 개발하고, 그 작동 원리에 대해서 알아보고자 한다. Dibenzofuran 과 dibenzothiophene 을 출발 물질로 palladium 촉매를 이용한 Sonogashira coupling 을 이용하여 2-ethynyldibenzofuran 과 2-ethynyldibenzothiophene 을 합성하고 이를 이용하여  $U^{DBF}$  와  $U^{DBT}$  를 합성하였다. 또한 DNA 센서로서 SNP 탐침의 유용한 시스템을 찾기 위해  $U^{DBF}$  와  $U^{DBT}$  를 DNA 에 도입하여 상보적인 염기 서열과의 혼성화에 따른 형광 세기의 변화를 알아보았다.



$\text{U}^{\text{DBF}}$  ( $\text{X}=\text{O}$ ),  $\text{U}^{\text{DBT}}$  ( $\text{X}=\text{S}$ )



일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-811

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Enantioselective Michael reaction of 3-substituted oxindoles catalyzed by binaphthyl-modified organocatalysts**

이현주 김대영

순천향대 화학과

The enantioselective conjugate addition reaction of 3-substituted oxindoles with Michael acceptors such as vinyl ketones and vinyl sulfones by binaphthyl-modified bifunctional organocatalysts was investigated. The corresponding Michael adducts, containing a quaternary center at C3-position of the oxindoles, were generally obtained in high yields with excellent enantioselectivities (up to 99% ee)

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-812

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Asymmetric fluorination of $\alpha$ -chloro- $\beta$ -ketophosphonates catalyzed by chiral nickel complexes

우섯별 김대영

순천향대 화학과

Fluorine-containing organic molecules are becoming increasingly important in medicinal chemistry. In particular, Very few methods for the preparation of  $\alpha$ -chloro- $\alpha$ -fluoro- $\beta$ -ketophosphonates are known. In this presentation, we wish to communicate the catalytic enantioselective fluorination of  $\alpha$ -chloroketophosphonates in the presence of air- and moisture-stable chiral nickel complex. The catalytic electrophilic fluorination of  $\alpha$ -chloroketophosphonates to give the corresponding chiral hetero dihalocompound with excellent enantiomeric excesses (up to 99 % ee).



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장소: 일산KINTEX

발표코드: ORGN.P-813

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Convenient synthesis of 1,2-dihydroquinoline derivatives



이다은 이현주 김대영

순천향대 화학과

Quinolines and their derivatives occur in numerous natural products, and many of them display interesting biological activities. In particular, one of the partially hydrogenated quinoline moieties namely dihydroquinoline is an important building block in various natural products and exhibits a broad range of biological activities and potential pharmaceutical applications. Herein we wish to report the results of our investigations on the Bronsted acid-catalyzed intramolecular cyclization of allylic alcohol derivatives to novel 1,2-dihydroquinoline derivatives

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장소: 일산KINTEX

발표코드: ORGN.P-814

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Organocatalytic enantioselective amination of ketones

**임영조 김대영**

순천향대 화학과

The efficient synthetic construction of  $\alpha$ -amino carbonyl compounds is one of the most intensely studied areas in organic synthesis. Enantioselective electrophilic amination of active methines is one of the most attractive reactions to generate quaternary stereocenters attached to a nitrogen atom. Recently, several groups presented the direct enantioselective amination<sup>1</sup> of active methine compounds in the presence of chiral Lewis acid complexes or chiral organocatalysts such as quinidine-derived alkaloids, cinchona alkaloids, ureas, and guanidines. As part of research program related to the development of synthetic methods for the enantioselective construction of stereogenic carbon centers, we wish to report the catalytic enantioselective amination of ester derivatives promoted by chiral catalysts. In this presentation, we wish to report the direct  $\alpha$ -amination of ketones catalyzed by organocatalysts with azodicarboxylates as the electrophilic nitrogen source.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-815

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Binaphthyl-derived organocatalytic asymmetric Michael addition reaction of $\alpha$ -ketoesters to vinylsulfones

이지현 이현주 김대영

순천향대 화학과

One of the ultimate goal and challenges in organic synthesis is the development of catalytic asymmetric transformation for the creation of functionalized optically active compounds with structural diversity from simple and readily available precursor molecules. The enantioselective conjugate addition reaction of  $\alpha$ -ketoesters with 1,1-bis(benzenesulfonyl)ethylene by binaphthyl-modified bifunctional organocatalysts was investigated. Treatment of  $\alpha$ -ketoesters with 1,1-bis(benzenesulfonyl)ethylene under mild conditions afforded the corresponding Michael adducts with excellent enantioselectivities.

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장소: 일산KINTEX

발표코드: ORGN.P-816

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Organocatalytic enantioselective Michael addition reaction of cyclic 1,3-dicarbonyl compounds to $\beta,\gamma$ -unsaturated $\alpha$ -ketoesters

한태현 이현주 김대영

순천향대 화학과

Coumarin derivatives are probably one of the most common skeletons found in natural products. Due to their extensive array of biological activities and pharmacological properties, the synthesis of this kind of compounds has been long-standing challenge in organic chemistry. In this presentation, we wish to report the direct enantioselective Michael addition of cyclic 1,3-dicarbonyl compounds to  $\beta,\gamma$ -unsaturated  $\alpha$ -ketoesters could be efficiently catalyzed by bifunctional organocatalysts

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-817

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Selective Fluorescence Turn-On Probe for Cu(I) through the Click Reaction

박석안 김해조

한국외국어대 자연과학대학 화학과

Copper is known to play an important role in organisms and sometimes, is toxic to higher organisms.[1] Click reaction has emerged as a highly fluorescent [2] and bioconjugation linkage,[3] by utilizing the copper catalyst.[4] Herein, we prepared a fluorescence probe (1), which showed a selective and sensitive response toward Cu(I) ions through the click reaction in aqueous solution. References[1]. Flemming, C. A.; Trevors, J. T. *Water, Air, and Soil Pollution*. 1989, 44, 143.[2]. Sivakumar, K.; Xie, F.; Cash, B. M.; Long, S.; Barnhill, H. N.; Wang, Q. *Org. Lett.* 2004, 6, 4603.[3]. Tornøe, C. W.; Christensen, C.; Meldal, M. J. *Org. Chem.* 2002, 67, 3057.[4]. Stefani, H. A.; Viera, A. S.; Amaral, M. F. Z. J.; Cooper, L. *Tetrahedron Lett.* 2011, 52, 4256.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-818

발표분야: 유기화학

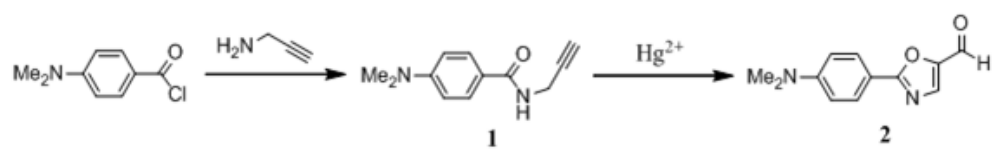
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Simple Ratiometric Fluorophore for the Selective Detection of Mercury through Hg(II)-Mediated Oxazole Formation

이희진 김해조

한국외국어대 자연과학대학 화학과

Mercury is known for very harmful metal to humans due to their bioaccumulation, biomagnification.<sup>1</sup> Above all mercury bioaccumulates in freshwater and marine foodwebs with health consequences for exposed wildlife and humans.<sup>2</sup> Therefore, selective detection of mercury ions is very important. So, we prepared a simple propargylamide functionalized chemodosimeter for the fluorescence detection of mercuric ions.<sup>3</sup> The probe 1 has shown highly selective ratiometric response to mercury(II) ions over other metal ions and fluorescence changes of 1 were observed with  $17 \text{ ?M}$  of mercury(II) ions as the detection limit in aqueous solution. This phenomenon was the result from propargyl amide to oxazole transformation mediated by the mercury(II) ions. Reference[1]. E. M. Nolan, S. J. Lippard, Chem. Rev. 2008, 108, 3443[2]. T. W. Clarkson, L. Magos, Crit. Rev. Toxicol. 2006, 36, 609.[3]. H. Lee, H-J. Kim, Tetrahedron Letters. 2011, 52, 4775



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-819

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ratiometric Detection of Cysteine by Ferrocenyl Enone

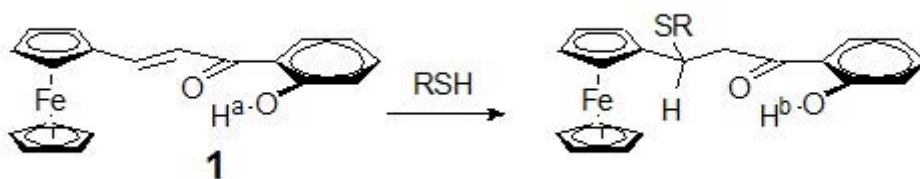
임수연 김해조<sup>1</sup>

한국외국어대 화학과 <sup>1</sup>한국외국어대 자연과학대학 화학과

Biothiols such as cysteine (Cys), homocysteine (Hcy), and  $\gamma$ -glutamylcysteinylglycine (GSH) are involved in a myriad of vital cellular processes, including redox homeostasis and cellular growth.[1,2] In particular, Cys is an essential biological molecule required for the growth of cells and tissues in living systems. The deficiency of Cys is associated with the retarded growth, hair depigmentation, edema, lethargy, liver damage, muscle and fat loss, skin lesions, and weakness.[3] Therefore, the selective detection of Cys is very important as a disease-associated biomarker.[4] Herein we report a ferrocenyl enone type of Michael acceptor 1 that is activated by an intramolecular hydrogen bond and exhibits selective response to Cys over other natural amino acids. Reference[1]. T. P. Dalton, H. G. Shertzer, A. Puga, Annu. Rev. Pharmacol. Toxicol. 1999, 39, 67.[2]. (a) Z. A. Wood, E. Schroeder, J. R. Harris, L. B. Poole, TransBiochem. Sci. 2003, 28, 32. (b) R. Carmel, D. W. Jacobsen, Homocysteine in Health and Disease, Cambridge University Press, UK, 2001.[3]. (a) S. Shahrokhian, Anal. Chem. 2001, 73, 5972.[4].



(a) M. Tomasulo, S. Sortino, A. J. P White, F. M. J. Raymo, *Org. Chem.* 2006, 71, 744. (b) R. Badugu, J. R. Lacowicz, C. D. Geddes, *Anal. Biochem.* 2004, 327, 82.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-820

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Selective Visible Probe for Cyanide ion

홍금희 김해조<sup>1</sup>

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Cyanide ion is a highly toxic anion that dose damage to organism by absorption through the lungs, gastrointestinal tract, and skin, and can lead to death. The cyanide ion inactivates the cellular repiration by interacting heme in cytochrome-a3 [1]. Therefore, we designed a probe (1) for cyanide that applicated to activated Michael acceptor type of probe for cyanide ions The probe has shown selective response toward cyanide over various anions through 1,4-addition of cyanide to  $\alpha,\beta$  ? unsaturated ketone in the probe. When cyanide ion was added , the noticeable color changes of 1 were observed by the naked eyesReferences1. Kellin, D. Proc. R. Soc. London, Ser. B 1929, 104, 206

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-821

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Sensitive and Selective Coumarin-Based Fluorescent Thiol-probe for Biological Thiols in the Cells

나상윤 김해조<sup>1</sup>

한국의외국어대 화학과 <sup>1</sup>한국의외국어대 자연과학대학 화학과

Biological thiols, such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH), play essential roles in maintaining redox homeostasis.[1], [2] However, abnormal levels of Cys, Hcy, and GSH in the cells are implicated in many human diseases, such as Alzheimer's disease,[3] retarded growth, edema, liver damage, loss of muscle and fat, skin lesions, and weakness.[4] Herein, We report a new coumarin-based fluorescent probe (1) for biological thiols in the cells. The probe (1) is highly sensitive for thiols with a low detection limit of 44.2 nM in aqueous solution. The probe (1) has shown highly selective response to biological thiols over various amino acids through the Michael reaction in vitro. References[1]. Dalton, T. P.; Shertzer, H. G.; Puga, A. Annu. Rev. Pharmacol. Toxicol. 1999, 39, 67[2]. Wu, G.; Fang, Y.Z.; Yang, S.; Lupton, J.R.; Turnur, N.D. J Nutr. 2004, 134 (3), 489.[3]. Seshadri, S.; Beiser, A.; Selhub, J.; Jacques, P.F.; Rosenberg, I.H.; D'Agostino, R.B. et al. N Eng J Med. 2002, 346 (7), 476.[4]. S. Shahrokhian.; Anal. Chem. 2001, 73 (24), 5972.

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장소: 일산KINTEX

발표코드: ORGN.P-822

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient preparation of furan-based monomers from biomass

홍연우 김영규 조진구<sup>1</sup> 채다원 강은실 김백진<sup>2</sup>

서울대 화학생물공학부 <sup>1</sup>한국생산기술연구원 그린공정소재연구그룹 <sup>2</sup>한국생산기술연구원 그  
린공정소재 연구그룹

Human culture has developed with the growth of fossil fuel. Fossil fuel is not just a fuel, but also an important resource to prepare the compounds that are essential in modern man's life. However, its reserve is limited and getting exhausted. In recent years, biomass has been raised as a renewable alternative energy and resource, and lots of related studies have been in progress. Up to now, most of the commercial monomers in the polymer industry were obtained from petroleum. We will present our effort to synthesize more effectively the biomass-derived monomers with a furan skeleton, which have a great potential to replace the petroleum-based monomers. As alternative biomass-derived monomers, some furan derivatives have received recently the spotlight from the polymer industry.

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발표코드: ORGN.P-823

발표분야: 유기화학

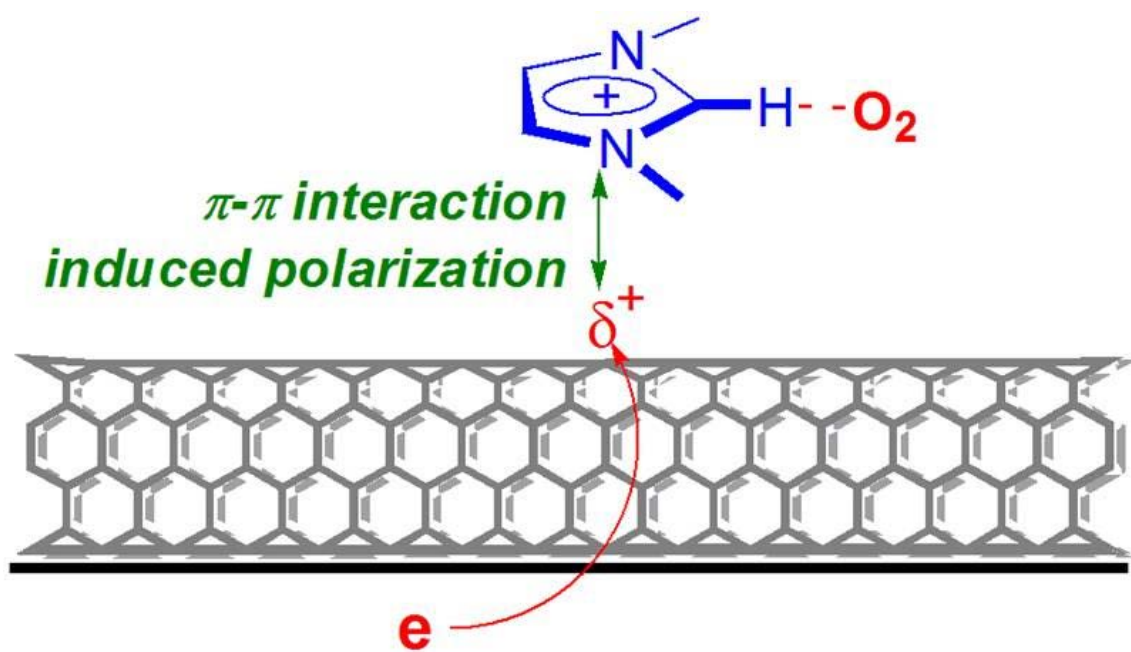
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of Metal-Free Electrocatalysts for Oxygen Reduction Reaction using Ionic Carbon Nanotubes

김연수 차아름<sup>1</sup> 전현지 신주연<sup>2</sup> 이종목<sup>3</sup> 이상기<sup>2</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 나노화학과 <sup>2</sup>이화여대 화학/나노과학과 <sup>3</sup>이화여대 화학  
과

The electrocatalytic oxygen-reduction reaction (ORR) is one of the most crucial factors in the performance of a fuel cell. The recent discoveries of metal-free electrocatalysts for ORR using the nitrogen- or boron-doped carbon nanomaterials have activated an exciting field for exploring the advanced metal-free electrocatalysts. The observed catalytic activity of these doped materials ascribed to the polarization of the carbon-nitrogen or carbon-boron bonds, which could create net charge on the carbon atoms in the  $\pi$ -conjugated carbon plane. In addition to the charge-induced favorable O<sub>2</sub> adsorption, the positively charged atoms can readily attract electrons from the anode to enhance the ORR. We found that the imidazolium salt-functionalized CNTs could also potentially be metal-free electrocatalysts for ORR as they induce polarization of CNT  $\pi$ -electrons increasing electron-transfer for ORR.



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장소: 일산KINTEX

발표코드: ORGN.P-824

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Au(I)-catalyzed oxidative-cyclopropanation reaction of propioamide with diphenyl sulfoxide**

염현석 신승훈

한양대 화학과

Since the initial discovery of the palladium-catalyzed Alder-ene reaction from 1,n-enyne substrates by the research group of Trost in 1984, extensive studies on a variety of catalysts and substrates have led to a large array of cycloisomerization or tandem addition. Among various cycloisomerization reactions of 1,n-enyne, the Pd-catalyzed oxidative cyclopropanation of 1,6-enyne was reported by the groups of Tse and Sanford in 2007 respectively. Recently, J. Zhang's group reported the redox reaction of 1,6-enyne substrate with pyridine-N-oxide as oxidant, which allowed the formation of cyclopropylketone derivatives. In our preliminary study, we investigated a reaction condition of terminal alkynes as substrate. This reaction involves the selective formation of two C-C bonds to afford annulated cyclopropylaldehyde derivatives, allowing for facile construction of pregnant quaternary centers. In addition, this quite simple strategy will provide a safe, mild and versatile avenue to numerous carbo- and heterocyclic frameworks possessing an intricate architecture. Unlike J. Zhang's report, when diphenyl sulfoxide cheaper than

pyridine-N-oxide was used as oxidant desired product was obtained in a good yield. Also we found that diphenyl sulfoxide was reacted with terminal alkyne selectively. Interestingly, although the redox reaction of diphenyl sulfoxide has been reported that it proceed through 3,3-sigmatropic rearrangement instead of gold-carbene intermediate by Ujaque, typical reactivity of carbene such as cyclopropanation was shown in our case. Therefore we present herein the mechanistic study about deference between diphenyl sulfoxide and pyridine-N-oxide as well as the scope of substrates.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-825

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Gold-catalyzed Ring Expansions of 1-Alkynylcyclobutanol Derivatives via Tandem Hydration and alpha-Ketol Rearrangement

신선웅 신승훈

한양대 화학과

In 2005, Toste group reported ring expansion reactions of 1-alkynyl cyclobutanol derivatives via 1,2-C-shift. Unlike this previous study where Au(I) induces a direct ring expansion, addition of small amount of water induces hydration followed by ring expansion. In this tandem reaction, Au(I)-catalysts perform a dual function, i.e. for the activation of alkyne toward hydration and as a Lewis-acid that mediate alpha-ketol rearrangement. With a number of substrates, these tandem reaction turned out to be faster than two competing processes, that is a direct expansion pathway mentioned above and Meyer-Schuster rearrangement. With intramolecular alcohol or amine nucleophiles in place of water, we could also obtain interesting hetero-spirocycles, efficiently.

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장소: 일산KINTEX

발표코드: ORGN.P-826

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

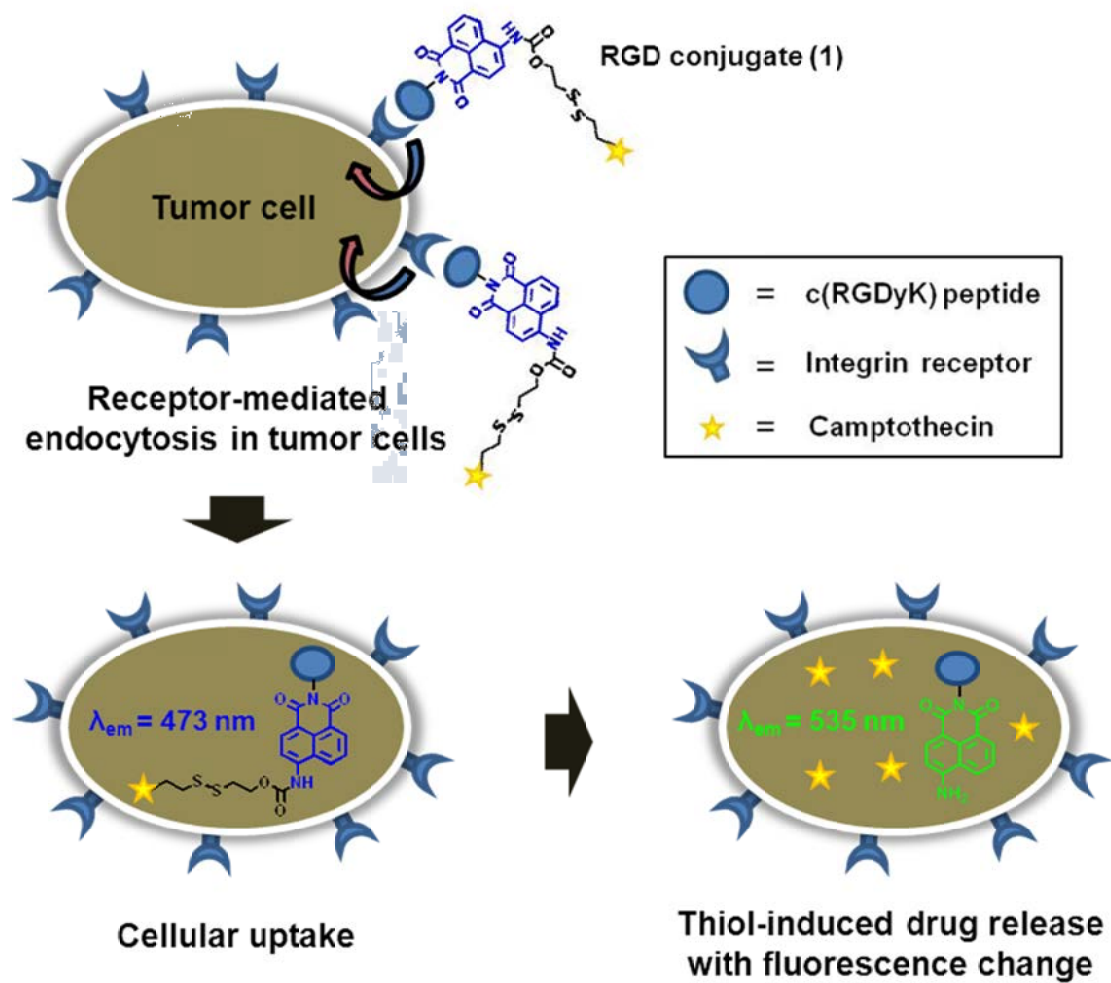
## A RGD peptide-appended naphthalimide fluorescent prodrug for monitoring of its uptake and drug release

이민희 장주희 양정호 강철훈<sup>1</sup> 김종승

고려대 화학과 <sup>1</sup>경희대 동서의학대학원

We herein present design, synthesis, spectroscopic characterization, and biological evaluation of a RGD peptide appended naphthalimide pro-CPT 1. Pro-CPT 1 is a multifunctional molecule composed of a disulfide bond as the cleavable linker, a naphthalimide moiety as the fluorescent reporter, a RGD cyclic peptide as a cancer-targeting unit, and camptothecin as the drug. Upon disulfide cleavage reaction with free thiols, most notably with GSH, 1 displays a red-shifted fluorescence at 535 nm and releases the drug concomitantly in an aqueous solution at pH 7.4. Confocal microscopic imaging experiments reveal that pro-drug 1 is preferentially taken up by U87 cells over C6 cells which is parallel with the order of drug potency based upon a cell viability test. The pro-CPT 1 is delivered intracellularly through a RGD dependent endocytosis and is cleaved in endoplasmic reticulum (ER), which is evident by its response to okadaic acid, an inhibitor of endocytosis, and its co-localization with ER tracker, respectively. This

new DDS system could provide a potential guideline for the construction of therapeutic drug delivery and monitoring system.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-827

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Organophosphorus and Carbamate Derivatives

정은빈 김현진 황민지 임기범 이상경

경상대 화학과

Organophosphorus (OP) and carbamates pesticides, a group of cholinesterase-inhibiting insecticides, have been widely used both in domestic settings and agricultural environments. Because, they exhibited broad-spectrum insecticidal activity and effectiveness. However, the extensive use of OP and carbamates pesticides has led to considerable poisonings of nontarget species including human fatalities. To help prevention further OP and carbamates pesticides poisonings, the addition of OP and carbamates pesticides residue determination in environment samples and agricultural products is urgently needed. So, many researchers tried to develop an immunoassay for determination of OP and carbamates pesticides using monoclonal antibodies against a genetic hapten. In this presentation, we want to report very simple organophosphorus and carbamates which were synthesized in our laboratory for aid of other researchers such as immunoassay and antiobesity.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-828

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design and Synthesis of New Organic Electronic Materials

황민지 김현진 정은빈 임기범 이상경

경상대 화학과

Organic thin film transistor (OTFT) has attracted considerable attention due to unique advantages such as low cost and ease of fabrication, light weight, and potential application in flexible large-area devices. However, the performance of OTFTs with semiconducting materials is still considerably limited by their relatively large band gaps. One important strategy for tuning the band gaps and the energy levels is utilization of donor-acceptor (D-A) type alternating copolymer. In this strategy, due to the interactions of HOMO and LUMO of the electron-donating and electron-deficient building blocks, the HOMO energy of the resulting copolymer is raised, while the LUMO energy is lowered, and resulting in a small band gap. For these reasons, we designed and synthesized a series of fluorene unit with electron-withdrawing groups for control the LUMO energy level. In this presentation, we will report synthesized and physical property.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-829

발표분야: 유기화학

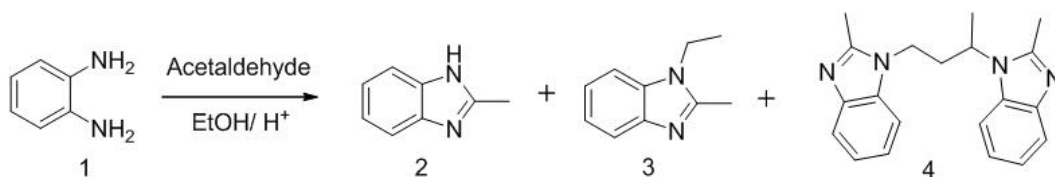
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Formation of benzimidazoles from o-phenylenediamine and acetaldehyde

이태희 박희정<sup>1</sup> 박균하

충남대 화학과 <sup>1</sup>한국기초과학지원연구원

Benzimidazoles 2-4 are formed from one-pot reaction of o-phenylenediamine and acetaldehyde. In order to find out the optimum conditions which afford compound 4 in maximum yield, we studied reaction conditions by varying the relative ratio of acetaldehyde and o-phenylenediamine, and by changing reaction temperatures. The relative yields of products 2-4 were determined by proton NMR spectra based on those of authentic samples.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-830

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Substituent Effects on Hydride Transfer Reactions of Benzothiazolium Ion with Benzimidazoline Derivatives

한인숙 정은정<sup>1</sup>

강원대 과학교육학부 <sup>1</sup>강원대 화학과

Abstract The kinetics of hydride transfer reactions of 3-benzyl-2-methylbenzothiazolium ion (BT<sup>+</sup>) with a series of 1,3-dimethyl-5-benzoyl-2-(substituted phenyl)benzimidazoline (p-CH<sub>3</sub>, H, p-F, p-Cl, m-F, m-Cl, m,m'-Cl<sub>2</sub>) and 1,3-dimethyl-2-substituted phenyl-1-H-anthra[2,1-d]imidazoline-6,11-dione benzimidazoline (p-CH<sub>3</sub>, H, p-F, p-Cl, m-F, m-Cl, m,m'-Cl<sub>2</sub>) have been measured spectrophotometrically in 2-propanol-H<sub>2</sub>O (4 : 1, v/v) at 25 ± 0.1 °C in order to explore the substituent effect the carbonyl group at the 5-position of benzimidazole ring. The reactivity is decreased when the carbonyl group is added in the benzimidazole ring as we expected. The rate constants for the reactions of BT<sup>+</sup> with X-BIH are linearly correlated with the Hammett parameters with the slopes of -0.599 and -0.300. 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 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-831

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A new Di(2-pyridylmethyl)amine based colorimetric and fluorescent chemosensor for $\text{Cu}^{2+}$

ZHENGXU

성균관대 화학학과

The development of new colorimetric and fluorescent molecular sensors for the detection of metal ions has been an attractive subject, for its diverse applications. Hence, we proposed that such fluorescent molecules complexed with desired metal ions. A new di(2-pyridylmethyl)amine derivative [1] was synthesized as a colorimetric and fluorescent chemosensor for  $\text{Cu}^{2+}$  ions. Experimental results indicate that [1] displayed the significant colorimetric and fluorescent changes upon binding with  $\text{Cu}^{2+}$  in aqueous solution. The  $\text{Cu}^{2+}$ -selective fluorescence quenching of [1] was detected with a 1:1 stoichiometry. The fluorescence behavior of [1] upon  $\text{Cu}^{2+}$  binding was explained based on electronic structure calculations. Overall, [1] can be useful for the study of the biological functions of  $\text{Cu}^{2+}$ .



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-832

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Physical Properties of OTFT Candidates

김현진 정은빈 임기범 황민지 이상경

경상대 화학과

Organic thin film transistors(OTFTs) have grown from a curiosity to a significant research area over the past two decade. Organic semiconductor materials used in OTFTs offer advantages of easy fabrication, mechanical flexibility and low cost. It is well known that the grafting of electron-withdrawing groups on the polythiophene backbone leads to a decrease of the HOMO and the LUMO levels. Recently, more semi-conducting organic compounds with rigid core units which exhibit good intermolecular ordering have been reported. In this presentation, we presented a new structure of OTFT candidates which including alkylated oligothiophene attached to electron rich or poor fused acenes. And we studied physical properties of these structures what have different electronic enviromental.

Electron rich or  
poor fused acene

Oligothiophene



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-833

발표분야: 유기화학

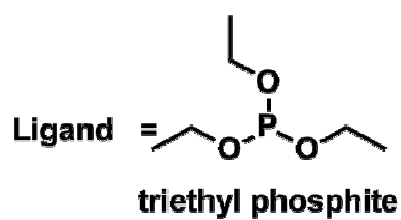
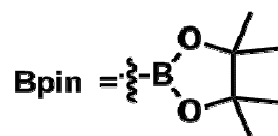
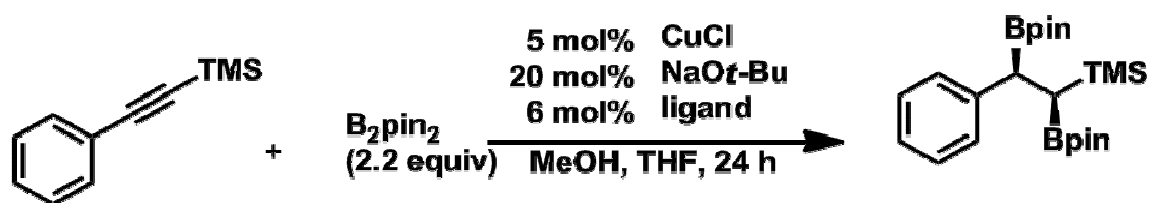
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Copper-Catalyzed Stereoselective Double Boration of Silyl Aryl Alkynes

정호영 윤재숙

성균관대 화학과

The boration of alkynes provided the most efficient synthetic access to alkenylboron compounds, which serve as useful building blocks in organic synthesis. Transition metal-catalyzed boration of internal alkynes using symmetrical diboron reagents in the presence of alcohol, generates formally mono-hydroborated alkenylboron compounds with excellent regio- and stereoselectivity. However, 1-aryl-2(trimethylsilyl)acetylenes were reacted to produce diborated compounds shown below without generating an intermediate alkenylboron compound. The double addition reactions led to regio- and stereoselective formation of the syn- product. More results will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-834

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Fullerene Derivative by Using Carbazole Moiety for P3HT-based Bulkheterojunction Solar Cells

김희운 황도훈 윤성철<sup>1</sup>

부산대 화학과 <sup>1</sup>한국화학연구원 화학소재연구단

A new fullerene derivative was synthesized with C60 and used as an electron acceptor material for P3HT-based bulkheterojunction solar cells. We have modified the basic structure of PC60BM by replacing the aromatic part by electron donating group with higher solubility and remain the aliphatic part. The new synthesized fullerene derivative showed good solubility in common organic solvents. The synthetic new fullerene derivative was characterized by <sup>1</sup>H-NMR and <sup>13</sup>C-NMR, UV-vis, DSC, TGA and Cyclic Voltammetry. Photovoltaic devices were fabricated using the configuration as follow ITO / PEDOT: PSS / P3HT: Acceptor / LiF / Al.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-835

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of Characterization of Photocleavable Linker for Solid-Phase Peptide Synthesis

김재희 여세원 이윤식

서울대 화학생명공학부

One-bead one-compound (OBOC) peptide libraries have been widely used for the screening of enzyme substrates. For the screening and identifying the peptide sequences from OBOC peptide library, special linkers which have orthogonal releasing property during solid-phase peptide synthesis condition, should be developed. Some linkers which release the peptide products by UV irradiation are known. The linkers are suitable for on-bead assay because they are stable until the side chain deprotection step and release peptides as amide form under UV. However, they have not been widely used because of some difficulties for their synthesis. In this presentation, we report on a facile synthesis of photocleavable linker (PCL), and its application in SPPS. The linker was prepared in good yield without any laborious column chromatography step.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-836

발표분야: 유기화학

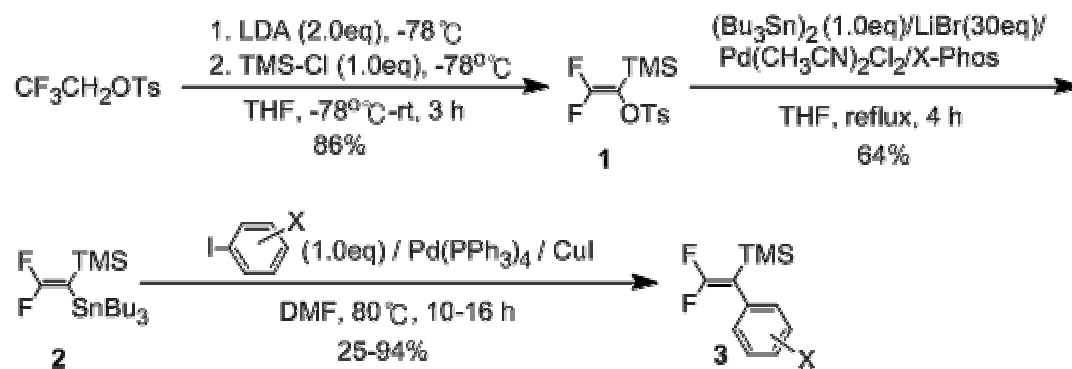
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Novel Approach to The Synthesis of 2,2-difluoro-1-tributylstannylethenyltrimethylsilane and Its Coupling Reaction

전종희 정인화

연세대 화학및의화학과

2,2-difluoro-1-trimethylsilylethenyl *p*-toluenesulfonate 1 was easily prepared in 86% yield from the reaction of 2,2,2-trifluoroethyl *p*-toluenesulfonate with 2 equiv of LDA in THF at  $-78^{\circ}\text{C}$ , followed by treatment with chlorotrimethylsilane. When the compound 2 was reacted with  $(\text{Bu}_3\text{Sn})_2$  (1.0 equiv) and LiBr (30 equiv) in the presence of  $\text{Pd}(\text{CH}_3\text{CN})_2\text{Cl}_2$  (3 mol%) and X-Phos (3 mol%) in THF at reflux temperature, stannylated product 2 was obtained in 64% yield. The cross-coupling reactions of 2 with aryl iodides in the presence of  $\text{Pd}(\text{PPh}_3)_4$  (10 mol%) and CuI (10 mol%) in DMF at  $80^{\circ}\text{C}$  afforded 2,2-difluoro-1-arylethenyltrimethylsilane 3 in 25-94% yields. The scope and limitation will be presented.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-837

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Allyl-Platinum Mediated Cyclization of N-allyl carbamates

김주혜 윤효상<sup>1</sup> 장혜영<sup>2</sup>

아주대 에너지시스템 응용화학 <sup>1</sup>아주대 에너지시스템학부 <sup>2</sup>아주대 화학과

Oxazolidinones have been widely used as chiral building blocks for asymmetric reactions and as biologically active units. So, selective and efficient synthesis of oxazolidinones has been intensively studied. Platinum complexes can be utilized for the synthesis of synthetically and biologically important 5-vinyloxazolidinones via cyclization of allylic carbamates. Platinum complex, SnCl<sub>4</sub>, and allyl bromide generate electrophilic allyl platinum intermediates in the presence of the pendant carbamate oxygen. The addition of oxygen nucleophile to an allyl platinum affords an active 5-vinylsubstituted oxazolidinones in good yield.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-838

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Copper-Catalyzed Synthesis Of Aromatic Amines From Ammonium salts/Amine derivatives

Wang Xi 장혜영<sup>1</sup>

아주대 에너지시스템학부 <sup>1</sup>아주대 화학과

Efficient catalytic protocols for the synthesis of aromatic amines are required. Thus, a general and simple metal-catalyzed amine arylation protocol has been intensively studied. In this study, with the combination of copper acetate, benzoic acid and carbonate ions, a variety of amines including ammonium salts, 1o and 2o aniline derivatives, 1o and 2o aliphatic amines, benzimidazole, phthalimide, and sulfonamide were efficiently arylated in the presence of phenyl boronic acid. By utilizing this copper catalyst, ammonium salts and 1o and 2o amines were successfully converted to monoarylamines, symmetric and unsymmetric diaryl amines in good yield.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-839

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 7-Triazolylcoumarin-Based Fluorescent Tag System for Stepwise, Comparative Assessment of Small Molecule Microarrays

전문국 구수진

한국화학연구원 의약화학연구센터

A fluorescent tag system based on 7-(1H-1,2,3-triazol-4-yl)coumarin fluorophore having a fluorous moiety and a polyethylene glycol (PEG) spacer at opposite ends was devised to assess the fabrication process of small molecule microarrays and to facilitate the interpretation of the relative binding data in the subsequent screening stage. The potential use of this system as a tool for a stepwise and comparative evaluation of small molecule microarrays was illustrated by the qualitative analysis of the results of the fluorescence detection obtained from the microarray experiments using the tagged biotins and streptavidin-Cy3 (and avidin-Cy5) as the binding partners. The influences of the following parameters on the results of the microarray experiment were investigated: i) the replacement of a fluorous moiety by a simple alkyl chain, ii) the PEG spacer, iii) the substitution pattern around the triazolylcoumarin fluorophore, and iv) the medium of the spotting solution.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-840

발표분야: 유기화학

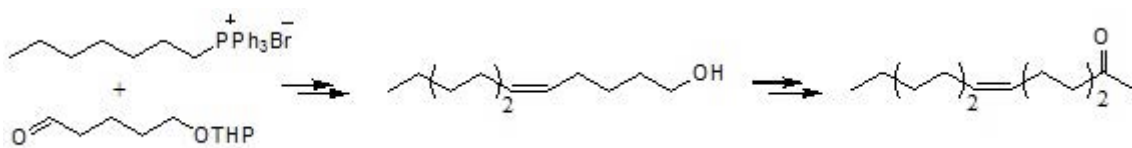
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Synthesis of Oriental Beetle Sex Pheromone via typical Wittig reaction and Grignard reagent

홍용표 권영빈<sup>1</sup> 유건상

안동대 응용화학과 <sup>1</sup>그린아그로텍 연구개발팀

Sex pheromone of oriental beetle, (Z)-7-tetradecen-2-one was efficiently synthesized from cheap 1,5-pentanediol and n-heptyl bromide. C5-protected pentanal and heptyltriphenylphosphonium bromide were stereoselectively coupled and then, deprotected to give (Z)-dodecen-5-en-1-ol. After bromination of the alcohol, the Grignard reagent, (Z)-5-dodecenylmagnesium bromide was easily acetylated to produce oriental beetle sex pheromone, (Z)-7-tetradecen-2-one.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-841

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Quantitative Electronic and Steric Effect on the Functionality Preference of Metathesis Ru Carbenes

이옥숙 손정훈 이희윤<sup>1</sup> 박창문 김경환<sup>1</sup>

충남대 화학과 <sup>1</sup>KAIST 화학과

Metal-catalyzed tandem coupling reactions with multifunctionalities are undoubtedly of importance to synthetic chemists for rapid synthesis of target compounds. However, one of the major hurdles for development of these reactions is very little information on the functionality preference of a catalyst, which dictates the identity of initial intermediate that can direct the key propagating species and the formation of the final product. As an effort to solve this fundamental issue, we determined the quantitative electronic and steric effect on the preference of metathesis Ru carbenes to their functionalities, alkene, alkyne, and allene, using FRET-based method. In addition, we describe the relationships between functionality preference of catalyst and final metathesis product, derived from metathesis reactions with substituted alkenes and alkynes.

일시: 2012년 4월 25~27일(수~금) 3일간

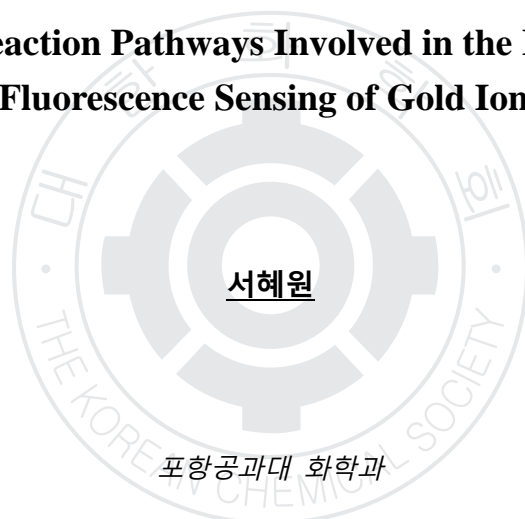
장소: 일산KINTEX

발표코드: ORGN.P-842

발표분야: 유기화학

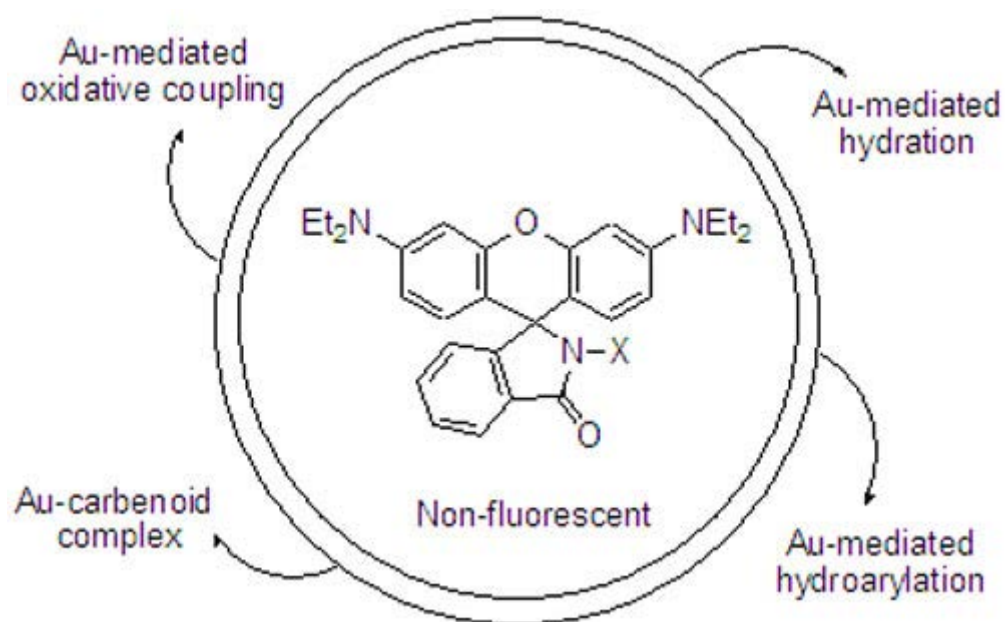
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies on the Reaction Pathways Involved in the Rhodamine-Based Fluorescence Sensing of Gold Ions



Gold chemistry has experienced renaissance in the last years because of unique and interesting properties of supported gold nanoparticles and catalytic and biological activities of gold complexes. Gold ions are soft Lewis acids, so they can easily activate carbon-carbon triple bonds in various bond-forming reactions.[1] We and others reported fluorescent molecular probes for gold ions. We found that the sensing reaction, however, involves several different reaction pathways which casts potential problems in applying the sensing protocol in certain conditions. To address those undesired chemical reactions in sensing gold ions, we investigated the gold-mediated reaction pathways involved in the rhodamine-based sensing. We have found that several undesired side reactions can interfere with the design spirolactam-ring-opening reaction. We characterized these side reactions, which are hydration of the triple bond, dimerization of the vinylgold intermediate, and nucleophilic participation of the aminophenyl moiety.[2] More importantly, we have characterized several vinylgold intermediates and their reaction pathways by

NMR and X-ray crystallography.[3] These results would contribute to not only the development of a well-designed fluorescence molecular probe for gold ions but also study of gold mediated organic transformations. References[1] Jimenez-Nunez, E.; Echavarren, A. M. Chem. Commun. 2007, 333-346.[2] Unpublished work[3] Egorova, O.; Seo, H.; Ahn, K. H. Angew. Chem. Int. Ed. 2011, 50, 11446.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-843

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Selective Fluorescent Recognition of $\text{HSO}_4^-$ via Pure C-H Hydrogen Bondings Based on Cyclic Benzbisimidazolium Derivative in Aqueous solution

최지영 이진용<sup>1</sup> 윤주영<sup>2</sup>

이화여대 바이오융합과학(화학)<sup>1</sup> 성균관대 화학과<sup>2</sup> 이화여대 화학·나노과학과

The fact that C-H hydrogen bonds can play determining roles in receptor?anion recognition is an exciting and unexpected discovery among the various artificial host molecules reported so far. However, there is increasing proof that even charge-neutral C-H donors may be strong enough for use in anion recognition chemistry. In addition, despite an urgent need for the development of simple methods for the detection of  $\text{HSO}_4^-$  ion, compared to other anions, there are relatively few chemosensors available that can detect sulfate species. Thus, to maximize these C-H hydrogen bonding interactions mentioned above and to recognize  $\text{HSO}_4^-$  ion in aqueous solutions, we designed and synthesized a novel cyclic benzbisimidazolium receptor, in which preorganized C-Hs can efficiently engage in binding and, most importantly, the C-H hydrogen bonding ability was increased by two adjacent imidazolium groups. Herein, a pure C-H hydrogen receptor that can selectively recognize  $\text{HSO}_4^-$  in aqueous solution was developed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-844

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ozonolysis of terminal alkynes

김서초 구본석 정인찬

한서대 화학과

For a long time studies concerned with the preparation and properties of ozonides were predominantly of academic interest, since ozonides have found no applications as such, and since they also played only a minor role as supposed or actual intermediates in synthetic reactions or in structural elucidations by their conversion into non-peroxidic products. In recent years, however, a number of naturally occurring organic peroxides have been found to play a role in biochemical reactions. A case in point is the naturally occurring cyclic peroxide artemisinin, which exhibits antimalarial activity. The Synthesis of ozonides could be rationalized by cycloaddition of carbonyl oxide, commonly called criegee-zwitterions and the carbonyl compounds which are derived from the primary ozonide of olefins.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-845

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nucleic acid sensitive and selective probe : Cytosol staining fluorescent dye

이상욱 홍종인

서울대 화학부

Although many commercially available cell imaging probes exist, new imaging probes with improved property and selectivity are still being developed. Nevertheless, there are rare RNA sensitive probes. Herein, we report a yellow nucleic acid sensitive cell imaging probe that selectively stains cytosol and nucleolus, where RNAs are more abundantly distributed than dsDNAs. Simple condensation of commercially available picolinium iodide derivatives and benzaldehyde derivatives led to styryl-based fluorescent probes, which showed fluorescence enhancement in the presence of nucleic acids. Some of our probes showed abnormally intense fluorescence in the presence of double stranded DNA (dsDNA) or RNA. Interestingly, one of our probes stained cytosol and nucleolus in cell imaging experiments, which indicates that our probe is more sensitive to RNAs. Synthesis of probes, their photophysical properties with nucleic acids, and cell imaging experiments will be presented in the poster.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-846

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies on the discrimination of redox-related biomolecules



오진록 홍종인

서울대 화학부

Phosphate-containing biomolecules are recognized as very important ones in living system because of their roles involved in a variety of process in biological system. Particularly, molecules such as NAD<sup>+</sup> or FAD have drawn much attention because of their crucial roles in cellular redox chemistry. And their sensing systems were not established well, thus the discrimination and sensing of them become important. Recently, our group synthesized PyDPA and achieved selective sensing of ppGpp among various phosphate-containing biomolecules by excimer formation induced by two pyrophosphate moieties in close proximity. Also, another sensor molecule, PTZ-DPA, was able to discriminate between FMN and FAD, by the photoinduced electron transfer mechanism. Being inspired by their sensing mechanism, we thought that PyDPA can be also utilized as a new sensing system for the discrimination of redox molecules, NAD<sup>+</sup>/NADP<sup>+</sup> and FMN/FAD. Details of the study will be discussed in the presentation.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-847

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **New Donor Materials based on Benzothiadiazole and Thiophene for Heterojunction Solar Cells**

**전용준 홍종인**

서울대 화학부

Since the first report of organic solar cells (OSCs) by Tang, the development of OSCs has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene were used as donor materials for heterojunction solar cells due to good charge transport ability. Also benzothiadiazole unit was used as low band gap donor materials due to their broad absorption spectra. To improve performance of heterojunction solar cells, we introduced new low band gap donor materials, consisting of benzothiadiazole and thiophenes. Details of the synthesis, photophysical study and device data will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-848

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrogenerated Chemiluminescent Sensor for Hydrogen peroxide Based on a Cyclometalated Ir(III) Complex

김훈준 홍종인

서울대 화학부

Reactive oxygen species (ROS) such as hydrogen peroxide ( $H_2O_2$ ) play fundamental roles in physiology, aging and disease in living organisms but are difficult to study because of their reactive and transient nature. When misregulated these species in cellular levels can cause oxidative damage to cellular protein, nucleic acids and lipid molecules, thereby contribute to aging and age-related disease states ranging from neurodegeneration to diabetes to cancer. Moreover, unregulated increases in cellular levels of  $H_2O_2$  have been linked to DNA damage, mutation, and genetic instability. Herein, we demonstrate a new sensing strategy based on electrogenerated chemiluminescence (ECL) analysis. In this case, an organometallic probe undergoes selective chemical reaction with hydrogen peroxide ( $H_2O_2$ ), and then it subsequently produces efficient emission by electrochemical triggering. Details of synthesis and photophysical studies will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-849

발표분야: 유기화학

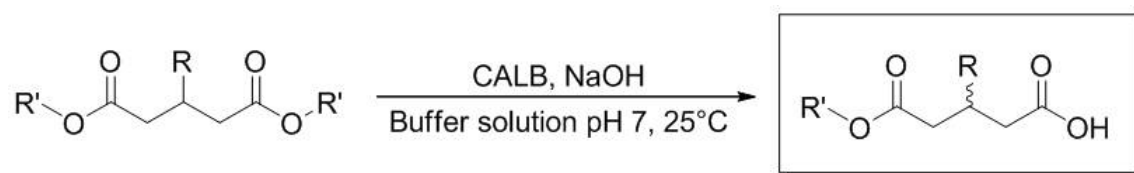
발표종류: 포스터, 발표일시: 수 18:00~21:00

## CALB catalyzed hydrolysis of 3-alkylpentanedioate: “allyl effect” and asymmetric synthesis of pregabalin

정재훈 엄희성 윤두하 하현준 이원구<sup>1</sup>

한국의국어대 화학과 <sup>1</sup>서강대 화학과

CALB-catalyzed desymmetrization of prochiral 3-alkylpentanedioic acid diesters was succeeded for the preparation of optically active 3-alkylpentanedioic acid monoesters bearing various alkyl substituents including methyl, ethyl, propyl and allyl. Allyl esters among many alkyl esters showed far better stereoselectivity implying the possible pi-pi interaction between the olefin of substrate and the side chains of Trp104 at the active site. This interaction called “allyl effect” was calculated through computational simulation. On the basis of this reaction was achieved the asymmetric synthesis of (S)-(+)-3-aminomethyl-5-methylhexanoic acid known as pregabalin in 70% overall yield.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-850

발표분야: 유기화학

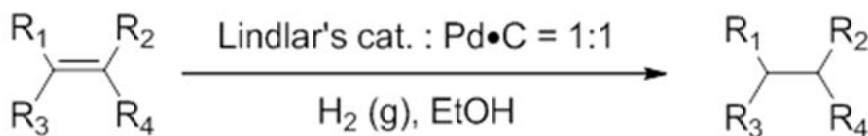
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemoselective reduction of olefin

지미경 윤두하 하현준 이원구<sup>1</sup>

한국외국어대 화학과 <sup>1</sup>서강대 화학과

Chemoselective reduction of olefins free from debenzylation and aziridine ring-opening was achieved by hydrogenation in the presence of mixed commercial catalysts Pd · C and Lindlar's.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-851

발표분야: 유기화학

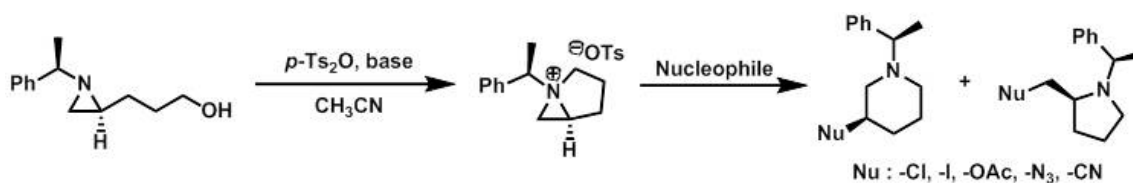
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of the stable azoniabicyclo[3.1.0]hexane and its ring-opening reaction

윤두하 하현준 이원구<sup>1</sup>

한국외국어대 화학과 <sup>1</sup>서강대 화학과

We developed a method for the preparation of the stable (5S)-1-((R)-1-phenylethyl)-1-azoniabicyclo[3.1.0]hexane from 3-((S)-1-((R)-1-phenylethyl)aziridin-2-yl)propan-1-ol with p-toluenesulfonyl anhydride. The nucleophilic ring-opening reaction of the stable bicyclic intermediate afforded either (R)-3-substituted-1-((R)-1-phenylethyl)piperidine and/or (R)-2-substituted-1-((R)-1-phenylethyl)pyrrolidine.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-852

발표분야: 유기화학

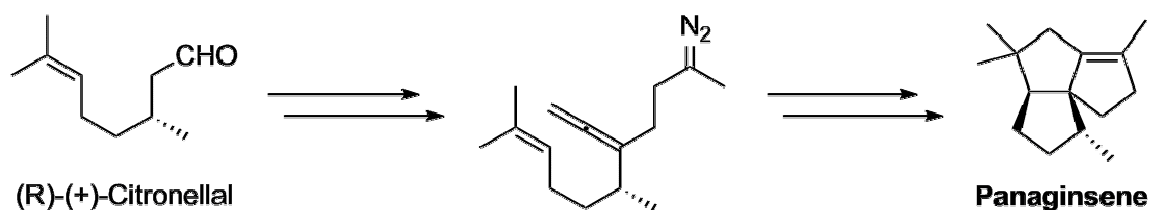
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Total Synthesis of Panaginsene

금수정 이희윤

KAIST 화학과

Panaginsene is one of the sesquiterpene hydrocarbons isolated from the roots of *Panax ginseng* C. A. Meyer (Wilfried A.Konig et al. 2005) which are pharmaceutically used in Asia for a long time. The first total synthesis of Panaginsene starting from (R)-(+)-Citronellal was accomplished stereoselectively with intramolecular trimethylenemethane(TMM) diyl [2+3]cycloaddition reaction. Using this tandem cycloaddition reaction, quaternary carbon center of Panaginsene can be easily assembled with high efficiency and stereoselectivity.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-853

발표분야: 유기화학

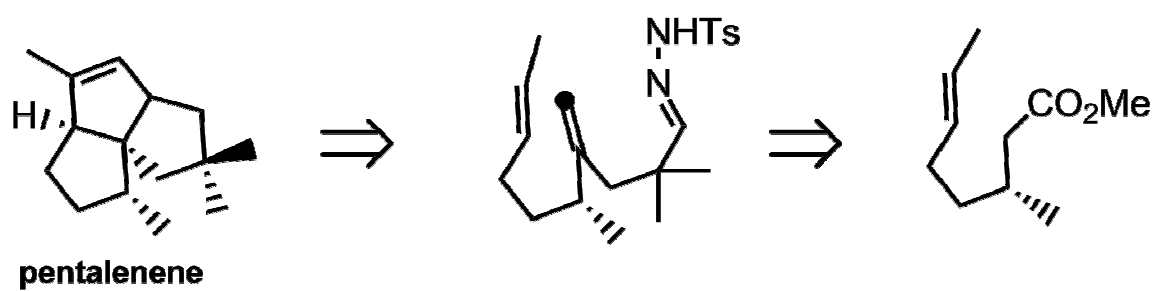
발표종류: 포스터, 발표일시: 수 18:00~21:00

## The total synthesis of (+)-Pentalenene

김윤정 이희윤

KAIST 화학과

In 1980, Seto and Yonehara reported the isolation from *Streptomyces Griseochromogenes*. It is the parent hydrocarbon of the pentalenene antibiotic family of fungal metabolites. Pentalenene is biosynthetic precursor of the pentalenolactone, antibiotic metabolites, produced by several *Streptomyces* species.<sup>1</sup> Due to its inherently interesting structures together with biological activities, it has attracted great attention. The tandem cycloaddition reaction of allenyl diazo compound<sup>2</sup> was applied to the stereoselective total synthesis of natural (+)-pentalenene. For synthesis of (+)-pentalenene, we prepared the cyclization precursor through introduction of the chiral center using enantioselective CuI-Tol-BINAP-catalyzed conjugate addition of Grignard reagent and the successful tandem cycloaddition reaction lead to the total synthesis of (+)-pentalenene.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-854

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of Trisubstituted Alkenes via Gold(I)-Catalyzed Hydrophosphoryloxylation

엄다한 강동진 이필호

강원대 화학과

Synthesis of stereodefined trisubstituted alkenes are 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-mediated cross-coupling reactions of stereodefined alkenyl derivatives and depends very much on the regio- and stereospecific synthesis of alkenyl derivatives from alkynes. In this regard, highly regio- and stereoselective synthesis of trisubstituted alkenes using boration, bromoboration, and iodination of alkynes or haloalkynes has been reported. During our investigation of Au(I)-catalyzed hydrophosphoryloxylation and hydroacyloxylation of alkynes, we have been interested in the possibility of hydrophosphoryloxylation of haloalkynes because the regio- and stereoselective hydrophosphoryloxylation would provide alkenyl halophosphates. We have developed a new stereoselective synthesis of trisubstituted alkenes, which is based on metal-catalyzed regio- and stereoselective hydrophosphorylation of haloalkynes and subsequent transition metal-catalyzed cross-

coupling reactions. The present approach provides an easy access to structurally diverse trisubstituted alkenes and will find many useful applications.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-855

발표분야: 유기화학

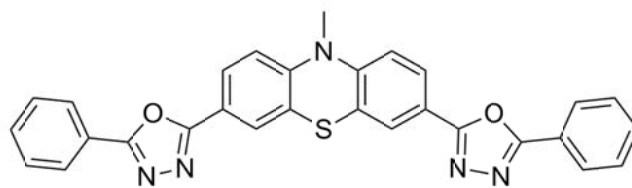
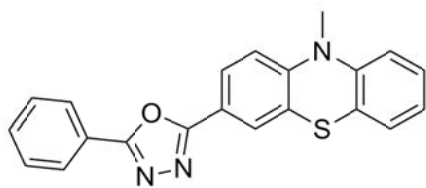
발표종류: 포스터, 발표일시: 수 18:00~21:00

## DDQ-Mediated Synthesis of New Materials for OLED containing Oxadiazole Derivatives

김진아 안광현<sup>1</sup>

경희대 화학과 <sup>1</sup>경희대 응용화학과

Oxadiazole ring is an electron-deficient functional group that can be used as an excellent electron-transport material (ETM) in organic multilayer electroluminescent (EL) diodes. We developed a new method of oxadiazole ring synthesis. A one-pot procedure for 1,3,4-oxadiazole ring formation from acyl hydrazide and aldehyde has been accomplished through oxidative cyclization using DDQ as an oxidant. The symmetric and asymmetric 2,5-disubstituted-1,3,4-oxadiazoles were obtained in high yields up to 99%. This non-metallic method will be useful for the synthesis of oxadiazole derivatives for those electronic applications requiring extremely low metal impurity. The highly fluorescent phenothiazine derivatives that can be utilized as a green light-emitting material in an OLED device were successfully prepared with a good yield using this method.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-856

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Selective recognition of $\text{H}_2\text{PO}_4^-$ by a cholestane-based imidazole-zinc ensemble

Jadhav Jyoti 김홍석

경북대 응용화학과

There is currently a great interest in the design and synthesis of receptors capable of binding anionic guest, as anions are well known to play numerous fundamental roles in a range of chemical, biological, and environmental processes. Of all the anions the recognition of phosphate anion is vital because of its significant role in signal transduction, energy storage and gene construction in biological system. Recently our group synthesized cholestane-imidazole-based motifs 1, 2 and 3 as building blocks in the construction of molecular receptors. Metal ion based receptors are relatively new and particularly attractive in this aspect, as the presence of metal ion not only provides additional binding sites for the guest anion but also pre-organize the binding sites of the receptor conformationally for most favorable anion binding through hydrogen binding and metal ion coordination. Herein, a new facial cholestane-based imidazole-zinc complex receptor 4 has been synthesized and assessed its binding properties toward anions.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-857

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

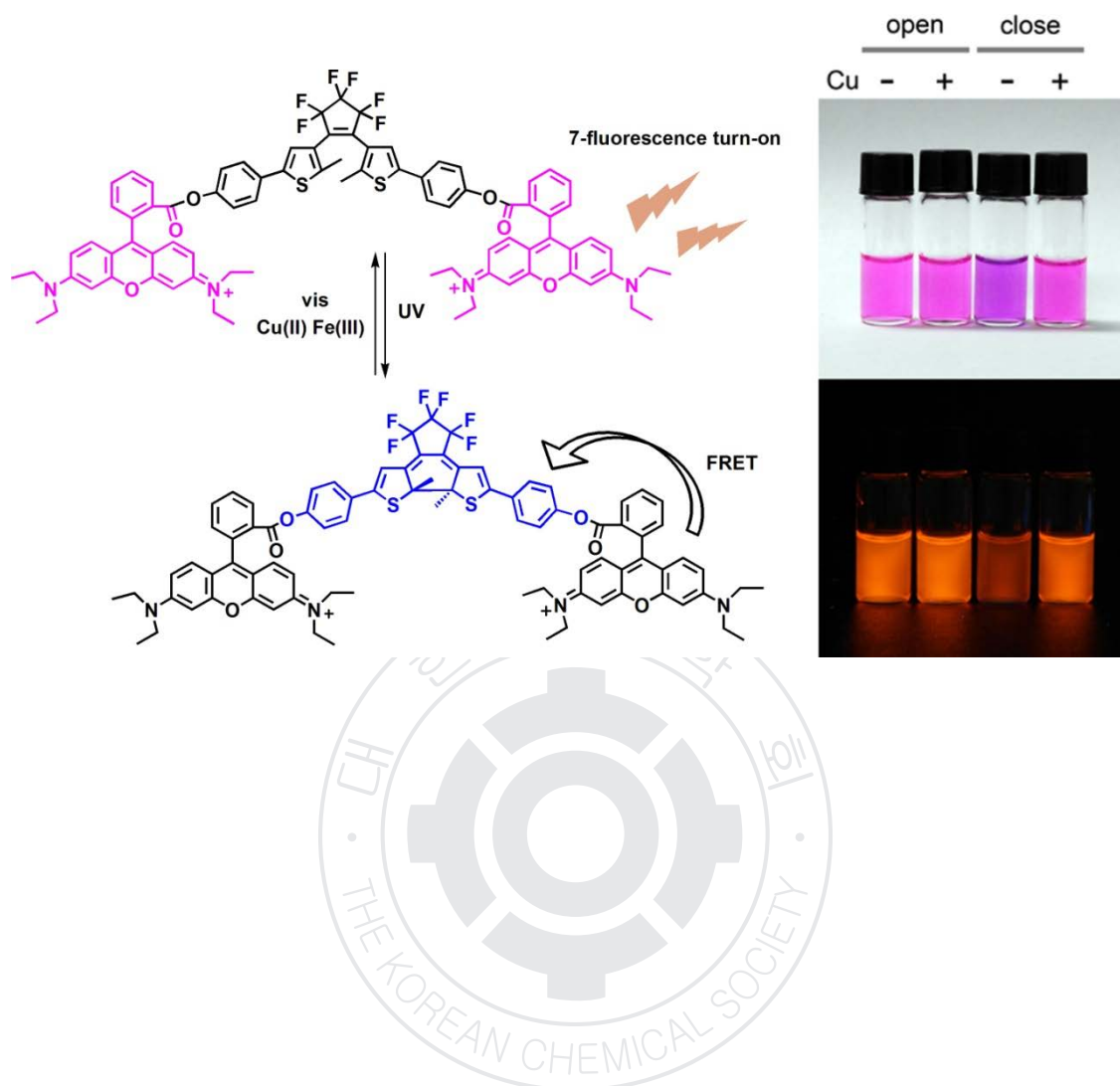
## Mechanism and sensory application of electrochemical switching of photochromic dithienylethenes

이수민 유명민<sup>1</sup> 남원우

이화여대 화학과 <sup>1</sup>이화여대 바이오융합과학과

Electrochemical ring opening of photochromic dithienylethenes (DTEs) is of prime importance because the process provides additional means to address bistable states. Its mechanism has, however, not been fully understood to date, and there are strong arguments about chemical identity of reactive intermediates. In order to investigate the mechanism, we have synthesized a series of DTEs with varying electron density of the photochromic core. We observe that the closed forms undergo ring-opening reaction by one-electron oxidants such as  $\text{Fe}(\text{bpy})_3^{3+}$  and  $\text{Cu}(\text{ClO}_4)_2$  in acetonitrile. Studies including ESR, stopped-flow UV-vis absorption, NMR, and spectroelectrochemical measurements establish the mechanism that radical cation of the closed form is the reactive intermediate of the oxidative ring opening. We have employed the mechanism to determine redox potentials by means of fluorescence turn-on signals. Specifically, conjugation of red-fluorescent rhodamines to the DTEs facilitates nonradiative FRET to the closed form, producing suppressed fluorescence emission. In contrast, presence of oxidizing metal ions

such as Cu(II) and Fe(III) triggers ring-opening reaction with a 7-fold fluorescence turn-on. It should be emphasized that the fluorescence response is fully reversible.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-858

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Synthetic Method of Heterocyclic Compounds via Intramolecular Hydroarylation

엄다한 서정민 이필호

강원대 화학과

Recently, transition metal-catalyzed intramolecular hydroarylation of alkynes, alkenes, and allenes by the addition of a C-H bond across a  $\pi$ -bond has received considerable attention for its synthetic application. These reactions have been demonstrated to be one of the effective green chemistries since hydroarylation shows ideal atom economy. After Pd-catalyzed intramolecular hydroarylation of alkynes was first described, a wide range of transition metal- and Lewis acid-catalyzed hydroarylation were reported. Still, hydroarylation of alkynyl arenes was achieved by a variety of transition metal catalysts such as Ru, Ga, Pd, Au, Pt, Fe, and Hg. In addition, we developed Pt-catalyzed hydro-arylation through a 6-endo mode for preparation of 1,4-dihydronaphthalenes. Although intramolecular hydroarylation is observed for alkynyl arenes, for arenes having a functionalized alkynyl group, there are regioselectivity and reactivity issues, which are difficult to expect and are a challenging problem. Herein, we report iron-catalyzed

intramolecular hydroarylation of alkynyl phenyl sulfides and alkynyl sulfonamides through a selective 6- and 7-*endo* mode



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-859

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chitosan-coated Gold nanoflowers: Fabrication and application

Tran Thi Nhung 이상화

경원대 화학생명공학과

This paper focused on a facile method to fabricate gold nanoflowers (AuNFs) with the 50-120 nm and plasma resonance in NIR band. In this method, chitosan served as a capping agent and ascorbic acid as a reducing agent at room temperature. The size, shape and NIR absorption of AuNFs were controlled by the concentration of chitosan, the pH of chitosan solution and the amount of ascorbic acid. AuNFs with many round corners and protrusions on the surface were prepared and checked for surface-enhanced Raman scattering (SERS). Key words: gold nanoflowers, chitosan, ascorbic acid, SERS.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-860

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Molecular dyads for fluorescence ratiometric sensing of biological zinc ions

우하나 유영민<sup>1</sup> 남원우<sup>2</sup>

이화여대 대학원 바이오융합과학과 <sup>1</sup>이화여대 바이오융합과학과 <sup>2</sup>이화여대 화학과

Fluorescence ratiometric sensors allow for quantitative detection of intracellular species because their response directly dictates the extent of analyte binding. We have prepared two fluorescence ratiometric sensors (HN1 and HN2) for biological zinc ions. The zinc probes are designed to possess either facilitated FRET (HN1) or frustrated FRET (HN2), which, in each case, produces fluorescence ratiometric response. In particular, HN1 displays the ratiometric change through zinc-induced disaggregation of self-assembled nanoaggregates. The studies including dynamic light scattering, field-emission scanning electron microscopy, and photophysical measurements support the mechanism by the aggregation/disaggregation. Meanwhile, the ratiometric response of HN2 is constructed by combination of a zinc-responsive probe signal and a reference signal that are invariant to zinc binding. The bioimaging utility of the zinc probes has been demonstrated by visualization of intracellular zinc ions in live HeLa cell

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-861

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies on the Selective Sensing of Nucleotides Using $\text{Zn}^{\text{II}}$ (cyclen)-Functionalized Poly(diacetylene) Liposomes

마동희

포항공과대 화학과

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. Poly(diacetylene) liposomes (or PDA liposomes) are unique sensing platforms that show blue-to-red color change as well as fluorescence change in response to environmental perturbations (heat, organic solvents, mechanical stress, and the ligand-receptor interaction). In addition, PDA liposomes can be readily immobilized on solid substrates. In our efforts to explore functionalized PDA liposome's properties, we developed new  $\text{Zn}^{\text{II}}$ (cyclen)-functionalized PDA liposomes for the selective sensing of nucleotides. The  $\text{Zn}^{\text{II}}$ (cyclen) moiety can recognize the thymine base and the phosphate group in the nucleotides. Our approach is to introduce second liposome component to modulate the surface morphology as well as the functional groups. We have demonstrated such a “multi-component” liposome approach can provide a selectivity pattern different from the conventional “mono-component” liposome



approach, which has been explained by a subtle change in the recognition environment on the surface of the liposome. The  $\text{Zn}^{\text{II}}$ (cyclen)-functionalized PDA liposomes show color changes from blue to red-purple upon interaction with ATP, ADP, TTP, CTP and GTP in solution. A microarray chip system fabricated with the liposomes, however, show red fluorescence only in the presence of ATP down to 1 pM level. Such a selectivity behavior manifests again that the recognition behavior can be modulated by changing the receptor environment, from solution to the solid state. A further investigation on the multi-component liposomes would provide us selective sensing systems for nucleotides.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-862

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Novel Catalyst System for Hydrostannation of Alkynes

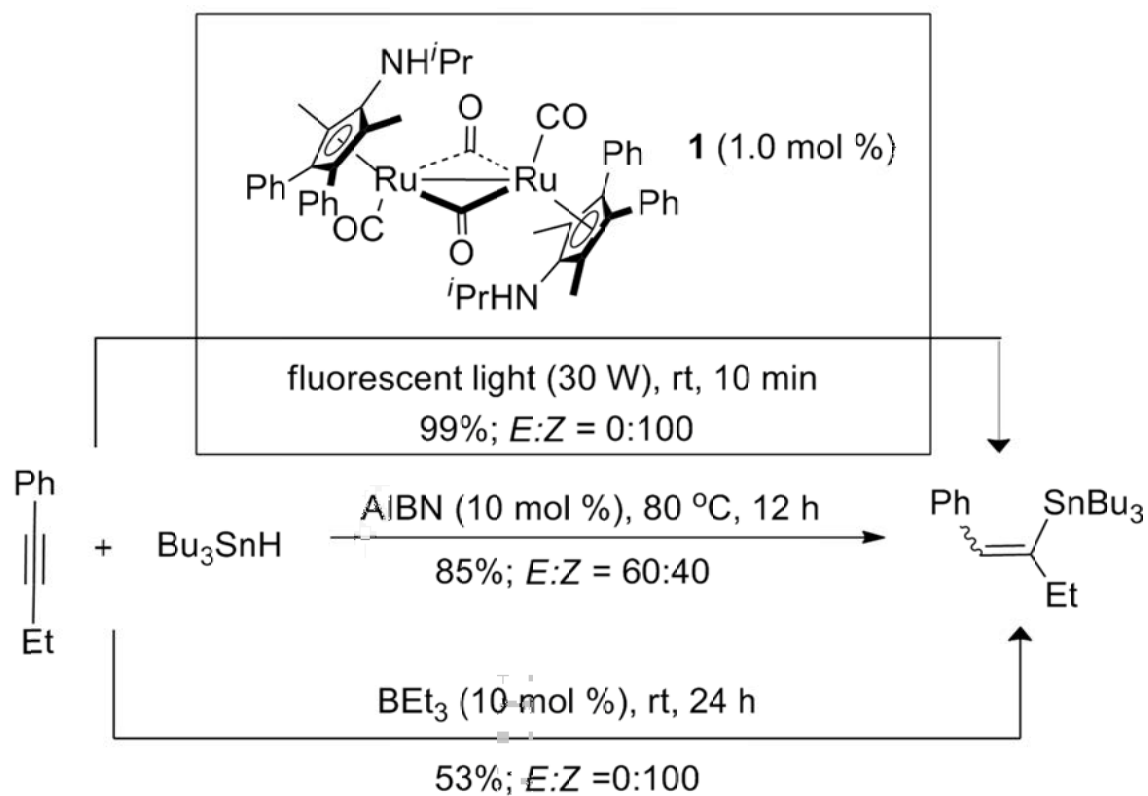
한정훈 이영호 박재욱

포항공과대 화학과

Organostannanes are valuable intermediates in organic synthesis due to their versatility in organic reactions. Particularly, vinylstannanes are useful substrates of metal-catalyzed carbon-carbon cross-coupling reactions. Moreover, vinylstannanes have been used frequently as vinyl anion synthons in various organic synthesis. Although there are many methods for preparing vinylstannanes, the direct addition of tin hydride to alkynes (hydrostannation) is the most attractive one in the view of efficiency and atom-economy.

Herein we describe a novel and efficient ruthenium catalyst system for the selective hydrostannation of alkynes, which is generated from a diruthenium complex (1) under simple illumination with household fluorescent light. The catalyst hydrostannation gave distinctive results under mild conditions in comparison with other methods. Most notably, even  $\text{Bu}_3\text{SnH}$  could be successfully engaged in the hydrostannation at room temperature. The complete hydrostannation of 1-phenyl-1-butyne with  $\text{Bu}_3\text{SnH}$  was achieved in only 10

min with 1.0 mol % of **1** under mild condition with excellent regio- and stereoselectivity.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-863

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Multifold Carbon-Sulfur Cross-Coupling Reactions

류태규 박영철 이필호

강원대 화학과

The transition-metal-catalyzed carbon-sulfur cross-coupling reaction is one of the fundamental processes in organic synthesis because the sulfide functional group is widely used in pharmaceuticals, functional materials, and synthesis of natural products. Sarandeses et al. developed an atom-efficient Pd-catalyzed cross-coupling reaction with triorganoindiums( $R_3In$ ). We have developed an efficient Pd-catalyzed multifold (2-, 3-, and 4-fold) carbon-sulfur cross-coupling reaction of indium tri(organothiolates) with polybromonated aromatic and heteroaromatic compounds in a one-pot procedure, producing di-, tri-, and tetrasulfides. These results indicate that indium tri(organothiolates) transfer all of three alkyl- or arylthio groups attached to indium metal to electrophilic coupling partners. These novel features, which is carried out with only a small excess of organometallic reagent and a low catalyst loading, make indium tri(organothiolates) highly useful alternatives to other organo-metallic reagents used in transition-metal-catalyzed multifold carbon-sulfur crosscoupling reactions and also mark them out as promising reagents for organic synthesis.

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발표코드: ORGN.P-864

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fluorescence turn-on $\text{H}_2\text{O}_2$ sensor exhibiting lysosome-localized fluorescence signals

조소민 송다영 유영민 남원우<sup>1</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 화학과

We have developed a new fluorescence turn-on  $\text{H}_2\text{O}_2$  sensor (ZP1Fe<sub>2</sub>) based on a paramagnetic iron complex of a fluorophore. The sensing platform can be readily constructed by complexation of paramagnetic iron ions and Zinpyr-1 (ZP1), a fluorescent metal ion sensor. The fluorescence turn-on mechanism by  $\text{H}_2\text{O}_2$  involves oxidative cleavage of the fluorescence-quenching iron ionophore. Under simulated physiological condition at pH 7.0 and 25 °C, the probe displays a 22-fold fluorescence turn-on with exceptional selectivity for  $\text{H}_2\text{O}_2$  over other reactive oxygen species such as  $\text{O}_2^-$ ,  $^-\text{OCl}$ , t-BuOOH, NO, t-BuO $\cdot$ , HO $\cdot$ , and  $^1\text{O}_2$ . In addition the fluorescent detection ability is not affected by presence of biologically abundant metal ions and pH change between 6.25 and 7.81. The probe is nontoxic to live HeLa cells and proved to detect intracellular  $\text{H}_2\text{O}_2$  at the lysosomes.

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발표코드: ORGN.P-865

발표분야: 유기화학

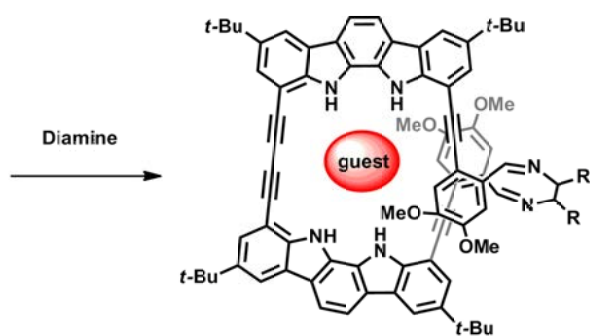
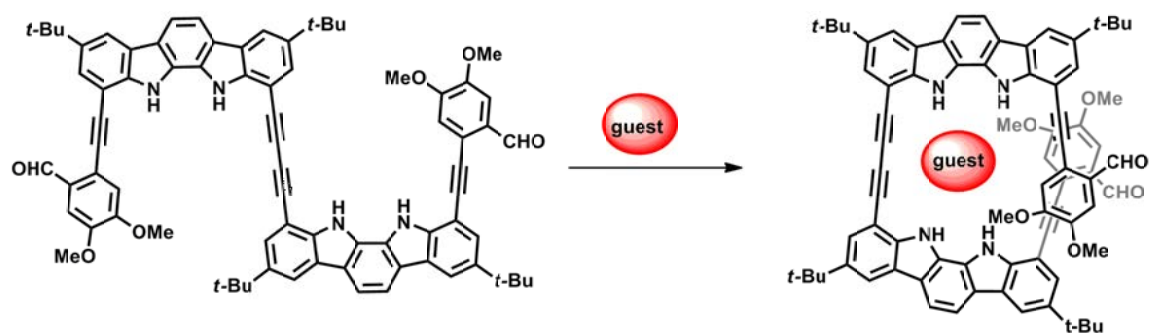
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A helical indolocabazole-imine macrocycle as a molecular sensor for chiral amines and carboxylates**

**김민준 석재민 정규성**

연세대 화학과

A large number of macrocycles have been prepared for synthetic receptors. Herein, we prepared a new imine macrocycle of helical chirality by folding of an indolocarbazole dimer. This imine macrocycle of helical chirality has great potentials as synthetic receptors and sensors of chiral molecules. This dimer consists of two indolocarbazole moieties connected by the butadiynyl spacer, which fold into a helical conformation in the presence of an anion as template. Anion binding makes two benzaldehydes close enough to form reversible imine bonds with diamines. When 1,2-diaminoethane was used, imine macrocycle were synthesized to racemic mixture. Also when R,R-isomers of diamine were used, imine macrocycle were induced to conformation of P-helix. Otherwise, when S,S -isomers of diamine were used, imine macrocycle were induced to conformation of M-helix. Moreover, when chiral anions were used as a template, these anions induced one side of helicity of imine macrocycle. The details of studying this imine macrocycle will be described in the poster.



*M*- or *P*-helix



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발표코드: ORGN.P-866

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Toward fluorescence ratiometric sensors for singlet oxygen

송다영 유영민 남원우<sup>1</sup>

이화여대 바이오융합과학과 <sup>1</sup>이화여대 화학과

Highly reactive oxygen species (hROS) such as singlet oxygen ( $^1\text{O}_2$ ) are closely linked to many of pathophysiological processes in the human body, but their molecular mechanisms have not been fully understood to date. Therefore probes that are capable of detection and quantification of hROS are urgently required. We have synthesized new fluorescence ratiometric probes for  $^1\text{O}_2$ . The  $^1\text{O}_2$  sensors have been constructed based on isobenzofuran which undergoes a [2+4] pericyclic reaction with  $^1\text{O}_2$ . We found that reaction rates increase in proportional to the conjugation length linked to the isobenzofuran moiety. The probes are photostable and selective for  $^1\text{O}_2$  over other reactive oxygen species including  $\text{H}_2\text{O}_2$ ,  $\cdot\text{OH}$ ,  $t\text{-BuOOH}$  and  $\text{O}_2\cdot^-$ . Finally,  $^1\text{O}_2$  detection utility in aqueous solutions has been demonstrated by fabricating nanoaggregates of the probe.



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발표코드: ORGN.P-867

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Palladium-Catalyzed Allyl Cross-Coupling Reactions with Organoindium Reagents

이구연 류태규<sup>1</sup> 이필호<sup>1</sup>

강원대 생명건강공학과 <sup>1</sup>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 triflates.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Recyclable Metal Nanoparticle-Catalyzed Selective Transformation of Silanes into Silanols using Water

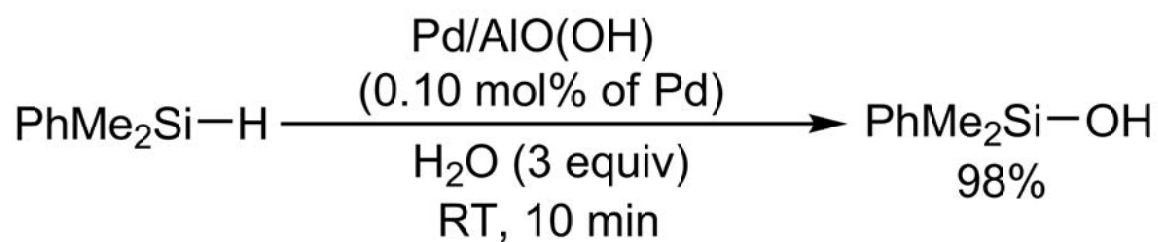
전미나 한정훈<sup>1</sup> 박재욱<sup>1</sup>

포항공과대 화학<sup>1</sup> 포항공과대 화학과

Silanols are widely used for synthesis of silicon-based polymers and nucleophilic partner for carbon-carbon cross coupling reactions. Various methods have been developed for synthesis of silanols. Among them, the catalytic oxidation of organosilanes by water and/or molecular oxygen, which produce H<sub>2</sub> and/or H<sub>2</sub>O as bi-products, would be clearly preferable to conventional methods. Recently, many results have been reported for this reactions using metal nanoparticle catalyst because of efficiency and reusability.

In this research, highly selective and efficient transformation of organosilanes into silanols was achieved using readily available heterogeneous metal nanoparticle catalysts on an

aluminum oxyhydroxide support [M/AlO(OH), M=Pd, Au, Rh, Ru, and Cu]. The transformation was performed under ambient conditions with water. Among the catalysts investigated, the palladium catalyst showed the highest activity. Furthermore, the turnover number (TON=99000) and turnover frequency (TOF=20 000 h<sup>-1</sup>) are the highest among those reported so far. The palladium catalyst was effective for a wide range of silanes, and the catalyst could be reused at least ten times without any loss in activity.



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발표코드: ORGN.P-869

발표분야: 유기화학

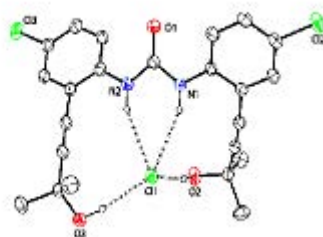
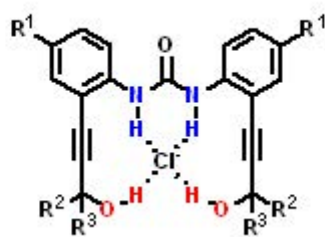
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Phenylurea-based synthetic receptors that transport chloride through lipid membranes

최예린

연세대 화학과

Membrane transport of anions is an important biological process which is closely associate with a variety of severe diseases.<sup>1)</sup> In a ClC channel, the chloride ion travels by a virtue of four hydrogen bonds with two NHs and two OHs in cell membranes. We here designed and synthesized anion receptors that were based on the phenyl urea skeleton and possessed the same functional groups with the ClC chloride channel. To improve the transport efficiency, we tuned the properties of the receptors; binding strength and lipophilicity. The former was modified by changing the electronic properties of R1 side chains and the number of hydrogen bond donors, and the latter was also controlled by the modification of R2 and R3 side chain. The structure of a complex was determined by single-crystal X-ray diffraction, and the binding constants were measured by <sup>1</sup>H NMR titrations. Finally, the transport ability was detected by the decrease of the fluorescence intensity of the embedded lucigenin in vesicles as chloride ion came in.



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발표코드: ORGN.P-870

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Ratiometric fluorescence sensing of Zinc by thiazole ? imidazole receptor**

**Aasif Helal Sahan Gunasekara 김홍석**

경북대 응용화학과

Zinc (II) is the second most abundant transition metal form of cation in the biological system. Excited state intramolecular proton transfer (ESIPT) is one of the most common photophysical processes occurred in benzazoles and used to develop ratiometric probes. In this poster, design and development of a novel thiazole-imidazole based fluorescent chemosensor for zinc ion in aqueous media will be reported.

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발표코드: ORGN.P-871

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Novel Synthesis of Indolizine Derivatives

모준태 류태규 이필호

강원대 화학과

Development of synthetic method of indolizine, which exhibit intriguing molecular structures featured by an *N*-bridgehead bicyclic ring system, has received much attention in recent years. Many of the synthetic and natural indolizines have displayed important biological activities which can find a variety of applications in pharmaceutical use. They are also useful in the field of material science owing to their unique photophysical properties. Although a number of methods are available for the synthesis of indolizine, the development of general and efficient synthesis of functionalized indolizines is still highly attractive. In this poster, we describe an efficient synthetic method of indolizines.

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장소: 일산KINTEX

발표코드: ORGN.P-872

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Synthesis of Cyclic Compounds via Double-Hydroarylation

모준태 이의철 이필호

강원대 화학과

Catalyst activation of aromatic C-H bonds leading to new and useful reactions such as C-C bond formations remains a long-term challenge to chemists and is of considerable interest for the chemical and pharmaceutical industries. It would provide simple, clean, and economic methods for making many useful aryl-substituted compounds directly from simple arens since prefunctionalization like a halogenations is involved. Over the past decade a variety of hydroarylation reactions were studied and published. In 2000, Fujiwara reported the catalytic hydroarylation of alkenes and alkynes using  $M(OAc)_2$  [ $M=$ Pd,Pt] in trifluoroacetic acid. In 2005, Tunge properly suggested two mechanism of hydroarylation of alkynes using transition metal. One is C-H activation system and the other is alkynes activation system. In 2010, our group was developed intramolecular hydroaylation of 2,3-allenoate using Platinum catalyst through alkynes activation. We efficiently produced 1,4-dihydronaphthalene derivatives. In continuation of our studies directed toward the development of efficient transition metal catalyzed hydroarylation reaction,



we found Au-catalyzed intramolecular cyclization of dialkynes. Herein, we report preparation of dicromens and polygon compounds via hydroarylation of dialkynes derivatives.



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발표코드: ORGN.P-873

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Tandem Addition/Cyclization Reaction

모준태 이도형 이필호

강원대 화학과

2-Pyrones are important structural subunits in a wide variety of biologically active natural products, as well as useful versatile synthetic intermediates. Recently, the activity of 2-pyrones as potent HIV protease inhibitors invoked additional interest in the investigation of 2-pyrones and their analogues. Phosphorus 2-pyrones are particularly interesting due to their similarity in reactivity and bioactivities with the carbon species. However, until 2004, only five phosphorus 2-pyrone analogues have been reported in the literature. Unfortunately, their methods have not been thoroughly examined and they are usually lengthy procedures which suffer from low yields. In 2005, Ding et al. prepared 2*H*-1,2-oxaphosphorin 2-oxides to show efficient cyclization reaction using  $\text{Ag}_2\text{CO}_3$  from (*Z*)-2-alken-4-phenylethynyl-phosphonic monoesters. However, only six examples were shown and the synthesis of (*Z*)-2-alken-4-phenylethynyl-phosphonic monoesters is complicated. Therefore, this has led us to develop a novel method for the synthesis of versatile phosphorus 2-pyrone.

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발표코드: ORGN.P-874

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Ethyl 2-Aryl-2,3-alkadienoates via Palladium-Catalyzed Cross-Coupling Reactions

강동진 오수성 이필호

강원대 화학과

Transition-metal-catalyzed cross-coupling reactions represent an extremely versatile tool in organic synthesis. Cross-coupling reactions leading to C-C bond formation are often key steps in a wide range of organic processes. During the past decades, a variety of organometallic reagents, such as alkyl-, allyl-, allenyl-, benzyl-, vinyl-, and arylmetals, have been used as nucleophiles in cross-coupling reactions. Recently, because allenes have been widely used in organic reactions, development of novel synthetic methods of allenes has been required. We demonstrated an efficient synthetic method for the preparation of ethyl 2-aryl-2,3-alkadienoates through Pd-catalyzed selective allenyl cross-coupling reactions of aryl iodides with organoindiums.

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발표코드: ORGN.P-875

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cycloisomerization of 1,3-Butadiene Derivatives

박상준 박성국 이필호

강원대 화학과

Indene derivatives, in particular multiply substituted ones, have been attractive, and synthetically useful methods for their synthesis have been developed. Among these known procedures, the most frequent attempts to result in the formation of indene derivatives are the photo or thermo rearrangement of 3-arylcylopropenes and the cyclization of phenyl vinyl derivatives or phenyl-substituted allyl alcohols. When treated with acids, the phenyl-substituted allyl alcohols afford phenyl-substituted allyl cations, which undergo electrocyclic ring closure to form indene derivatives by the elimination of a proton. However, the introduction of different substituents onto the indene ring encountered difficulties especially when the highly substituted indene derivatives and their yields are concerned. Herein, we report a very simple and efficient method for the synthesis of diaryl substituted indenenes in excellent yields.

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장소: 일산KINTEX

발표코드: ORGN.P-876

발표분야: 유기화학

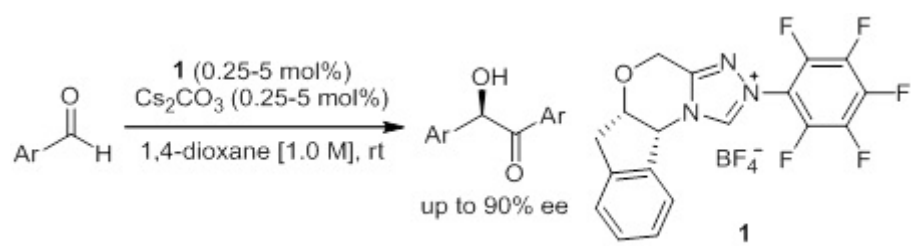
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Inverse Enantioselectivity with Catalyst Loading in Enantioselective Self-Benzoin Condensation using Triazaolium-based N-Heterocyclic Carbene Catalyst**

maohui 김선민 An ShuLan 양정운

성균관대 에너지과학과

Asymmetric self-benzoin condensations of aromatic aldehydes was achieved using 0.25-5 mol% of a cis-2-aminoindanol-based chiral triazolium N-heterocyclic carbene catalyst, affording high yield benzoin derivatives with high enantioselectivity. Remarkably, lower catalyst loading resulted in higher yields and enantioselectivities.



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발표코드: ORGN.P-877

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New Synthetic Method of Cyclic Compounds

박영철 김진식 이필호

강원대 화학과

The ene reaction between an enol and an alkyne is an established synthetic reaction with respect to its five-membered rings formation, known as the Conia-ene reaction. However the high temperature required for this reaction limits its application in organic synthesis. This cyclization methodology has been expanded in recent years by the use of transition-metal catalysts, which has allowed the reaction to proceed at lower temperatures. Unfortunately, these transition-metal-catalyzed cyclizations are often needed additives, such as strong base, strong acid, and photochemical activation. Herein, we have developed that iron catalyze the cyclization of 1,3-dicarbonyl compounds to provide an efficient method for five-membered rings formation. And organostannanes enjoy extensive use in organic synthesis due to the multitude of transformations. Recently, vinyl-, alkenyl-, and benzylstannanes have been used nucleophilic species, for coupling with various electrophiles under mild and neutral conditions in palladium-catalyzed carbon-carbon bond formation methods. We have reported an efficient synthetic method of stannyl derivatives catalyzed by transition-metal.

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발표코드: ORGN.P-878

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 니트로 방향족 화합물의 수소화 반응을 통한 아민 유도체 제조

오승근 장상은 김용진

한국생산기술연구원 그린공정소재연구그룹

시클로헥실아민 및 N-알킬시클로헥실아민은 고무용 약품, 농약, 계면활성제, 염료, 향료, 산소흡수제, 방식제 등 다양한 공업적인 용도로 널리 사용되는 화학물질이다. 기존의 시클로헥실아민의 제조는 시클로헥사놀 또는 페놀을 암모니아로 아미노화 하는 방법이나 아닐린의 수소화를 통해 제조되었으며, 주로 아닐린의 수소화를 통한 방법이 널리 사용되었다. 이때 사용되는 아닐린은 니트로벤젠의 수소화를 통해 제조된다. 따라서 기존의 방법으로 니트로벤젠으로부터 아닐린을 생산하기 위해서는 두 단계의 공정을 거쳐야 하는 단점이 있다. 본 연구에서는 이를 극복하기 위해 한 단계의 반응으로 니트로벤젠으로부터 시클로헥실아민을 직접 제조하는 실험을 진행하였다. 또한, 반응 조건의 조절을 통해 N-알킬시클로헥실아민을 제조하기 위한 실험도 진행하였다. 스테인리스 고압 반응기에서 수소 기체를 사용하여 반응을 진행하였으며, Ru/C 를 촉매로 사용하였다. 이소프로판올을 용매 및 alkylation agent 로 사용하였고, 반응 물질은 니트로벤젠 이외에 nitroaniline, nitrotoluene,



halogen-nitrobenzene, dinitrobenzene 등 다양한 니트로 방향족 화합물을 사용하여 실험을 진행하였다. 반응 후 생성물을 GC 및 GC mass spectrometer 를 이용하여 전환율 및 선택율을 계산하였다.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-879

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of a New Class of Taurine Derivatives as Antioxidants

김범태 조익수<sup>1</sup> 채민선<sup>1</sup> 황기준<sup>2</sup>

전북대 생리활성물질연구소, 생리활성소재과학과 <sup>1</sup>전북대 생리활성소재과학과 <sup>2</sup>전북대 화학과

Taurine, a sulfur-containing amino acid, has been reported to demonstrate a variety of bioactivity such as anti-inflammatory and antioxidant effect. A new class of taurine derivatives were prepared, and their DPPH radical scavenging activities as a primary antioxidant activity were evaluated. Some of taurine derivatives were synthesized by the reaction of cinnamic acid analogues with taurine tetrabutylammonium salt via Curtius rearrangement. The results of DPPH radical scavenging activity shows that taurine derivatives demonstrate remarkable increase in activity compared with those of cinnamic acid derivatives. The use of taurine tetrabutylammonium salt was turned out to be much more effective as a taurine source than taurine itself in Curtius rearrangement reaction condition

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-880

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Unsymmetric Ketones through Cross-Coupling Reaction



이도형 손익환 이필호

강원대 화학과

The development of palladium-catalyzed cross-coupling reaction has revolutionized the formation of carbon-carbon bonds. These coupling reaction have found many applications in natural product synthesis, material science, and medicinal chemistry. The Suzuki reaction, which involves organoboron compounds, has been widely used because of the ready availability of boronic esters and their excellent compatibility with many functional groups during the cross-coupling reaction. Herein, we studied palladium-catalyzed cross-coupling reaction of organoindium reagents with aryl halides and a preparation of acyl indium reagents.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-881

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Bulk-Heterojunction Solar Cells with Benzimidazole-Based Novel Polymers as Electron Donors

심주영 박혜지 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

The PININEBBTMBI was used as the electron donor for the PSCs (ITO / PEDOT:PSS / polymer:PC71BM(1:4) / TiO<sub>x</sub> / Al). The unique structure of PININE, incorporating the vinylene unit with bicyclic [2.2.0] system, can overcome the basic degradation problem of the common type of vinylene units in PPV series<sup>1</sup>. The solar cells made from conjugated PININEs with benzimidazole and bithiophene units, which are new conjugated polymers for the application in polymer solar cells (PSCs), exhibit high PCEs even in basic PSC device structure. The absorption spectra of PININEDTMBI with thiophene units exhibit two maximum peaks at about 418 and 637 nm in solution. The solutions of PININEBBTMBI show two absorption peaks at about 438 and 634 nm which is red-shifted about 20 nm as compared to PININEDTMBI caused by the introduction of bithiophene units. The best solar cell performance obtained has a layered structure of ITO / PEDOT:PSS / PININEBBTMBI:PC71BM(1:4) / Al. Under white light

illumination (AM 1.5 G, 100 mW/cm<sup>2</sup>), the obtained J<sub>sc</sub> is 6.66 mA/cm<sup>2</sup>, V<sub>oc</sub> is 0.78 V, FF is 41%, and PCE is 2.11%.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-882

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Correlation of the Rates of Solvolysis of 2-Phenylethyl and 2,2-Diphenylethyl Chloroformate and a Consideration of the Branching $\beta$ -Alkyl Group Effects

성미혜 양기훈 박경호 유찬주 경진범

한양대 응용화학과

Specific rates for solvolyses of 2-phenylethyl chloroformate (1) and 2,2-diphenylethyl chloroformate (2) have been measured in a wide range of solvents. When the extended Grunwald-Winstein equation [ $\log(k/k_0) = lN + mY + c$ ] is applied, the solvolyses of 1 and 2 have a satisfactory correlation in all of the solvents. The sensitivities toward changes in solvent nucleophilicity and solvent ionizing power are consistent with a rate-determining addition-elimination pathway. The kinetic solvent isotope effects (KSIEs,  $k_{MeOH}/k_{MeOD}$ ) for the methanolyses of 1 and 2 show trends similar to those observed previously for the solvolyses of other primary alkyl haloformates. The enthalpy and entropy of activation were also determined for the solvolyses of 1 and 2 in ethanol, methanol, 80% ethanol, and 70% TFE. The results are compared with those reported earlier for ethyl chloroformate and other alkyl haloformate esters.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-883

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Apoptozole that binds to an ATPase domain of Hsc70 promotes  
membrane trafficking of mutant cystic fibrosis transmembrane  
conductance regulator**

**백경화 고성균 신인재**

연세대 화학과

Cystic fibrosis transmembrane conductance regulator (CFTR) is a cell-surface anion channel that permeates chloride and bicarbonate ions. The most frequent mutation of CFTR that causes cystic fibrosis is the deletion of phenylalanine at position 508 ( $\Delta F508$ ), which leads to defects in protein folding and cellular trafficking to the plasma membrane. The lack of the cell-surface CFTR results in a reduction in the lifespan due to chronic lung infection with progressive deterioration of lung function. Hsc70 plays a crucial role in degradation of mutant CFTR by the ubiquitin-proteasome system. To date, various Hsc70 inhibitors and transcription regulators have been tested to determine whether they correct the defective activity of mutant CFTR. However, they exhibited limited or questionable effects on restoring the chloride channel activity in cystic fibrosis cells. Herein, we show that a small molecule apoptozole (Az) has high cellular potency to promote membrane trafficking of mutant CFTR and its chloride channel

activity in cystic fibrosis cells. Results from affinity chromatography and ATPase activity assay indicate that Az inhibits the ATPase activity of Hsc70 by binding to its ATPase domain. In addition, a ligand-directed protein labeling and molecular modeling studies also suggest the binding of Az to an ATPase domain, in particular, an ATP-binding pocket. It is proposed that Az suppresses ubiquitination of  $\Delta F508$ -CFTR maybe by blocking interaction of the mutant with Hsc70 and CHIP, and, as a consequence, it enhances membrane trafficking of the mutant.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-884

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Facile Synthesis of Pyrazole

박성국 박영철 이필호

강원대 화학과

The pyrazole moiety is present in a plethora of natural and synthetic compounds. It is involved in a number of biologically active molecules and can act as an efficient coordinating ligand. In this regard, pyrazoles have been studied for over a century as an important class of heterocyclic compounds and still continue to attract considerable attention due to the wide range of medicinal activities they possess, such as analgesic, antimicrobial, antiviral, anti-inflammatory, hypoglycemic, antihypertensive and antitumor properties. While there are many new and novel methods available for the assembly of the pyrazole nucleus, we have developed a new synthesis of pyrazole. We report that cross-couplings of various pyrazole derivatives with arylboronic acids, terminal alkynes, and stannane give 3,5-disubstituted pyrazoles.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-885

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Fluorene-Based Donor-Acceptor Narrow Band-Gap Polymers and Their Derivatives for Bulk-Heterojunction Polymer Solar Cell Applications

심주영 박혜지 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

The advantage of dimethyl-2H-benzimidazole compared to the benzothiadiazole moiety of PCDTBT is to improve the solubility of the polymer while keeping the 1,2-quinoid form to lead coplanarity of the backbone. The PFDTMBIs in solid films show two maximum peaks at about 420?427 and 626?641nm. 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 caused by the introduction of bithiophene units. The device with PFBBTMBI5:PC61BM blend demonstrated a VOC value of 0.68 V, a JSC value of 3.10mA/cm<sup>2</sup>, and a FF of 0.35, leading to the efficiency of 0.74%, improved performance relative to other copolymers of the series.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-886

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

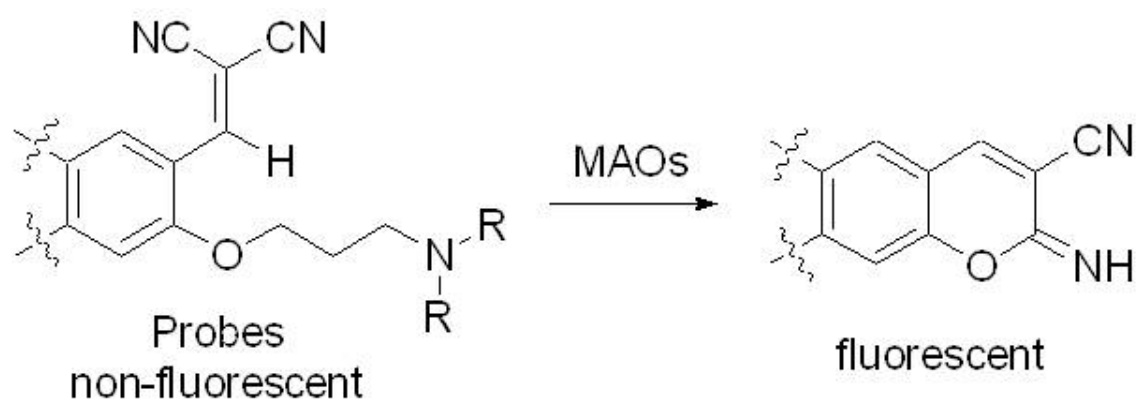
**Synthesis of a two-photon absorbing compound toward reactive  
fluorescent probes : An application to probing monoamine oxidase  
activity**

**김도경 안교한**

포항공과대 화학과

Monoamine oxidases (MAOs) play an important role in regulating tissue levels of amine neurotransmitters and dietary amines. Much efforts have been made to search for MAOs inhibitors, which have potential for the treatment of neurological disorders such as Parkinson's disease and schizophrenia. It is thus important to develop homogeneous and highly sensitive assay systems for MAOs' activity, which may be used for drug discovery and for monitoring enzymatic activities in complex biological systems. The known fluorescent probes for MAOs are based on one-photon fluorophores, for example, resorufin and quinazolinone derivatives. Two-photon probes for MAOs, however, remain unexplored, in spite of their advantageous features over the one-photon probes. We have developed a novel type of fluorescent probes, with which MAOs' activity can be assayed in vitro and imaged in cells by both one- and two-photon microscopy. Coumarin precursors (the probes) thus undergo a MAO-catalyzed oxidation

reaction followed by hydrolysis to afford a  $\beta$ -aryloxyaldehyde intermediate, which further undergoes  $\beta$ -elimination followed by an intramolecular cyclization to afford an imino-coumarin product (Imino-POS) that emits fluorescence in the turn-on mode, either by one-photon or by two-photon excitation



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-887

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Benzimidazole-Based Low Bandgap Small molecules for Efficient Polymer Solar Cell

심주영 박혜지 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

In the past decade, polymer solar cells (PSCs) have attracted considerable attention for their unique advantages over traditional silicon-based solar cells, such as low cost, light weight, and the potential for making flexible large area devices by roll-to-roll manufacturing. Bulk heterojunction(BHJ) films has been dominated by polymeric donor materials, as they typically have better film-forming characteristics and film morphology than their small-molecule counterparts. 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. Three small organic molecules, 5-hexyl-2,2'-bithiophene (HS5431), benzo[b]thiophene(HS5438) and tri phenyl amine(HS5439), with 2,2-dimethyl-2H-benzimidazole unit as new electron-deficient unit, were synthesized by Suzuki coupling reaction. The spectra of HS5431 and HS5439 in the solid thin films show absorption bands with maximum peaks at 399, 617 and 378, 602 nm.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-888

발표분야: 유기화학

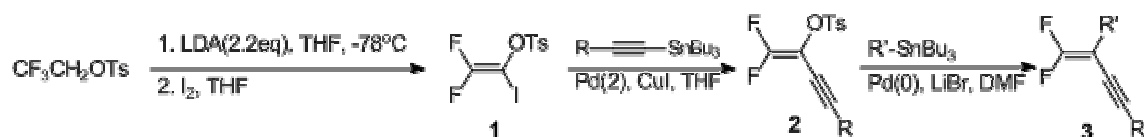
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of 1-alkynyl-2,2-difluoroethenyl p-toluenesulfonate and its reactivity

이효영 정인화

연세대 화학및의화학과

2,2-Difluoro-1-iodoethenyl p-toluenesulfonate **1** was synthesized in 66% yield from the reaction of 2,2,2-trifluoroethyl p-toluenesulfonate with 2.2 equiv of LDA at  $-78^{\circ}\text{C}$ , followed by treatment with iodine. Alkynylation reaction of 2,2-Difluoro-1-iodoethenyl p-toluenesulfonate **1** with alkynylstannane in the presence of  $\text{PdCl}_2(\text{PPh}_3)_2$  and  $\text{CuI}$  in THF afforded 1,1-difluoroenynes **2** in 52~73% yields. The cross-coupling reaction of 1-alkynyl-2,2-difluoroethenyl p-toluenesulfonate **2** with organostannane reagents provided the 1,1-difluoroenynes **3**. The scope and limitation will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-889

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of Allenes via Palladium-Catalyzed Selective Cross-Coupling Reactions

손익환 박상준 이필호

강원대 화학과

Transition metal-catalyzed cross-coupling reactions represent an extremely versatile tool in organic synthesis. We demonstrated an efficient synthetic method for the preparation of allenes through Pd-catalyzed selective allenyl cross-coupling reactions of aryl iodides with organoindiums. Because introduction of aryl group to allene is difficult, this method would pave a new way to synthetically valuable processes of a wide range of functionalized allenes.

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장소: 일산KINTEX

발표코드: ORGN.P-890

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 1D and 2D NMR Spectroscopy Study on Dynamic Self Assembly of Pd(II) metal Coordinated Macrocycle

김동환 임춘우<sup>1</sup> 김태우<sup>1</sup>

경희대 동서의과학과 <sup>1</sup>경희대 동서의학대학원

Dynamic self-assembly of 1,3-bis(4-pyridyloxy)propane and cis-protected Pd(II) metal with ethylenediamine is presented. <sup>1</sup>H NMR spectra have revealed that the formation of [2]catenane is dependent on the concentration of macrocyclic ring. We have performed the structural analysis of macrocyclic ring and [2]catenane using H<sup>1</sup>H COSY and ESI MS. The dynamic process of the catenation has been elucidated by van't Hoff plot and the formation of [2]catenane is enthalpically favored in D<sub>2</sub>O, strongly suggesting the hydrophobic interactions for the formation of [2]catenane. Diffusion-ordered NMR spectroscopy (DOSY) distinguishes between dinuclear self-assembled macrocyclic ring and [2]catenane, indicating that [2]catenanes diffuse slower than macrocyclic rings in D<sub>2</sub>O.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-891

발표분야: 유기화학

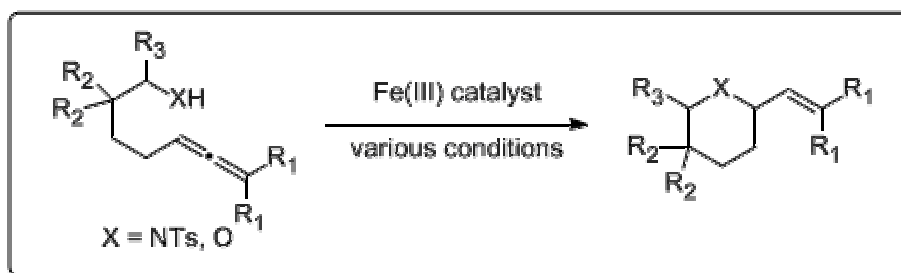
발표종류: 포스터, 발표일시: 수 18:00~21:00

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

정민석 진하정 김영삼<sup>1</sup> 신예호<sup>1</sup> 강은주

경희대 응용화학과 <sup>1</sup>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.



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장소: 일산KINTEX

발표코드: ORGN.P-892

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Donor Polymers Containing Cyclopenta[def]phenanthrene in Their Units with Improved Photovoltaic Performance

심주영 박혜지 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

The research for the achievement of efficient organic photovoltaics (OPVs) has become one of the most popular topics in recent years caused by their potential to be an alternative source of green energy. Polymer solar cells have many desirable features including large-scale fabrication utilizing low cost solution processability. The development of novel materials is necessary to enhance the coverage of the solar spectrum and the absorption coefficients, which can improve the lower power- conversion efficiency and smaller photocurrent as compared to the case of inorganic solarcells. New conjugated polymers containing electron donor-acceptor pairs for organic photovoltaic device utilizing a new type of acceptor are reported to show good solubility at room temperature in organic solvents. These donor-acceptor conjugated polymers were synthesized by palladium catalyzed stille coupling reaction of 4,4-bis(2-ethylhexyl)-4H-cyclopenta[def]phenanthrene (CPP) and dimethyl-2H-benzimidazole. The new type of acceptor was fabricated in PCPPDTMBIs and PCPPBBTMBIs

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-893

발표분야: 유기화학

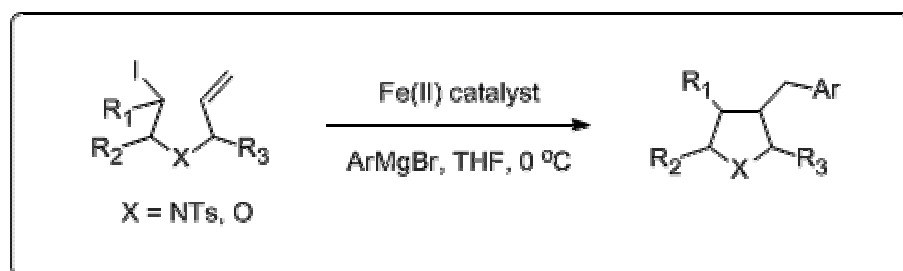
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Tandem Radical Cyclization and Cross-coupling Reaction with Fe(II) Catalyst and Aryl Grignard Reagent

김재곤 정시현<sup>1</sup> 강은주<sup>1</sup>

경희대 화학과 <sup>1</sup>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 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-894

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

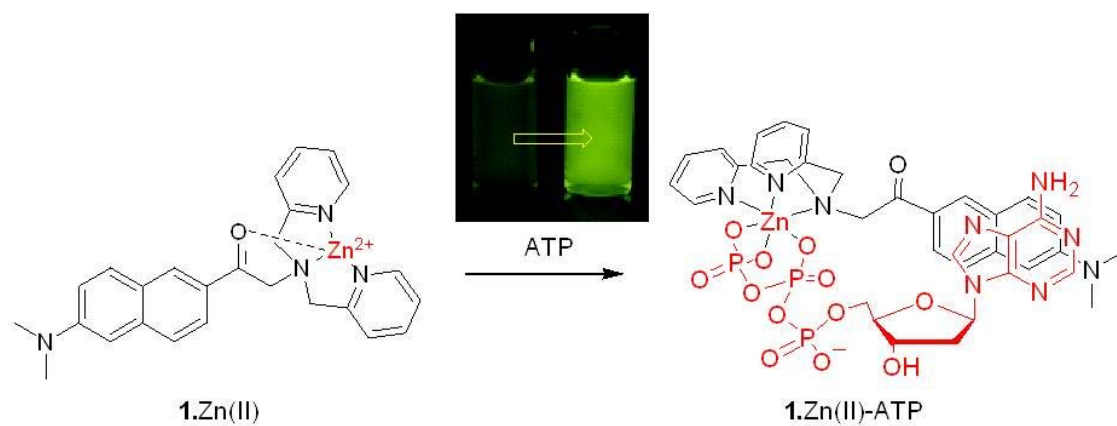
## Acedan based Two-photon Fluorescent Probe for ATP and ADP

alla sreenivasa rao 김도경 안교한

포항공과대 화학과

Adenosine triphosphate (ATP) is perceived as the “molecular unit of currency” for intracellular energy transfer in the living cells; it transports chemical energy within the cells for metabolism. Deficiency in the ATP level, results ischemia, Parkinson’s disease and hypoglycaemia. Monitoring of the ATP concentration level is thus important for the study of different cellular mechanisms, enzymatic processes, and even cell apoptosis. For the detection of ATP, various colorimetric and fluorescent probes have been developed. Most of these fluorescent probes, however, work with one-photon microscopy (OPM) that requires a short excitation wavelength which can cause unfavorable features such as shallow penetration depth, photo-bleaching, photo-damage, and cellular auto-fluorescence. These problems can be mostly alleviated by the two-photon microscopy (TPM) that employs two near-infrared photons for excitation. In spite of the advantageous features, so far no two-photon probe for nucleotides such as ATP has been developed. For this purpose, we developed a two-photon probe based on acedan, which selectively detects

ATP/ADP among various anions examined including PPi and AMP. The probe is permeable to cell membranes and thus can be directly used for TP imaging of ATP and ADP in living cells.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Construction of new perylenequinone core, 1,12-bis((benzoylamino)methyl)-3,10-perylenequinone

김범태 김효연<sup>1</sup> 이윤아<sup>1</sup> 황기준<sup>2</sup>

전북대 생리활성물질연구소, 생리활성소재과학과 <sup>1</sup>전북대 생리활성소재과학과 <sup>2</sup>전북대 화학과

The multisubstituted naphthoquinones have attracted much attention due to their potential as key intermediates in the synthesis of the naturally occurring and biologically important perylenequinoids such as calphostins and Hypocrellins. we synthesized 3-(benzoylamino)methyl-1,2-naphthoquinones as a key intermediate to develop new perylenequinone class of compounds with diverse substitution pattern at 1,12-position and improved photosensitizing activity. Finally, the novel perylenequinone core, 1,12-bis((benzoylamino)methyl)-3,10-perylene quinone, was successfully prepared from the dimerization of the key intermediate, 3-(benzoylamino)methyl-1,2-naphthoquinones. For the optimum dimerization condition, several attempts such as oxidative (FeCl<sub>3</sub>) or acid-catalytic (Trifluoroacetic acid) coupling has been performed.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Total synthesis of carvotanacetones and confirmation of their absolute stereostructures

이재연 정시원 이희윤

KAIST 화학과

Carvotanacetone family contains natural products with the basic skeleton of Carvone. Carvone, 6-hydroxycarvone, and 4-hydroxycarvone belong to this family of compounds. The absolute stereochemistry of these compounds has been elucidated by Circular Dichroism (CD) spectral data. The method using CD is based on an empirical rule called Snatzke's Rule. The absolute stereochemistry of natural products containing Carvotanacetone structure also has been assigned in the same way. However, the absolute stereochemistry of some of the natural products in this family had to be corrected through total synthesis or X-ray crystallography. Alotaketol A, Phorbasin C, and Phorbaketol A are the examples. To confirm the absolute Stereochemical structures of Carvotanacetones, the total synthesis of these compounds from Pinene which has the known absolute stereochemistry was studied. In this presentation, we will discuss the relationship of the absolute stereochemistry of Carbotanacetones with CD spectroscopy.

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발표코드: ORGN.P-897

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and photovoltaic properties of copolymers based on 2,2-(1,5-pentamethylene)-2H-benzimidazole designed for efficient photovoltaic applications

박혜지 심주영 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

The sunlight is a clean, abundant and virtually limitless energy source which can be used to address the growing global energy needs. We report synthesis and photovoltaic properties of two new conjugated copolymers with benzimidazole prepared by Stille coupling reaction. The advantage of PMBI is high solubility of the polymer while keeping the coplanarity of the backbone. The electrochemical bandgaps of PCDTPMBI5 and PCBBTPMBI5, calculated from cyclic voltammetry data, are about 2.11 and 2.00 eV, respectively. The optical band gap of the synthesized PCDTPMBI5 (1.43 eV) was smaller than that of PCBBTPMBI5 (1.56 eV), caused by lower ICT effect contributed by low molecular weight of PCBBTPMBI5. The devices comprising PCDTPMBI5:PC61BM (1:2) and PCBBTPMBI5:PC61BM (1:3) with thermal treatment showed an open-circuit voltage (VOC) of 0.27 and 0.30 V, a short-circuit current

density (JSC) of 1.09 and 1.75 mA/cm<sup>2</sup>, and a fill factor (FF) of 0.29 and 0.38, giving an power conversion efficiency of 0.09 and 0.20%, respectively.



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발표분야: 유기화학

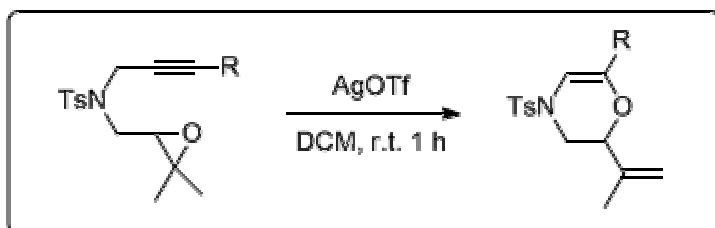
발표종류: 포스터, 발표일시: 수 18:00~21:00

## AgOTf-catalyzed Isomerization of Oxo-alkynes

Muchchintala Maheswa 이윤영 강은주

경희대 응용화학과

Several alkynyl epoxides were isomerized to cyclic allyl vinyl ethers (3,4-dihydro-2H-1,4-oxazines) using AgOTf as the catalyst.



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발표분야: 유기화학

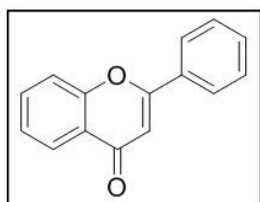
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis Of Various 3-Hydroxyflavone Derivatives Using a Modified AFO reaction

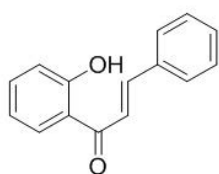
김보정 정현주<sup>1</sup> 김학원<sup>1</sup>

경희대 화학과 <sup>1</sup>경희대 응용화학과

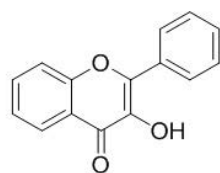
Flavonoid 는 식물계에 널리 분포되어 있으며, 2 번 위치에 phenyl 기를 포함하는 chromone 계열, 즉 flavone 을 기본 구조로 갖는 화합물을 일컫는다. 이 중에서도 3 번 탄소 위치에 hydroxyl group 을 가지고 있는 flavone 은 flavonol 이라고도 하며, 여러 가지 생리활성을 나타내는 것으로 잘 알려져 있다. Myricetin, Quercetin, Kaempferol 등의 천연물들이 대표적인 3-hydroxylated flavones 유도체들이다. 그러나, 현재까지 잘 알려진 chalcone 으로부터 flavonol 을 합성하는 방법인 AFO reaction 은 다양성과 재현성면에서 제한점이 많으며, 출발물질의 치환기에 대해서도 많은 영향을 받는다. 따라서, 본 연구진은 chalcone 유도체로부터 1 step 으로 직접 3-hydroxyl flavone 유도체들을 합성할 수 있는 AFO reaction 을 다양한 chalcone 유도체들에 대해서 조사, 정리하였고, 기존 방법보다 개선된 AFO 반응을 개발, 적용하였다.



Flavone<sup>21</sup>



AFO reaction



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-900

발표분야: 유기화학

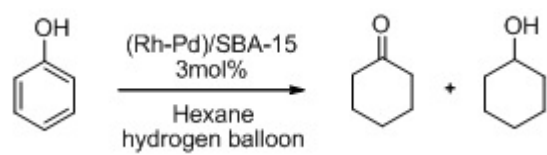
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nanosized (Rh-Pd)/SBA-15 Catalyzed Hydrogenation of Arenes

권현지 이강우 이희석<sup>1</sup> 정희진 변송호 김학원<sup>1</sup>

경희대 화학과 <sup>1</sup>경희대 응용화학과

학문적으로나 상업적 목적으로 많은 연구가 진행되어지고 있는 catalytic hydrogenation 은 반응의 결과로 생성되는 화합물이 상업적으로 중요한 물질의 중간체로 사용되어지고 있는 중요한 유기반응이다. 이러한 수소화 반응 중에서 aromatic compound 의 exhaustive hydrogenation 의 예로, phenol 의 hydrogenation 반응으로 얻어지는 cyclohexanone 과 cyclohexanol 은 nylon-6 를 합성하는 과정에서 caprolactom 을 만드는 중요한 중간체로 사용되어지고 있다. Catalytic hydrogenation 에 사용되어지는 금속 촉매에는 Pd, Rh, Pt, Ir 등이 있으며, 그 중 Rh 은 arenes 의 benzene ring 을 reduction 시키는데 많이 이용되어지고 있다. 본 발표에서는 기존에 이미 알려진 mesoporous silica 인 SBA-15 지지체를 이용하여 Rh 과 Pd 의 alloy 착물을 담지 시킨 후, 환원과정을 통해 nano 크기의 Rh-Pd alloy metal 이 담지 된 금속 촉매 (Rh-Pd)/SBA-15 을 합성하였으며, Rh 과 Pd 의 비율에 따른 촉매의 arene 유도체 수소화반응의 효율을 연구한 결과를 설명하고자 한다.





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발표코드: ORGN.P-901

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Photovoltaic Properties of Conjugated Copolymers PCDTMBIs Based on poly(N-9'-heptadecanyl- 2,7-carbazole-alt-5,5- (4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)) and Various Thiophene

박혜지 심주영 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

Dimethyl-2H-benzimidazole unit was designed to substitute the BT unit of poly(N-9'-heptadecanyl- 2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole))(PCDTBT). A series of new semiconducting polymers with 2,2-dimethyl-2H-benzimidazole, 9-heptadecanyl-9H-carbazole, and thiophene (or bithiophene) units was synthesized using Stille polymerization to generate PCDTMBIs (or PCBBTMBIs). In dimethyl- 2H-benzimidazole, the sulfur at 2-position of BT unit was replaced with dialkyl substituted carbon, while keeping the 1,2-quinoid form, to improve the solubility of the polymers. The absorption spectra of PCDTMBIs with thiophene units exhibit two maximum peaks at about 430 and 613?645 nm in solution. The solutions of PCBBTMBIs show two absorption peaks at about 445?456 and 630?645 nm which is red-shifted about 20 nm when compared with PCDTMBIs caused by the introduction of bithiophene units. In most efficient polymer PCBBTMBI3, the device

annealed at 100 °C for 10 min demonstrated a VOC value of 0.60 V, a JSC value of 4.31 mA/cm<sup>2</sup>, and a FF of 0.35, leading to the power conversion efficiency (PCE) of 0.91%, under white light illumination (AM 1.5 G and 100 mW/cm<sup>2</sup>).



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발표코드: ORGN.P-902

발표분야: 유기화학

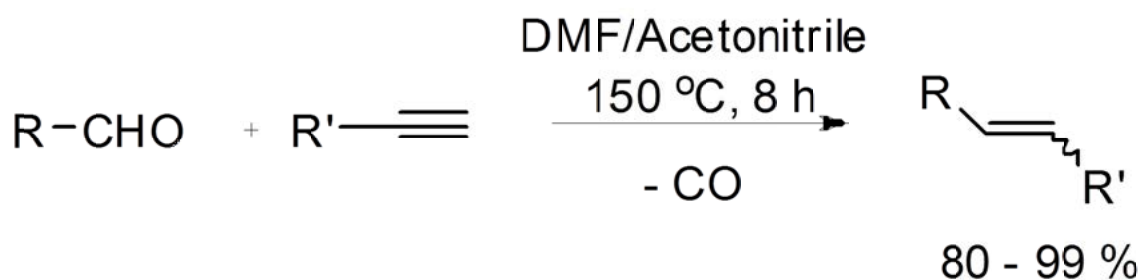
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Studies about Decarbonylative Olefination of Aldehydes and Terminal Alkynes

송정아 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

We have synthesized various olefins through the decarbonylative addition reaction of aldehydes to terminal alkynes using ruthenium catalyst. E/Z mixture of olefin products are obtained at high yields. The results of our study will be discussed at the presentation in details. This work is supported by the NRF (WCU project R33-10169).





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발표코드: ORGN.P-903

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Position effect of substituent group on the characteristics of two novel  
fulleropyrrolidine derivatives and the efficiency of organic  
photovoltaic devices**

미동보 김희운 김지훈 FEI XU<sup>1</sup> 황도훈<sup>1</sup>

부산대 <sup>1</sup>부산대 화학과

In the quest for finding alternative solar energy conversation devices in place of expensive silicon photovoltaic cells, organic photovoltaic (OPV) cells using the mixture of conjugated polymeric materials and acceptors have been proving themselves the front runner. In this paper, two novel fullerene derivatives used as electron acceptors were synthesized through 1, 3-dipolar cycloaddition. The new synthesized fullerene derivatives showed good solubility in common organic solvents and the synthetic products were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR and FAB-Mass. Photovoltaic devices were fabricated using the traditional configuration as follows: ITO/ PEDOT: PSS/ active layer/ LiF/ Al. The weight ratios of the electron donor to the acceptor in the active layer were 1:0.5, 1:0.7 and 1:1. We have found that in the case of the two novel synthesized fullerene derivatives, abbreviated as p-HOPF and o-HOPF,

substituent groups onto C<sub>60</sub> core have position effects on the characterization of fullerene derivatives and on the efficiency of OPV devices.



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발표코드: ORGN.P-904

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **New conjugated polymers based on dithienyl-2,1,3-benzothiadiazole with cyano group in vinylene as new donor materials for OPVs**

**박혜지** 심주영 송수희 진영읍<sup>1</sup> 서흥석

부산대 화학과 <sup>1</sup>부경대 공업화학과

Two alternating copolymers, PCVCNDTBT and PFVCNDTBT, with electron rich unit and electron deficient moiety for the efficient ICT were synthesized by Knoevenagel coupling polymerization and characterized. The high Voc value of the PSC of PCVCNDTBT (~0.91 V) is attributed to its lower HOMO energy level (5.6 eV) as compared to PCDTBT (5.5 eV). The optical band gaps of PCVCNDTBT (1.74 eV) and PFVCNDTBT (1.80 eV) are lower than those of PCDTBT (1.88 eV) and PFVDTBT (2.32 eV), which is advantageous to provide better coverage of the solar spectrum in the longer wavelength region. Bulk heterojunction solar cells based on blends of the polymer with PC61BM gave power conversion efficiency of 0.76% for PCVCNDTBT under AM 1.5, 100 mW/cm<sup>2</sup>.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **An efficient synthesis of enantiopure 3-aryl piperazine-2-carboxylic acids via diaza-Cope rearrangement (DCR)**

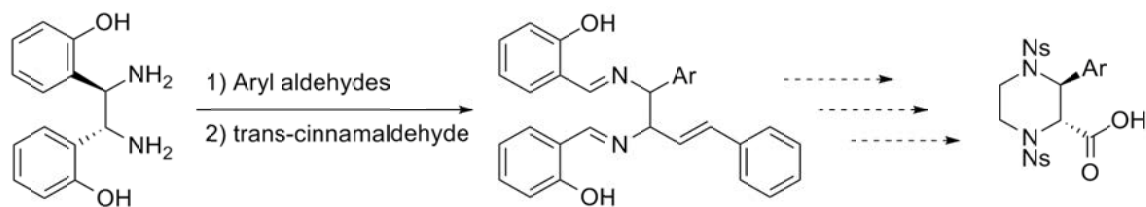
**권순호 변상문 김병문**

서울대 화학부

Piperazine ring is a common building block present in many bioactive molecules. This structural unit has been incorporated in many therapeutically important compounds such as HIV-protease inhibitors, monoamine reuptake inhibitors, MAP kinase inhibitors, CCK1R agonists, urotensin antagonists, GHSR antagonists and HIV integrase inhibitors. Although many compounds containing a piperazine moiety have been synthesized so far, preparation of chiral piperazine derivatives is still a challenging synthetic transformation. Typically, chiral piperazines have been synthesized through asymmetric hydrogenation of substituted pyrazines and various stereoselective cyclocondensations. Recently, there has been much interest in developing novel synthetic methods such as addition of Grignard reagents to pyrazine N-oxides, iridium-catalyzed synthesis from diols, synthesis starting from vicinal N-sulfinyl diamines and nosylamide-activated aziridines. However, some of these methods suffer from low ee of final compounds and complicated synthetic steps with low yields. We have developed an efficient route for enantiopure 3-



aryl piperazine-2-carboxylic acids starting from optically pure 1,2-bis(2-hydroxyphenyl)-1,2-diaminoethane (HPEN) via diaza-Cope rearrangement (DCR) using various aryl aldehyde and trans-cinnamaldehyde. Ring formation using vinyl sulfonium salt followed by oxidation using ruthenium(III) chloride monohydrate with sodium periodate provided the desired chiral piperazine derivatives.



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장소: 일산KINTEX

발표코드: ORGN.P-906

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and applications of benzimidazole based small molecules as donor materials for organic photovoltaics

박혜지 심주영 송수희 진영읍<sup>1</sup> 서홍석

부산대 화학과 <sup>1</sup>부경대 공업화학과

Organic photovoltaic technology, a low-cost, lightweight, and flexible thin film device toward inexhaustible renewable clean energy, has received great attention during the past years. Utilization of 2,2-dimethyl-2H-benzimidazole has received strong attention as the electron-deficient unit for the generation of electron donor material for organic photovoltaic cells (OPVs). This paper reports the first small organic molecules based on dimethyl-2H-benzimidazole, which can produce intramolecular charge transfer. Two soluble small organic molecules, MMM and OMO, with dimethyl-2H-benzimidazole unit were synthesized by Suzuki coupling reaction with Pd(0)-catalyst. The spectra of MMM and OMO in the solid thin films show absorption bands with maximum peaks at 374, 598 and 373, 588 nm, and the absorption onsets at 678 and 673 nm, corresponding to band gaps of 1.83 and 1.84 eV, respectively. The devices comprising MMM with PC61BM (1:3) showed a VOC of 0.66 V, a JSC of 2.03 mA/cm<sup>2</sup>, and a fill factor (FF) of 0.27, giving a power-conversion efficiency of 0.37%.

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발표코드: ORGN.P-907

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

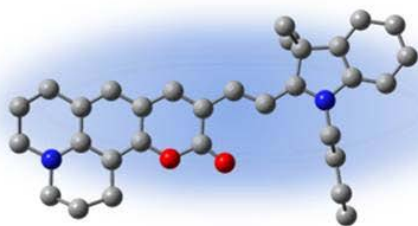
## Chromogenic and 'Turn-on' Fluorescent KCN Chemodosimeter

이재홍 정단비 장주희 김종승

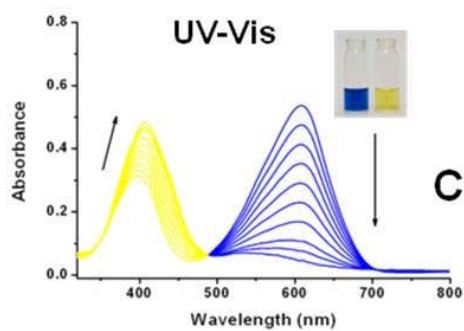
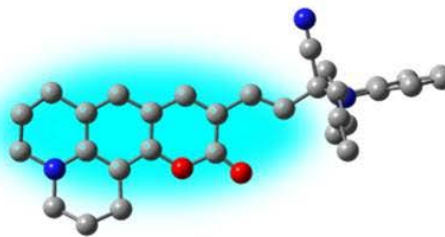
고려대 화학과

An indole conjugated coumarin derivative 1 for KCN chemodosimeter has been for the first time prepared. Compound 1 displayed considerable dual changes in both UV-vis absorption (blue-shift) and emission (turn-on) bands exclusively for KCN over other various potassium salt of anions in H<sub>2</sub>O/CH<sub>3</sub>CN (5:95, v/v) solution. DFT/TDDFT calculations support that the fluorescence enhancement of 1-KCN is mainly due to blocking of the ICT process from the coumarin N atom to the positive charged indole group with a conjugated spacer

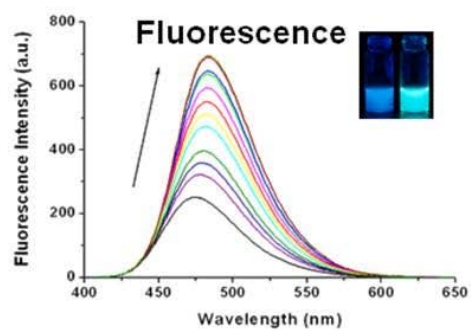
1



1+KCN



**Dual  
Changes!**



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-908

발표분야: 유기화학

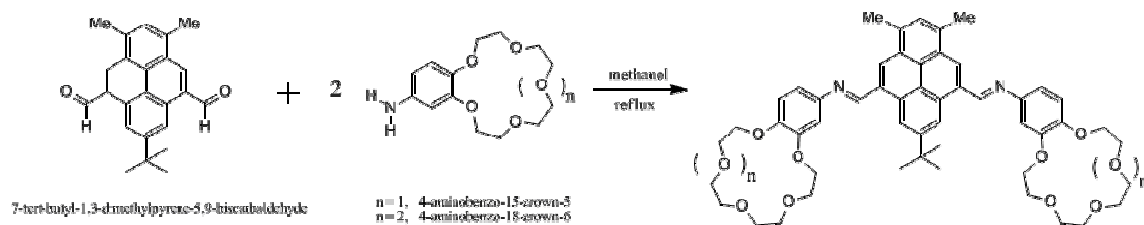
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and fluorescence properties of new bis-benzo crown ethers

주재운 장호 김기백 장우식 장승현

대구대 화학과

In this study, we synthesized new bis-benzo crown ether containing pyrene moieties. The synthesis of a novel 7-tert-butyl-1,3-dimethylpyrene-5,9-bis-4-aminobenzo crowns discotic and its binding properties to a series of alkali metal was studied. Syntheses, fluorescent properties will be discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-909

발표분야: 유기화학

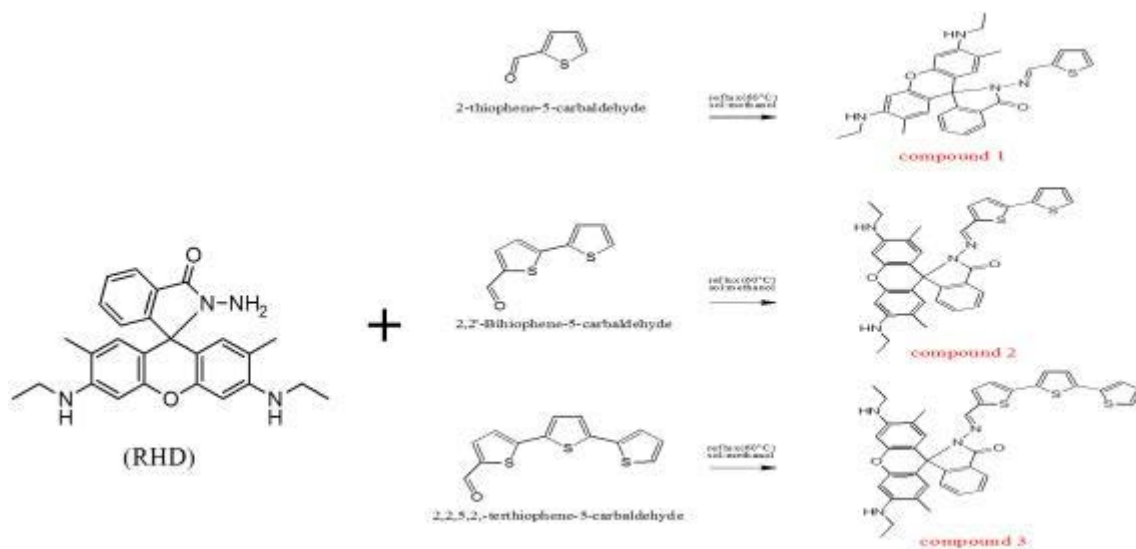
발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Synthesis and Properties of rhodamine 6G fluorescence sensors

김기백 주재운 장호 장우식 장승현

대구대 화학과

A new rhodamine 6G fluorescent sensors were synthesized by a two-step condensation reaction of rhodamine 6G and hydrazine compound(RHD). And this new compound(RHD) was synthesized with thiophene compounds(C1~C3). Compound 1 was synthesized by 2-thiophene-5-carbaldehyde (RHDT), Compound 2 was synthesized by 2,2'-Bithiophene-5-carbaldehyde(RHDB), Compound 3 was synthesized by 2,2,5,2-terthiophene-5-carbaldehyde(RHDTT). Syntheses, fluorescence properties will be discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-910

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

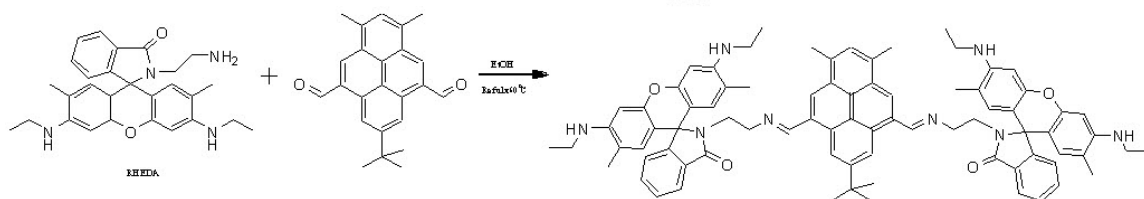
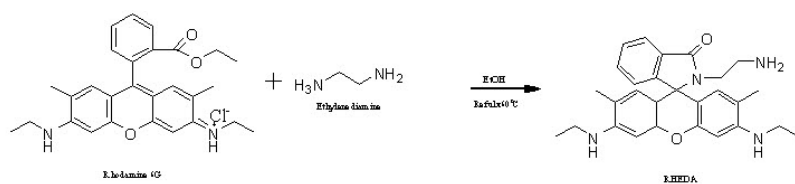
## Synthesis and fluorescent properties of new rhodamine compound containing pyrene

장우식 주재운 김기백 장호 장승현

대구대 화학과

We synthesized new kinds type of rhodamine 6G fluorescent sensors. A new rhodamine 6G fluorescent sensors were synthesized by imine reaction of rhodamine 6G and 7-tert-butyl-1,3-dimethylpyrene-5,9-biscarbaldehyde. The synthesized compounds were confirmed by FT-IR, NMR, FAB-MS, UV-Vis, Fluorescence spectrum.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-911

발표분야: 유기화학

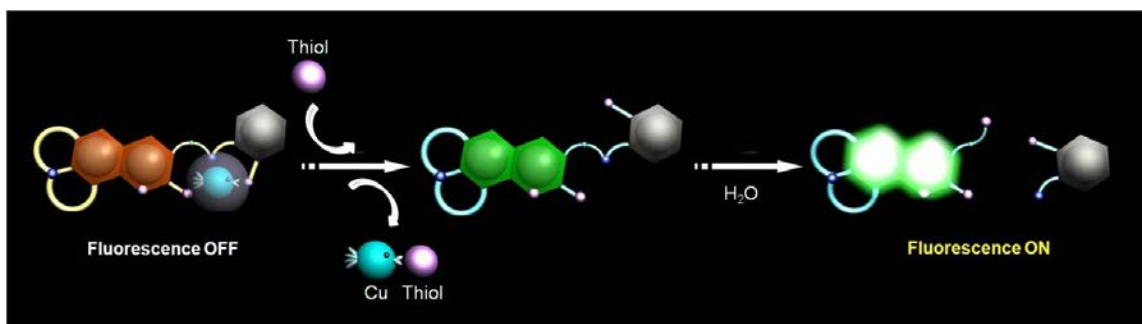
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Coumarin-Cu(II) ensemble-based thiol chemodosimeter

정효성 김수연 동방선 김태영 김종승

고려대 화학과

The new iminocoumarin-Cu(II) ensemble based chemodosimeter 1-Cu(II) selectively reacts with thiols over other amino acids at pH 7.4 under aqueous conditions. 'Off-On' fluorescence change of 1-Cu(II) is seen by addition of thiols which induces decomplexation of Cu(II) ion from non-fluorescent 1, followed by hydrolytic cleavage of the resulted Schiff base to give a strongly fluorescent coumarinaldehyde. From the confocal microscopy study, 1-Cu(II) showed marked fluorescence enhancement for thiols in HepG2 cells. It is thus the contention of the authors that this novel finding would be an important guideline in designing reaction-based fluorescent turn-on sensors for the biologically relevant thiols.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-912

발표분야: 유기화학

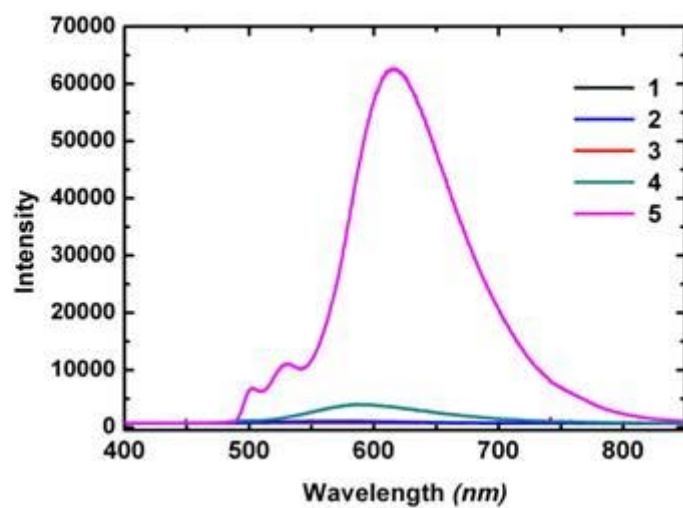
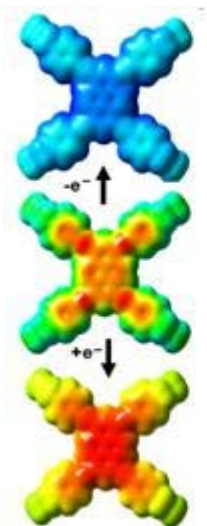
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient Electrogenenerated Chemiluminescence from New $\pi$ -Extended Pyrene Derivative

이연옥 이윤학<sup>1</sup> 양정호 김종승

고려대 화학과 <sup>1</sup>세종대 화학과

Photophysical, electrochemical, and ECL properties of pyrene derivatives (1-5) bearing (prophyphenyl)ethynyl unit were investigated. With increasing the conjugation length, absorption bands of the compounds show a gradual bathochromic shift in order of  $1 < 2 < 3 < 4 < 5$  and enhanced fluorescence quantum yield. From NMR and HOMO/LUMO orbital analysis, compound 5 was found to give the most optimized  $\pi$ -electron delocalization among five compounds tested. It was also supported by the redox reversibilities from cyclic voltametry and DFT calculations such as spin density distribution for cation/anion radicals, non-adiabatic reduction potential for cation radical, and vertical detachment energy for anion radicals. As a result, it is noted that the redox reversibilities depend on to the extent of conjugation of the pyrene compound. The ECL excimer emission remarkably enhances in order of  $1 < 2 < 3 < 4 < 5$ .



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-913

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A practical and high-yielding one-pot synthesis of 4-acyl-1,2,3-triazoles via TIPS-protected ynones

김수민 김상희

서울대 약학대학/약학과

1-substituted 4-acyl-1H-1,2,3-triazoles exhibit various interesting biological activities, and thus may serve as a novel structural scaffold for drug development. Herein, we developed an improved and convenient one-pot process for the synthesis of 1-substituted 4-acyl-1,2,3-triazoles. The first step of one-pot process was the Sonogashira cross-coupling of acid chlorides with triisopropylsilyl (TIPS)-acetylene to generate TIPS-protected ynones. The second and third steps were the in situ AgF-mediated desilylation to give terminal ynones and subsequent Cu-catalyzed Huisgen cycloaddition. We employed TIPS protecting group instead of the previously applied TMS group. The increased chemical stability of bulky TIPS-protected ynones allowed high-yielding one-pot process. The TIPS protected ynones could be desilylated and reacted with azides by exposure to a mixture of AgF/CuI under mild conditions. This one-pot process can be applied to various substrates and should be of general utility for the synthesis of a wide range of 1-substituted 4-acyl-1H-1,2,3-triazoles

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-914

발표분야: 유기화학

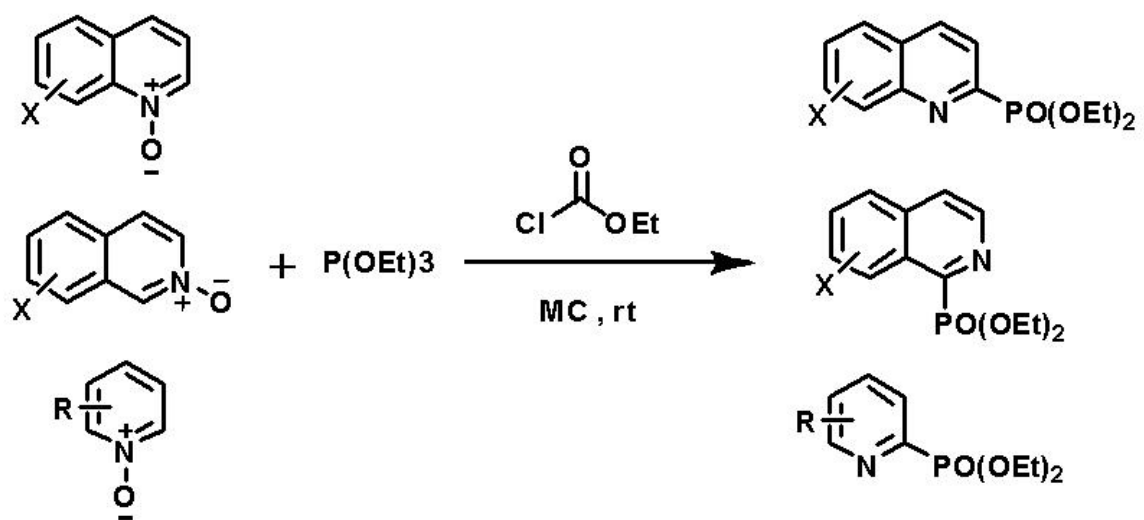
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Reductive phosphorylation of Pyridine, Quinoline or Isoquinoline N-oxide with triethyl phosphite

이상진 윤철민<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

N-oxide of nitrogen containing heteroaromatics such as pyridine, quinoline and isoquinoline undergo the reductive phosphorylation using a protocol of triethyl phosphite and ethylchloroformate at rt to give the corresponding ethyl ester of heteroaromatic phosphonic acid.



X = 3-methyl, 6-methyl, 7-methyl, 6-methoxy, 6-nitro, 6-chloro

R = 3-methyl, 4-phenyl





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-915

발표분야: 유기화학

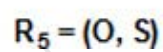
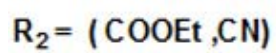
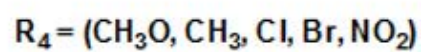
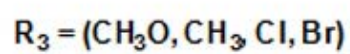
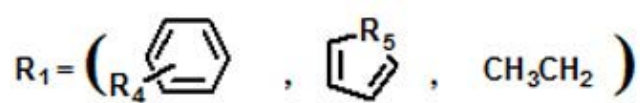
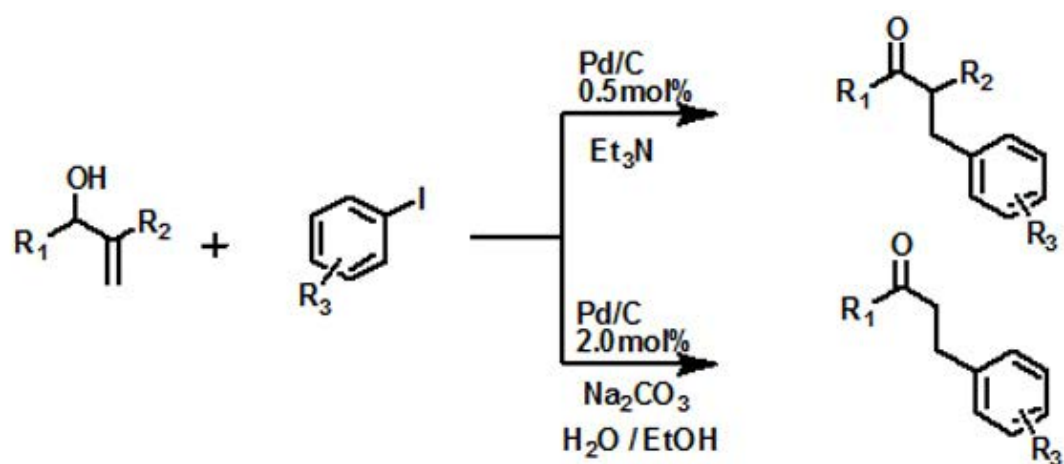
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Pd/C catalyzed Heck reaction of Baylis-Hillman adduct with iodobenzenes**

**김현수 윤철민<sup>1</sup>**

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

Morita-Baylis-Hillman adducts was coupled with a variety of iodobenzene under neat conditions or aqueous condition using Pd/C as a catalys to give corresponding products in good to excellent yields. The reactions under aqueous condtion (water and Ethanol 1:1) gave the decarboxylated Heck products and the reaction under neat condition gave coupling products,  $\beta$ -ketoesters. These reactions are simple, selective, environmentally benign and economical.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-916

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of a Zinc Complex from Quinaldic Acid and 8-Hydroxyquinoline for OLED

임영훈 김익환 이범종<sup>1</sup>

인제대 화학과 <sup>1</sup>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. Metal-chelate materials based on polycyclic aromatic ligands are attractive for tuning emission colors. The metal-chelate materials emit various luminescence colors depending on the molecular structure. In this work, quinaldic acid (QA) and 8-hydroxyquinoline (HQ) were employed as organic ligands and the corresponding zinc complex (Zn(HQA)) was synthesized. The structure of Zn(HQA) was determined by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, FT-IR, UV-Vis and XPS. The maximum UV-vis peak of Zn(HQA) was observed at 270nm. This compound shows the strong-yellow emission under excitation by UV lamp of 365nm. The photoluminescence (PL) and electroluminescence (EL) properties of Zn(HQA) will be discussed.

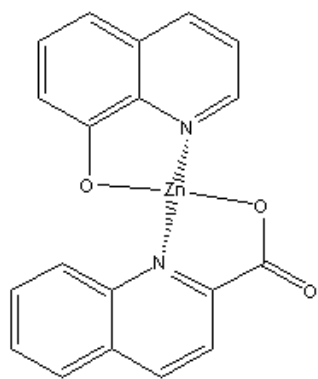


Fig 1. Synthesis of Zn(HQA)

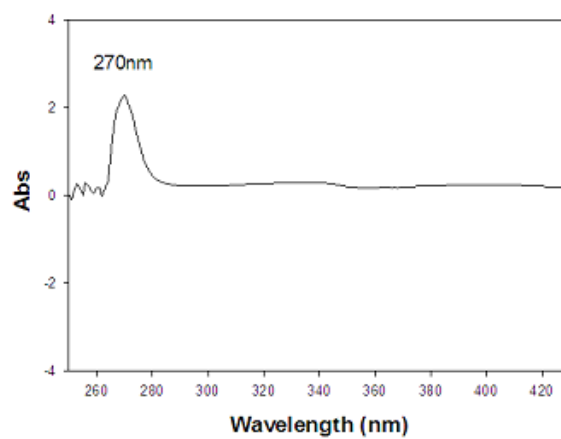


Fig 2. UV-vis spectrum of Zn(HQA) in DMF



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-917

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Copper(I)-catalyzed Azide-Alkyne Cycloaddition in a Cell Lysate

김태우 임춘우 Le Thi Hoa

경희대 동서의학대학원

Even though copper(I)-catalyzed azide-alkyne cycloaddition (described as “Click reaction” in this abstract) is thought as a reliable and efficient reaction, the click efficiency and bioorthogonality in a complex cell lysate context is still in a debate. To answer the question, we set up two Click monitoring systems: fluorescein-based FDA HPLC analysis and fluorogenic fluorescence microplate reading. Using these methods, we systematically tested the influence of Click reaction parameters on the Click efficiency:  $[Cu^+]$ ,  $[NaAsc]$ ,  $[Cu^+]/[NaAsc]$ , copper ligand,  $Cu^+/ligand$  ratio, buffer, reaction time etc. The reaction progress was real-time monitored by fluorogenic Wang’s azide and the reaction product was quantitatively analyzed by FDA HPLC. Unexpectedly, we observed that the Click reactions in cell lysate were not completely gone in many cases. That kind of observation implies that we should carefully optimize the cell-lysate Click condition.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-918

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of a Hybrid Zinc Complex from 3H-[1,2,3]triazolo[4,5-b]pyridin-3-ol and 8-Hydroxyquinoline for OLED

TRINH DAC HOANH 임영훈 이범종<sup>1</sup>

인제대 화학과 <sup>1</sup>인제대 의생명화학과

Organic light-emitting diodes (OLEDs) are believed to be the next-generation flat panel displays due to low driving voltage, high contrast, ease of fabrication, wide viewing angle and low cost. In this field, the development of novel luminescent organic/organometallic compounds is key to enhance the performance of organic and polymeric light-emitting devices. Since the first OLEDs with Zn complexes were reported in 1993, synthesis of novel zinc complexes as active materials for OLEDs have focused on improving electron mobility or producing a blue shift or red shift emission compared to Znq2. In this work, we synthesized a hybrid zinc complex of 3H-[1,2,3]triazolo[4,5-b]pyridin-3-ol (TP) and 8-hydroxyquinoline (H) ligands, Zn (TPH). The structure of Zn (TPH) was determined by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, FT-IR, UV-Vis, XPS and elemental analysis. Zn (TPH) shows a yellow emission under excitation by UV lamp of 365 nm. The photoluminescence and electroluminescence (EL) properties will be discussed. References [1] Y.

Hamada, T. Sano, M. Fujita, T. Fujii, Y. Nishio, K. Shibata, *Jpn.J. Appl. Phys.* 32 (1993) L514[2] A.  
Kraft, A.C. Grimsdale, A.B. Holmes, *Angew. Chem. Int. Ed.* 37 (1998) 402.

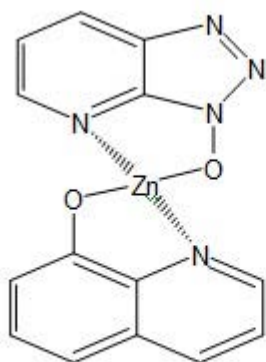


Fig. 1. Chemical structure of Zn (TPH)



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-919

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**The first intramolecular Fischer indolization and its combination with  
aromatic Claisen rearrangement for the synthesis of tricyclic  
benzo[cd]indole**

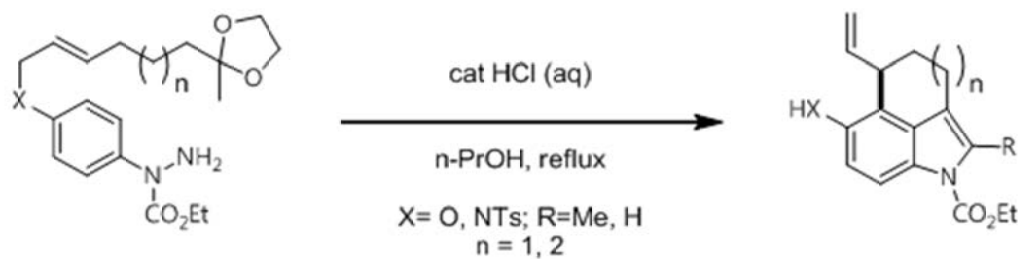
**박준 박인걸 조천규**

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. In addition, 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.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-920

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The total synthesis of ( $\pm$ )-lycorine and ( $\pm$ )- $\alpha$ -lycorane

정용근 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 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 ( $\pm$ )-lycorine and ( $\pm$ )- $\alpha$ -lycorane.

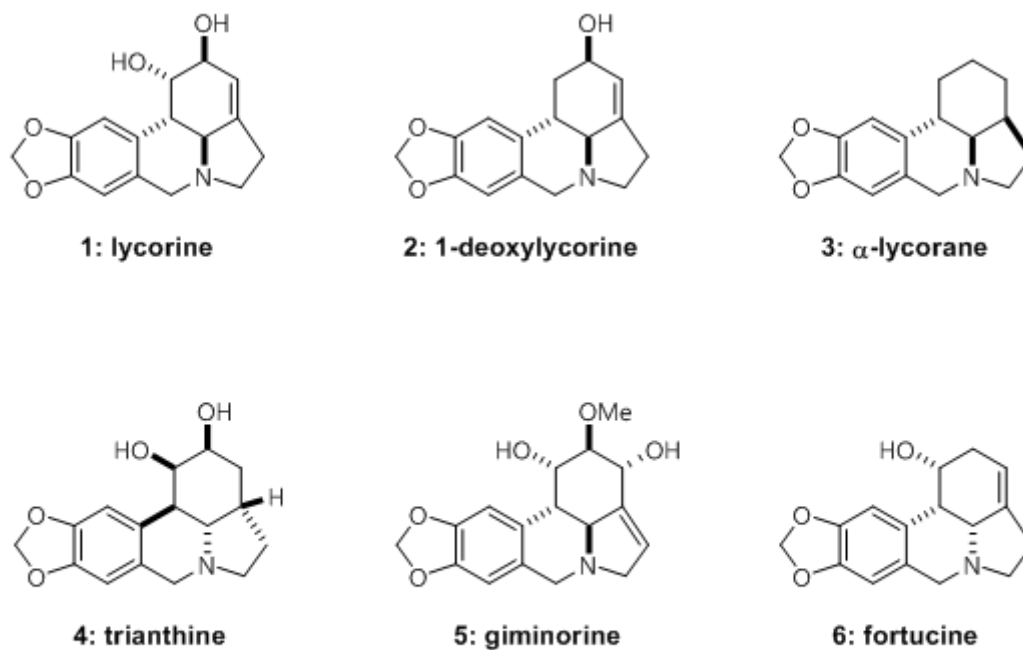


Figure 1. pyrrolo[de]phenanthridine-type natural alkaloids.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-921

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

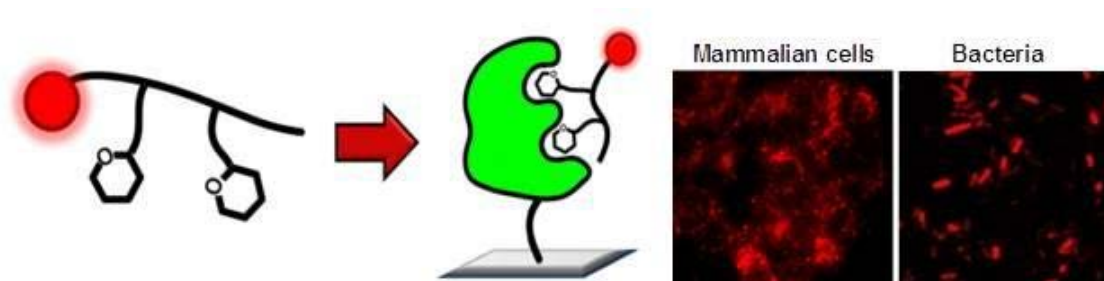
**An efficient solidphase synthesis of glycopeptide with various valences  
and different spatial arrangements of the sugar and analysis of density  
dependent binding of glycan**

**배재영 신인재**

연세대 화학과

Recognition of glycans present in the form of glycoconjugates (e.g. glycoproteins, glycosphingolipids, proteoglycans) in cells by proteins is a crucial biological event that is implicated in various physiological and pathological processes. Thus, understanding the role of glycan-mediated recognition events and blocking glycan-protein interactions associated with diseases, such as inflammation, cancer and pathogen infection, are of great importance for biological research and therapeutic applications. Typically, carbohydrate-binding proteins (lectins) interact with monovalent sugars with weak binding affinity (millimolar range) and poor selectivity. A facile and efficient solidphase synthesis of linear peptide-based glycoclusters with various valences and different spatial arrangements of the sugar ligands is described. Lectin binding properties of the glycoclusters were initially examined by using microarrays immobilized by various lectins. These glycoclusters were then employed to detect the cell-surface carbohydrate-

binding proteins in bacteria. Finally, the uptake of glycoclusters by mammalian cells through receptormediated endocytosis was evaluated. The results, obtained from the in vitro and in vivo studies, indicate that the binding affinities toward immobilized and cell-surface proteins are highly dependent on the valence and spatial arrangements of the sugar ligands in glycoclusters.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-922

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and light-controlled cation detection of rhodamine derivative with spiropyran unit

신은주 하종운<sup>1</sup>

순천대 화학과 <sup>1</sup>순천대 기초의 화학부

The design and synthesis of artificial receptors for sensing and recognition of heavy transition-metal ions have received considerable attention because these types of metal ions can produce diverse effects for health of human and other living organisms and environments. Spirolactam derivatives of rhodamine dyes are excellent sensing systems because the spirolactam ring-opening process by the addition of metal cation leads to a vivid color change enabling detection with the naked eye and a turn-on fluorescence change. Spiropyran(SP), nonpolar UV-absorbing form, is well-known photochromic compound accomplishing reversible molecular structural changes to merocyanine(MC), polar VIS-absorbing form, by the photochemical ring opening on UV irradiation. In turn, MC is reversed to SP by ring closure thermally or on irradiation of visible light. Reversible photochromic SP-MC transformation is one of subjects of active research on optical memory and switch, on the basis of significant difference in polarity, excited state energy, or molecular geometry between two forms. Spiropyran itself is chemosensor for CN-

anion. Incorporating photochromic molecules into chemosensor molecules might lead to a variety of light controlled ion detection systems. In this study, a rhodamine derivative with spiropyran unit was prepared and their light-controlled cation detection was investigated using absorption and fluorescence spectroscopy.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-923

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and photochromic reaction of Spiropyran-PAMAM dendron

신은주 허대영<sup>1</sup>

순천대 화학과 <sup>1</sup>순천대 기초의화학부

Since dendrimers are first envisaged by Flory in 1941 and first synthesized by Newkome and Tomalia, they have attracted much attention because of their fascinating structure and unique properties. Dendrimers show the most appealing characteristics such as size monodisperse, globular macrocyclic architecture, ample interior voids, and peripheral functional density, pH-dependent contraction and swelling, amphiphilicity, thermal stability, flexibility, low viscosity, high biocompatibility. Consequently, dendrimers have inspired active research activities in material science, sensors, nanoreactors, green catalyst supports, biomaterials, and drug delivery systems. Spiropyran(SP), nonpolar UV-absorbing form, is well-known photochromic compound accomplishing reversible molecular structural changes to merocyanine(MC), polar VIS-absorbing form, by the photochemical ring opening on UV irradiation. In turn, MC is reversed to SP by ring closure thermally or on irradiation of visible light. Reversible photochromic SP-MC transformation is one of subjects of active research on optical memory and switch,



on the basis of significant difference in polarity, excited state energy, or molecular geometry between two forms. Incorporating photochromic molecules into PAMAM dendron leads to a variety of photoresponsive systems, the properties of which can be manipulated by light. In this study, porphyrin-PAMAM dendron was prepared and their reversible photochromic reaction was investigated using absorption spectroscopy.



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발표분야: 유기화학

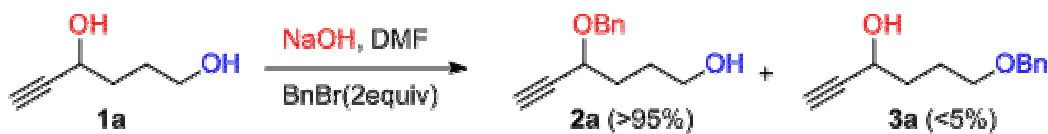
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemoselective benzylation of propargylic alcohols in the presence of various hydroxyl groups

이지호 오창호

한양대 화학과

Selective -OH protection has long been interested in synthetic organic chemists. We have observed highly selective benzylation of propargylic alcohols in the presence of the other hydroxyl groups under very usual conditions: benzyl bromide and sodium hydroxide in DMF at room temperature. This would have a high synthetic utility in selective protection of the hydroxyl group of propargylic position among various hydroxyl groups in complex molecule syntheses.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Bridging of two chromophores for enhanced performance of DSSC**

이상희 김동희 신정훈 김가영 유수창 최규석

군산대 화학과

Appropriate bridging of two monoanchoring dye molecules can give several positive effects on photovoltaic performance. Dianchoring mode of bridging dye caused strong binding to TiO<sub>2</sub> which not only increased the amount of adsorbed dye but also pushed the dye molecule to assume a rigid non planar conformation, thereby minimizing aggregation. Our results suggest that there is a room for the structural optimization by the appropriate bridging of the dye molecules.

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발표코드: ORGN.P-926

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Reactions of Tetrazole-5-thiones and 5-Amino-1,2,3,4-thiatriazoles

송대웅 박수용 이찬규 박태협 경영수

강릉원주대 화학신소재학과

Tetrazole-5-thiones and 5-amino-1,2,3,4-thiatriazoles were selectively prepared from the reaction of organic isothiocyanates and azide. We synthesized tetrazole-5-thiones and 1,4-disubstituted tetrazole-thiones from 5-aminothiatriazoles. Various nucleophiles were added selectively to N- or S-addition product of tetrazole ring of tetrazole-5-thiones depending on the character of the nucleophiles. In, addition, the structure of tetrazole-5-thione and 5-amino-1,2,3,4-thiatriazole were determined by X-ray crystallography.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Polymer-supported Electron-rich Oxime Palladacycle for Suzuki Reaction and Addition Reactions

조흥준 공새롬 박성준 이윤식

서울대 화학생물공학부

Previously, we reported stable and electron-rich oxime palladacycles by introducing electron donating groups on polymer supported oxime ligand. The catalyst showed potent catalytic activity and reusability in Suzuki reaction. For further development, the catalyst was evaluated by comparing the reaction rates and turn of numbers (TONs) to those of others. In Suzuki reaction, the catalysts performed well and gave high yields and TONs even though with deactivated aryl halides without severe leaching of Pd. Furthermore, the polymer supported electron-rich oxime palladacycle was very effective in addition reaction of phenylboronic acid to  $\alpha,\beta$ -unsaturated ketones,  $\alpha$ -ketoesters.

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발표분야: 유기화학

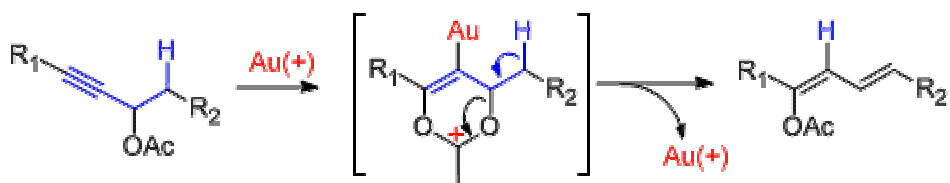
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Gold-catalyzed migration of propargylic acetates to the 1,3-dienoacetates

오부근 박종률 오창호

한양대 화학과

Propargylic acetates and carboxylates have been isomerized to the corresponding 1,3-dienocarboxylates under gold(I)-Ag(I) cocatalysis in very high yields. Depending on Ag(I) sources, some dienoacetates were in situ hydrolyzed to the corresponding  $\alpha\beta$ -unsaturated ketones.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**C-N bond rotatonal energy barrier of 1,3,5-triazine-2,4,6-triyl tris  
(dibutyl carbamo di thioate) and 1,3,5-triazine-2,4,6-triyl  
tris(dibenzylcarbamodithioate)**

이신호 김영준

충남대 화학과

우리는 마찰저감제로 사용할 수 있는 1,3,5-triazine-2,4,6-triyl tris(dibutylcarbamodithioate)와 1,3,5-triazine-2,4,6-triyl tris(dibenzylcarbamodithioate)을 합성하여 thiocarbamate 의 C-N bond rotation energy 를 Dynamic NMR (DNMR)로써 알아보았다. 화합물의 합성은 base 와 dithiocarbamate 3eq 사용하여 THF 용매 하에 합성하였다. 합성한 화합물은 X-Ray Diffraction(XRD)과 MALDI 를 통해 characterization 하였다. Dithiocarbamate 의 C-N 결합 회전에너지 측정은 Nuclear Magnetic Resonance (NMR)로 실험하여 NMR data 를 얻어 coalescence temperature 를 구하고 line shape analysis 로 약  $\Delta G = 18\text{KJ/mol}$  의 값을 얻을 수 있었다.

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발표코드: ORGN.P-930

발표분야: 유기화학

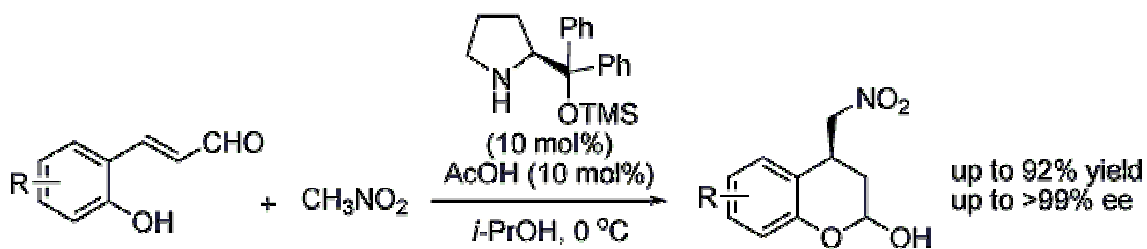
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Asymmetric Organocatalytic Michael Addition-Cyclization Cascade Reaction of Nitroalkanes with o-Hydroxycinnamaldehyde

김신애 김성곤

경기대 화학과

A catalytic enantioselective Michael addition-cyclization reaction of nitroalkanes with o-hydroxycinnamaldehydes has been established using a diphenylprolinol TMS ether as an organocatalyst. The reaction afforded the corresponding 4-substituted chroman-2-ols in excellent yields with high levels of enantioselectivities (95 - >99% ee).





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발표분야: 유기화학

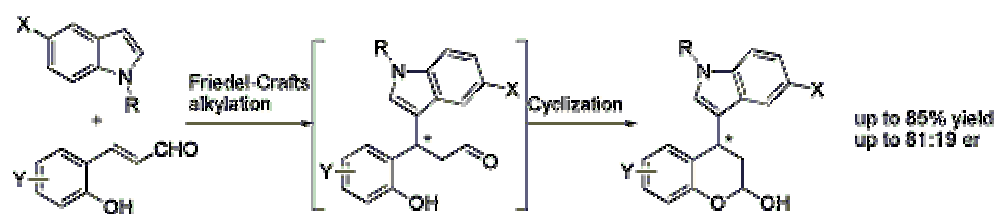
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Asymmetric Organocatalytic Friedel-Crafts Alkylation-Cyclization Cascade Reaction of Indoles with o-Hydroxyaromatic $\alpha,\beta$ -Unsaturated Aldehydes

권성혁 김성곤<sup>1</sup>

경기대 자연과학대학 화학과 <sup>1</sup>경기대 화학과

An asymmetric organocatalytic Friedel-Craft alkylation-cyclization cascade reaction of indoles with o-hydroxyaromatic  $\alpha,\beta$ -unsaturated aldehydes was developed to produce chiral 4-substituted chroman-2-ols in moderate to good yields with up to 81:19 er. A variety of chroman derivatives can be readily obtained through the subsequent transformation of these products having the biologically useful molecular scaffolds of indole and chroman.



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발표분야: 유기화학

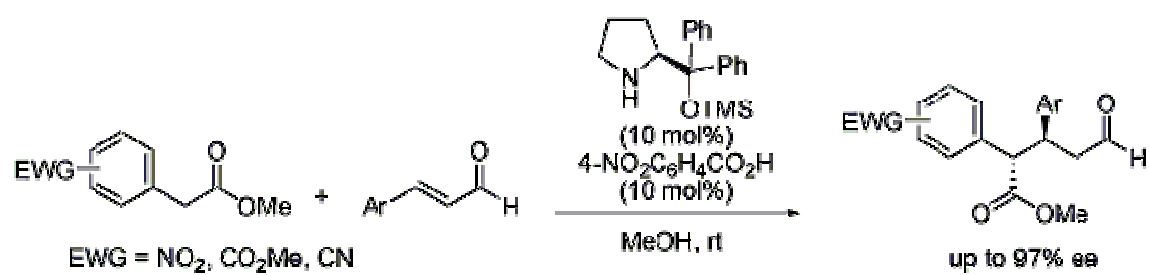
발표종류: 포스터, 발표일시: 수 18:00~21:00

**Enantioselective organocatalytic Michael addition of 2-arylacetates  
and 2-arylacetonitriles having an electron-withdrawing group to  $\alpha,\beta$ -  
unsaturated aldehydes**

서승우 김성곤

경기대 화학과

The asymmetric organocatalytic Michael addition reaction of 2-arylacetates and 2-arylacetonitriles having an electron-withdrawing group to  $\alpha,\beta$ -unsaturated aldehydes has been established using diphenylprolinol trimethylsilyl (TMS) ether as organocatalyst. The 2-arylacetates and 2-arylacetonitriles having NO<sub>2</sub>-, CO<sub>2</sub>Me-, and CN-functional groups on the aromatic ring can be used in this reaction. The desired products were obtained with good to excellent yields and high enantioselectivities (up to 97% ee).



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **An efficient synthesis of LipidGreen via microwave assisted selective allylation**

**HAUSHABHAU S PAGIRE 안진희<sup>1</sup>**

과학기술연합대학원대 의약 및 약품화학<sup>1</sup> 한국화학연구원 대사성질환연구팀

We previously developed a new lipid imaging probe, LipidGreen, which stained lipid droplet in 3T3L1 cell lines and zebrafish fat deposits. In this presentation, we report an efficient synthesis of LipidGreen via microwave assisted selective allylation

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발표분야: 유기화학

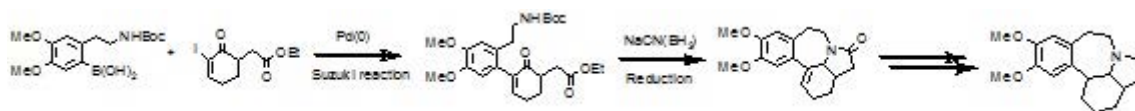
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of polycyclic Alkaloids using Suzuki reaction and reduction

김희동 김건철

충남대 화학과

Alkaloid 7-membered ring using transition metal cyclization of the structure was studied. In this study, cyclization followed by Suzuki reaction and reduction were confirmed by previous studies. As an extension of this methodology, the synthesis of polycyclic alkaloid hexahydroapoerysopine was achieved through an efficient synthetic route. And a structure similar to natural products of (+)- $\gamma$ -lycorane may be synthesized.



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발표코드: ORGN.P-935

발표분야: 유기화학

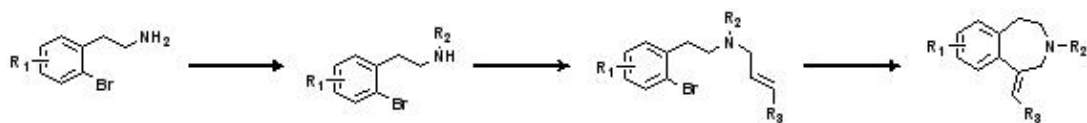
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of N-Heterocycles Using Heck reaction

민지영 김건철

충남대 화학과

Benzazepines and their derivatives are basis of framework of natural product and have biological activity. There are lots of effort to synthesis of benzazepines and their derivatives. Because they have unique structure consisting of 7-membered ring connected with benzene ring. Radical reaction, Heck reaction and intramolecular hydroarylation after A3-coupling are already known methods of synthesizing benzazepine. In this study benzazepine derivatives were synthesized by the intramolecular Heck Reaction. By introducing diverse allyl groups on nitrogen electronic and steric effects of the reaction products were investigated.



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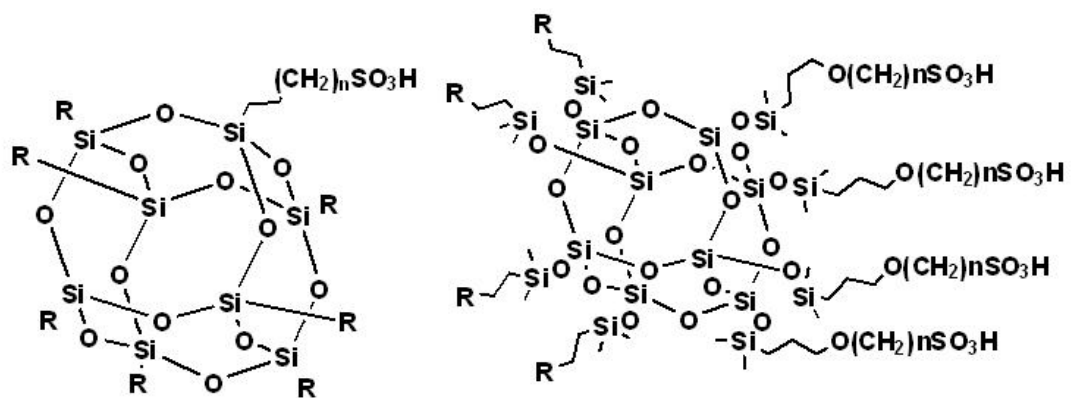
## Organic-inorganic Hybrid Composites of POSS and Sulfonic acid derivatives

B.Prem kumar Vijay kumar 최경민 신동수

창원대 화학과

Organo-composites of polyhedral oligomeric silsesquioxanes (POSS) and sulfonic acid derivatives and various alkyl groups can be synthesized by direct hydrosilylation of allyl alcohol alkenes with octakis(dimethylsiloxy)octasilsesquioxane,  $(\text{HSiMe}_2\text{O})_8\text{Si}_8\text{O}_{12}$  (Q8M8H), in presence of platinum divinyltetramethyldisiloxane [Pt(dvs)] as a catalyst. The hydrophilic sulfonic acid ( $-\text{SO}_3\text{H}$ ) group has been assembled in the POSS cages to provide ion conduction, while the hydrophobic portion (alkyl groups) has been incorporated in POSS cages to develop amphiphilic polymers for drug/gene delivery and formation of hydro gels.





R = Alkyl Chain, perfluoro alkyl chain

n = 1 to etc



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발표분야: 유기화학

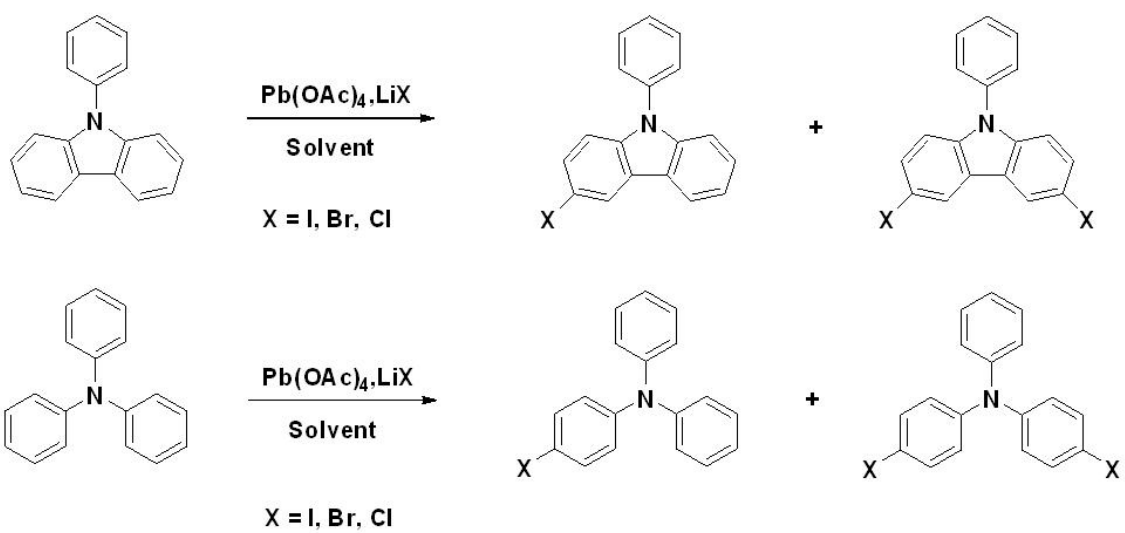
발표종류: 포스터, 발표일시: 수 18:00~21:00

## One-pot halogenation of aromatic compound having nitrogen using $\text{Pb}(\text{OAc})_4$

최경민 신동수

창원대 화학과

We have introduce a new and convenient halogenating agent for the direct halogenation of aromatic compound having nitrogen using  $\text{Pb}(\text{OAc})_4$ . we demonstrate to produce selectively the corresponding various halogenated aromatic compound.



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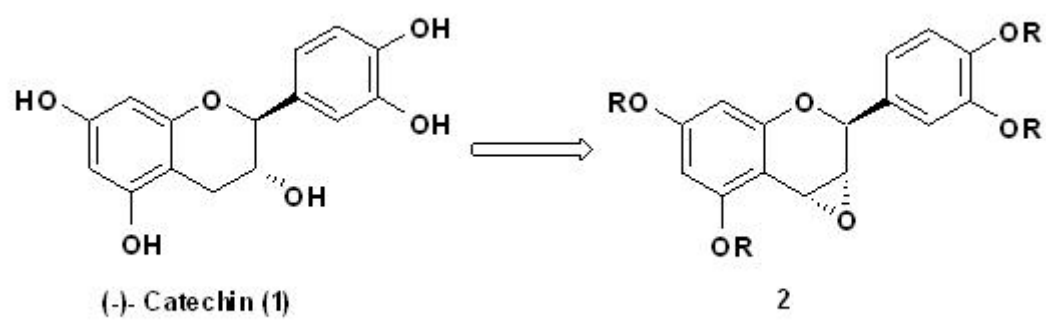
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Total synthesis of (-)-Catechin

kumar deepak B.Prem kumar 신동수

창원대 화학과

(?)-Catachin found to possess a wide range of biological activities includes anti-oxidant, anti-proliferative and anti-HIV etc. As a part of our research to design, synthesize and develop natural herbicides, we have initiated a program for the synthesis of (?)-Catachin and its analogs involving Jacobsen Asymmetric epoxidation as key step.



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발표분야: 유기화학

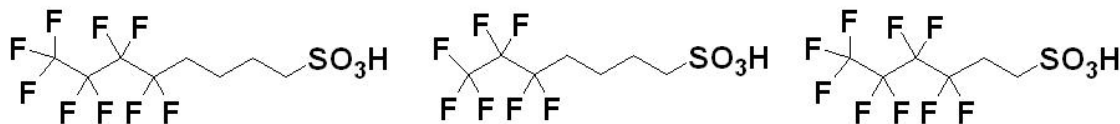
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Alternatives for PFOS (perfluorooctanesulfonic acid)

Vijay kumar B.Prem kumar 최경민 신동수

창원대 화학과

World has been using many bioaccumulative perfluorosurfactants as stain repellents over the decades. To overcome some draw backs of the well known perfluorosurfactant perfluorooctanesulfonic acid (PFOS), we initiated the synthesis of perfluorinated and partially fluorinated sulfonic acid derivatives involving radical conjugate addition of perfluoro/partially fluoro alkyl halides on vinylsulfonates.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of Electrospun Non-woven Mat of Dibutryl chitin/Poly(lactic acid) Blend on Wound Healing in Hairless mice

황희민 이덕희<sup>1</sup> 채규윤<sup>2</sup>

원광대 생명나노화학<sup>1</sup> 원광대 생명나노화학과<sup>2</sup> 원광대 화학과

The aim of this study was to examine the proliferative ability of dibutryl chitin (DBC) on scratch wound in HaCaT keratinocytes and to evaluate the effect of nanoporous non-woven mat (DBCNFM) on skin wound healing in hairless mice by use of advantages of DBCNFM, such as high porosity and high surface area to volume. The cell spreading activity of DBC was verified through a cell spreading assay in scratched human HaCaT keratinocytes. Scratch wound experiments showed that DBC notably accelerates the spreading rate of HaCaT keratinocytes in dose dependent. The molecular aspects of the healing process were also investigated by hematoxylin & eosin staining of the healed skin, displaying the degrees of reepithelialization and immunostaining on extracellular matrix synthesis and remodeling of the skin. Topical application of DBCNFM significantly reduced skin wound rank scores and increased the skin remodeling of the wounded hairless mice in dose dependent. Furthermore, DCENFM notably increased the expression of the type 1 collagen and filaggrin. These results demonstrate that DBC efficiently

accelerates the proliferation of HaCaT keratinocytes and DBCNFM notably increases extracellular matrix synthesis on remodeling of the skin, and these materials are a good candidate for further evaluation as an effective wound healing agent.





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발표분야: 유기화학

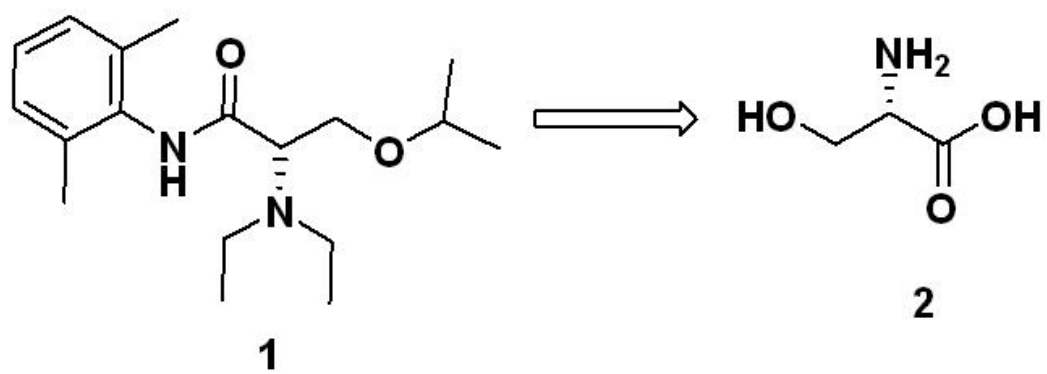
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Derivatives for $\alpha$ -Amino Acid Synthesis

정해동 신동수

창원대 화학과

These derivatives for  $\alpha$ -Amino Acid as a wide range of biological activity which were synthesized by D-Serine using selective protection and deprotection of functional groups to obtained a new amino acid derivatives. These derivatives show an antiepileptic drug.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of porous carbon material through hydrogen-bonding interaction and its application on ethylene adsorption

mayani suranjana mayani vishal jitendra bhal 이준영 김상욱

동국대 신소재화학과

The demand of porous carbon material has increased considerably in last decade due to their extensive usage in industrial adsorption purpose, gas separation, water purification and catalysis. In the present work, we have synthesized a new porous carbon material by solvent evaporation induced self assembly method (EISA) using hydroquinone/formaldehyde as a precursor which can help self assembly with template triblock copolymer PEO-PPO-PEO (F127). The template removal have resulted the porous carbon material (PCM) framework upon carbonization. We have also prepared porous carbon fibers (PCF) using kapok fibers along with hydroquinone/formaldehyde/F127 and observed its ethylene adsorption capacity. The characterization of PCM and PCF were accomplished by different physico-chemical characterization methods. The synthesized carbon materials showed excellent gas adsorption ability towards ethylene gas at room temperature as well as at 50°C.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Wet oxidation of phenol analogues using Fe/SBA-15 as catalyst

mayani suranjana mayani vishal jitendra bhal 이준영 김상욱<sup>1</sup>

동국대 신소재화학과 <sup>1</sup>동국대 나노소재화학화

The catalytic activity of Fe/SBA-15 for the oxidation of phenol analogues such as 2-chlorophenol (2-CP), 4-chlorophenol (4-CP), 2-nitrophenol (2-NP), 4-nitrophenol (4-NP) and 2,4,6-trichlorophenol (2,4,6-TCP) was investigated in an aqueous solution. Fe/SBA-15 was prepared by wet impregnation method. The heterogeneous green catalyst was calcined at 823K for 3h before catalytic run in high pressure stirred reactor under defined reaction conditions. Catalytic wet oxidation of 2-CP, 4-CP, 2-NP, 4-NP and 2,4,6-TCP was achieved 80.2, 71.2, 53.1, 62.8, 77.3 % in presence of H<sub>2</sub>O<sub>2</sub> and 85.7, 65.8, 61.9, 63.7, 78.1 % in absence of H<sub>2</sub>O<sub>2</sub>, respectively in 15-300 min. The reactions were followed pseudo first order kinetics. It is significant that the catalyst worked well without addition of external oxidant. Some of the products of oxidation were identified with GC-MS analysis and on the basis of the results, probable mechanisms for oxidation have been suggested.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-944

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of nano sized carbon gold silica composites and its potential multifunctional applications

mayani vishal jitendra bhal mayani suranjana 김상욱 고성현

동국대 신소재화학과

Pitches are thermoplastic 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 and material science. Presently, we preceded to the development of nano carbon cages (CC), carbon gold composite (CGC) and carbon gold silica (CGS) composite using template methods with nano silica ball (NSB), pyrolysis fuel oil (PFO) and 1%  $\text{HAuCl}_4$  solution. Due to their easy fabrication protocols and broad potential applications, the hybrid nanocomposites CC, CGC and CGS are choosy for specific interests. Here, CC and CGC nanocomposites commonly referred to be carbon cages and gold nanoparticles deposited into carbon cages respectively. 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 ethylene adsorption capacity and catalytic oxidation were studied with excellent selectivity and higher conversion respectively. The composites were characterized

by power X-ray diffraction (XRD), thermo-gravimetric analysis (TGA), N<sub>2</sub> adsorption-desorption isotherm, scanning electron microscopy (SEM) coupled with energy dispersive spectroscopy (EDS), transmitted electron microscope (TEM) and FT-IR.



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발표코드: ORGN.P-945

발표분야: 유기화학

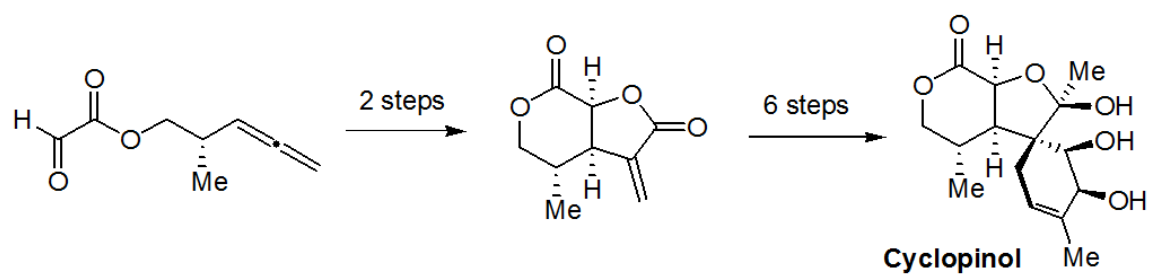
발표종류: 포스터, 발표일시: 수 18:00~21:00

## A New Cyclocarbonylation Catalyzed by Palladium Complex: Synthesis of Bicyclic Lactones

양보나 김지현 유찬모

성균관대 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of transition metals are some of the most attractive methodologies since reactions can directly construct complicate molecules from relatively simple starting materials. We would like to present herein several crucial points that have emerged from our recent investigations: 1) novel cyclization of allene-glyoxyaldehydes mediated by Pd or Ru complex to afford the bicyclic lactones; 2) synthetic studies toward an enantioselective synthesis of isocyclocalopin A.





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발표코드: ORGN.P-946

발표분야: 유기화학

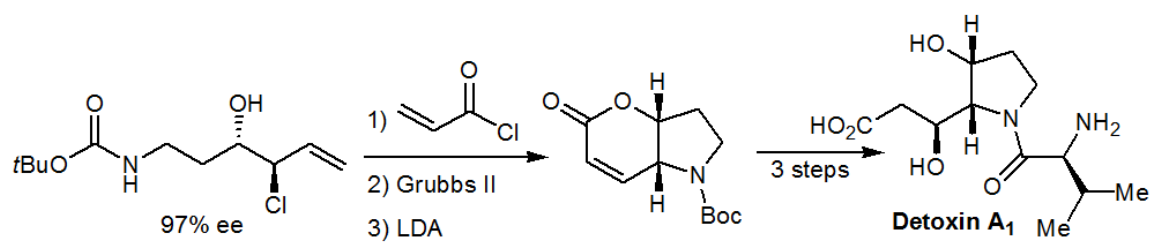
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enantio- and Diastereoselective Chloroallylboration for the Synthesis of Chlorohydrins: Synthesis of Detoxine

곽진호 김현아 유찬모

성균관대 화학과

Development of stereo-controlled consecutive processes can offer advantages over stepwise transformations by increasing chemical efficiency and saving effort due to a simple operation. Recently, we developed a new synthetic method for the synthesis of all 4 possible chlorohydrins stereoselectively. We would like to present herein several crucial points that have emerged from our recent investigations: 1) Construction of bicyclic system starting from the chlorohydrin. 2) enantio- and diastereoselective synthesis of Detoxin naturally occurring A.



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발표코드: ORGN.P-947

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Eco-friendly and efficient preparations of monomer for polyamide

고무현 김현정 신나라 김영규

서울대 화학생물공학부

TPEs (Thermoplastic Elastomers) are in the spotlight as the potential alternative materials of the natural rubber. Most of all, we are focused on polyamide type TPEs which have a wide range of applications because of their good thermal stability, and excellent chemical and hydrolytic resistance. Recently the interest in renewable polymer increased with natural resources such as vegetable oil. From this point of view, we will present eco-friendly and efficient process for synthesizing monomers of polyamide type TPEs.

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발표코드: ORGN.P-948

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Arylation of heterocycles via photoredox catalysis**

**Naeem Iqbal 조은진**

한양대 응용화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-949

발표분야: 유기화학

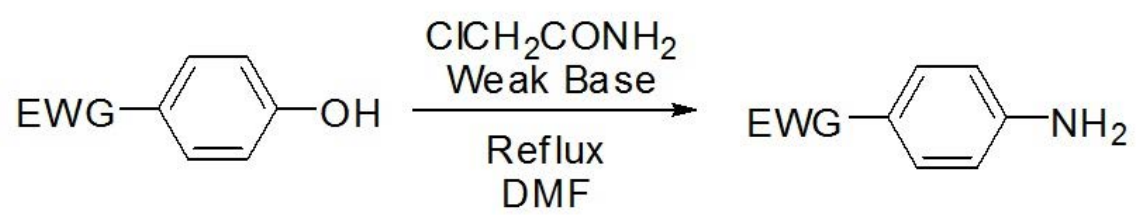
발표종류: 포스터, 발표일시: 수 18:00~21:00

## A convenient One-pot Direct Conversion of Phenols to Aniline via Smiles Rearrangement

xievongsheng 신동수 장희재<sup>1</sup> 문기철<sup>1</sup>

창원대 화학과 <sup>1</sup>창원과학고 화학연구실

A convenient one-pot direct conversion of phenols to anilines has been developed. Using our methodology, anilines can be obtained in moderate yields by a reflux reaction of electron-withdrawing substituted phenols with ClCH<sub>2</sub>CONH<sub>2</sub> and weak base in DMF via Smiles rearrangement. In this progress, the DMF solvent is easily recycled by distillation, and then the residue can be simply absorbed into the silica gel and purified directly. This method is also available for the synthesis of aminopyridine from the corresponding hydroxyl substrate.



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장소: 일산KINTEX

발표코드: ORGN.P-950

발표분야: 유기화학

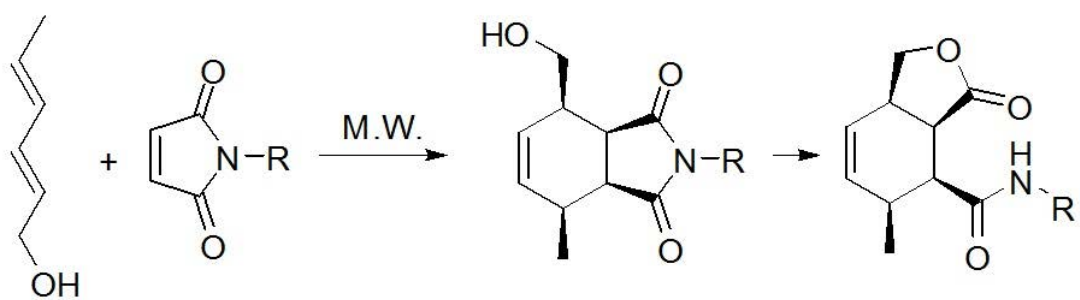
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Microwave-assisted One-pot Synthesis of (3aR, 4R, 5S,7aR)-5-methyl-3- oxooctahydroisobenzofuran-4-carboxamide

xievongsheng 신동수 장희재<sup>1</sup> 문기철<sup>1</sup>

창원대 화학과 <sup>1</sup>창원과학고 화학연구실

Using microwave irradiation, simply mixing 4-hexadien-1-ol and N-electron-withdrawing substituted maleimide together provide cis-fused bicyclic imide via intermolecular Diels-Alder reaction followed to form the titled product by intramolecular esterification. A one-pot multi-step process, which is green and convenient, can be carried out evolutionarily. Only the endo-stereoisomeric product can be observed by the investigation of <sup>1</sup>H NMR spectrum.





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장소: 일산KINTEX

발표코드: ORGN.P-951

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Rh-catalyzed acylation and intramolecular cyclization of benzamides and aldehydes: synthesis of 3-hydroxyisoindolin-1-ones**

김인수

경희대 약학과

3-Hydroxyisoindolin-1-one is an important core structure of numerous natural products and artificially synthesized bioactive molecules, such as chilenine, a natural isoindolobenzazepine alkaloid isolated from *Berberis empetrifolia*, and fumadensine, an isoquinoline from *Fumaria densiflora*. Additionally, 3-hydroxyisoindolin-1-one moieties have been found in other bioactive molecules such as a Raf kinase inhibitor, an MEK protein kinase inhibitor as well as an HIV integrase inhibitor. 3-Hydroxyisoindolin-1-ones are also useful precursors for synthesis of arylmethyleisoindolin-1-one compounds, which are important privileged structures of many biological active molecules. In addition, the products of dehydration of 3-hydroxyisoindolin-1-ones have been found to be useful intermediates in the total synthesis of isoindolobenzazepine alkaloids such as lennoxamine. Transition metal-catalyzed direct transformation of inactive C-H bonds has emerged as a powerful tool for the facile production of structurally diverse organic molecules. Since the pioneering efforts of Murai, great progress has been

made in transition metal-catalyzed C-H bond functionalization upon trapping with appropriate electrophiles or nucleophiles under oxidative or basic conditions, respectively. In particular, reactions involving the activation of C-H bonds by neighboring directing group have been extensively investigated. As results, the combination of transition metals and directing groups provides efficient conversion of C-H bonds to C-C, C-X, C-O, and C-N bonds. Although carbon-carbon bond formation reactions using unsaturated C=C or C≡C bonds as the coupling partners have been well established, the reactions of C-H bonds and C-heteroatom unsaturated bonds, (e.g., C=O and C=N bonds), remain relatively unexplored. Herein we describe a rhodium-catalyzed oxidative acylation and intramolecular cyclization of primary benzamides with aryl aldehydes via direct sp<sup>2</sup> C-H bond cleavage. In the presence of [Cp\*RhCl<sub>2</sub>]<sub>2</sub>, AgSbF<sub>6</sub>, and silver carbonate as an oxidant, primary benzamides can be effectively carbonylated to 3-Hydroxyisoindolin-1-ones in good to high yields.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-952

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Norlignan Derivatives and Inhibitory Effect of Antigen-Induced Degranulation

김인수

경희대 약학과

Norlignans are abundant in the heartwood of many coniferous trees and in some monocotyledonous plants, and possess a wide spectrum of biological activities such as anti-cancer/anti-inflammatory, anti-complement, anti-fungal activity, testosterone  $5\alpha$ -reductase inhibition, and cyclic AMP phosphodiesterase inhibition. Naturally occurring norlignan are a class of natural phenolic compounds with diphenylpentane carbon skeletons ( $C_6-C_5-C_6$ ). Hinokiresinol, the E-isomer of nyasol, is a typical example of such a norlignan. Hinokiresinol was first isolated from the heartwood of *Chamaecyparis obtuse* in 1965, and was found to display appreciable estrogen receptor binding activity and some antiparasitic activity. We recently found that nyasol and its derivatives, isolated from *Anemarrhena asphodeloides*, act as powerful inhibitors of antigen-induced degranulation, and have the potential to be useful therapies for allergic disorders such as asthma and atopic dermatitis. In view of these interesting

biological activities of norlignans, we report here the inhibitory activity of hinokiresionol derivatives including synthetic intermediates on antigen-induced degranulation.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enantioselective Synthesis of (?) -cis-Aerangis Lactone and (+)-trans-Aerangis Lactone

김인수

경희대 약학과

Lactones are important flavor and aroma constituents that are extensively used as additives in food and perfume. Many lactones exhibit interesting biological activities as attractants for pollination and seed germination stimulants. They also act as allergens, pheromones, antiseptics, and cardiogenic agents. In particular,  $\delta$ -lactones appear as a ubiquitous structural motif in a number of natural products that display a wide range of biological activity. As representative examples of  $\delta$ -lactones, cis-aerangis lactones and trans-aerangis lactones were first reported by Kaiser in 1993 as the main odoriferous components of the African moth orchids *Aerangis confusa* and *Aerangis kirkii*. Later, (?) -cis-aerangis lactone was found to be the sole stereoisomer present in the scent of living white flowering orchids (*Aerangis confusa*). All four stereoisomers were initially synthesized as a racemic mixture of cis- and trans-isomers through hydrogenation of dihydrojasmones and subsequent Baeyer-Villiger oxidation of the cyclopentanone moiety. In this paper, we present a new catalytic strategy for the asymmetric total synthesis of (?) -cis-

aerangis lactone and (+)-trans-aerangis lactone, that includes catalytic carbon-carbon bond formations, such as iridium-catalyzed diastereoselective and enantioselective carbonyl crotylation, ruthenium-catalyzed intermolecular or intramolecular metathesis reaction, and the organocatalytic Mitsunobu reaction.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-954

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

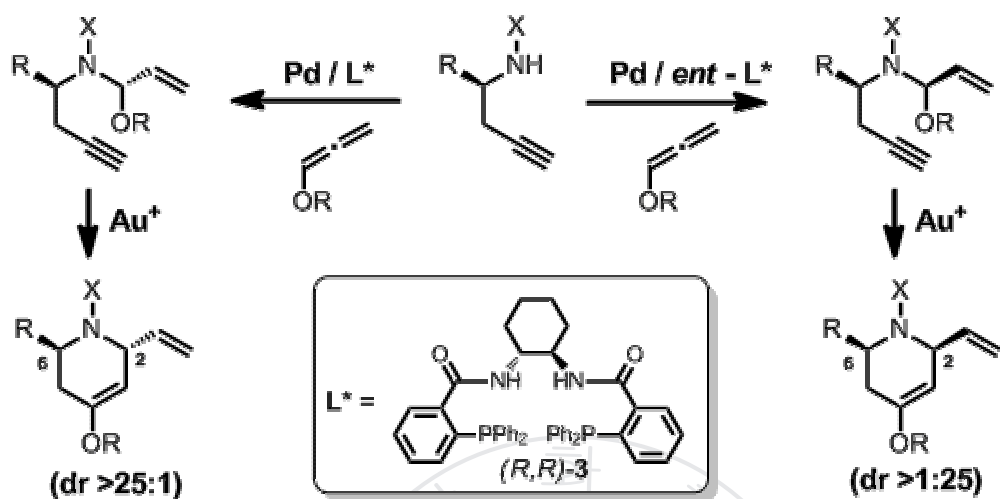
## **Stereodefined *N,O*-acetals: Pd-catalyzed Synthesis from Homopropargylic Amines and Utility in the Flexible Synthesis of 2,6-Substituted Piperidines**

**김해진**

포항공과대 화학과

The synthesis of organic compounds possessing heteroatoms substituent has been considered as a key topic in organic chemistry. In particular, *N,O*-acetals have been conceived as a precursor of the iminium ion-mediated C-C bond formation.<sup>1</sup> In most cases in this area, the stereochemical information of the *N,O*-acetal can be easily destroyed due to the instability of the *N,O*-acetals. We developed the synthesis of chemically labile *N,O*-acetals and utility for the first time.<sup>2</sup> The synthesis of stereodefined *N,O*-acetals was achieved by the Pd-catalyzed asymmetric hydroamination of alkoxyallene. Various tosyl-protected homopropargylic amines were converted into corresponding *N,O*-acetals in excellent yield with high regio- and stereoselectivity. In addition, we combined the stereodefined *N,O*-acetal with Au-catalyzed cycloisomerization.<sup>3</sup> The diastomeric *N,O*-acetals were converted into the corresponding *cis*- and *trans*-2,6-disubstituted piperidines. We expect that this unique strategy represents an important concept in

synthetic organic chemistry. Reference(1) Warriner, S. Category 4: *Compounds with Two Carbon-Heteroatom Bonds in Science of Synthesis: Houben-Weyl Methods of Molecular Transformations*; Eds.; Georg Thieme Verlag: Stuttgart; 2007; Vol 30, p 7. (2) Kim, H.; Rhee, Y. H. *J. Am. Chem. Soc.* Accepted for publication (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.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-955

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Spectroscopic Study of Donor-Acceptor Dyads Containing Diimides Connected by Aryl Spacers

김성식 M. Fujitsuka<sup>1</sup> T. Majima<sup>1</sup>

전북대 화학과 <sup>1</sup>Osaka University

Synthetic investigation of dyads containing diimides such as pyromellitic diimide and naphthalene diimide is described. Several spacers were introduced for the target molecules. Two dianhydrides such as pyromellitic dianhydride or naphthalenetetracarboxylic dianhydride were used to prepare intermediate compounds, i.e., monoimides having alkyl substituents. Two different types of reactions, which include 1:1 reaction and 1:1:1 reaction, were compared using two dianhydride and alkyl amine. N-Boc protecting group was also introduced to get intermediates as amine. Two different types of final intermediates were synthesized and compared for the target molecule. The spectroscopic investigation of the dyad were described as the preliminary study for a new electron transfer system.

일시: 2012년 4월 25~27일(수~금) 3일간

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발표코드: ORGN.P-956

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and Physical Properties of Chitosan Benzoic Acid Derivatives Using a Phosphoryl Mixed Anhydride System

정진아 이덕희 채규윤<sup>1</sup>

원광대 생명나노화학과 <sup>1</sup>원광대 화학과

Direct benzylation of the two hydroxyl groups on chitosan was achieved using phosphoryl mixed anhydride system, derived from trifluoroacetic anhydride (TFFA), benzoic acids (BAs), and phosphoric acid (PA). The reaction is operated as one pot process under mild conditions. And it does not requires neither inert atmosphere nor dry solvent. The structures of the synthesized compounds were confirmed by n.m.r and i.r spectroscopy. Solubility test on the compounds revealed that they were soluble in organic solvents such as N,N-dimethylformamide (DMF), dimethylsulfoxide (DMSO), acetone, and ethanol (EtOH). In the meantime, morphological study by a scanning electron microscorph (SEM) evidently indicated that the chitosan benzoates underwent significant structural change after the benzylation.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-957

발표분야: 유기화학

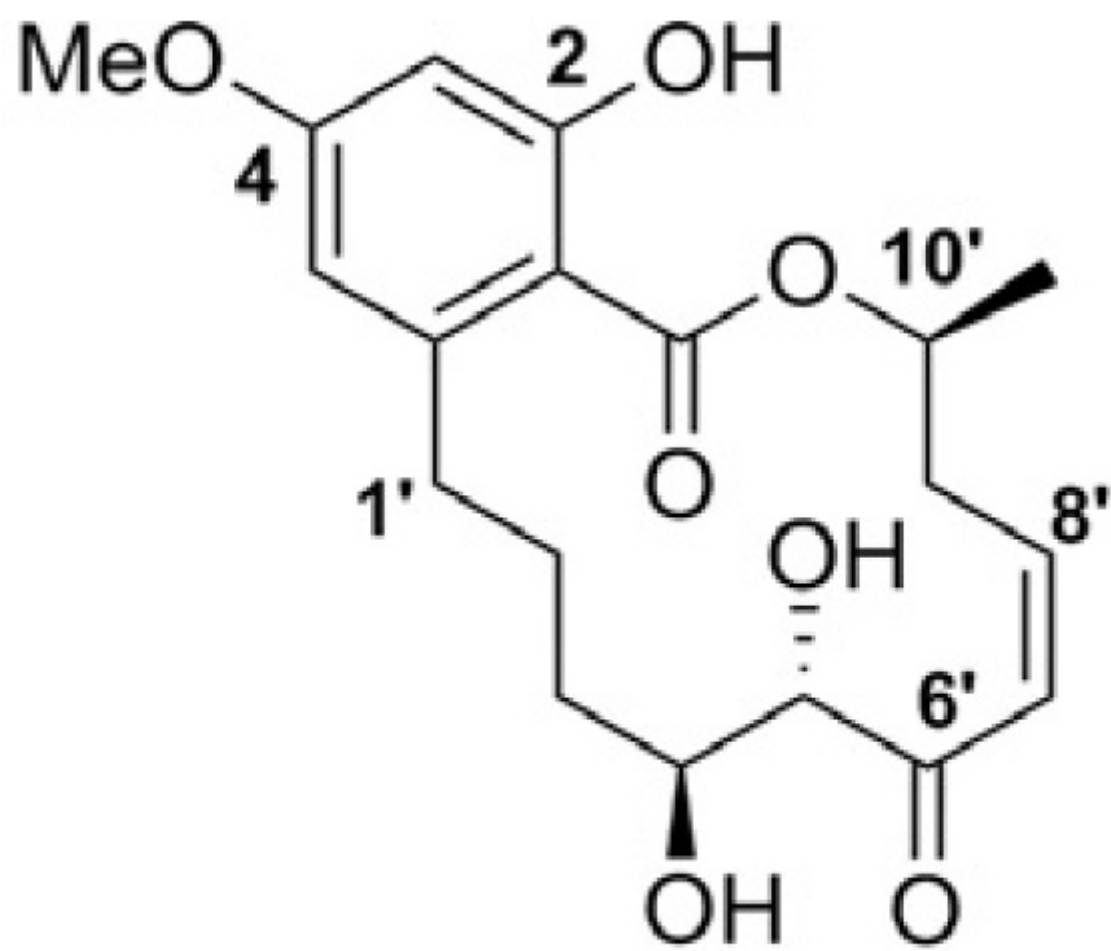
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Total synthesis of L-783277

김직녀 윤지혜 심태보<sup>1</sup> 이원구

서강대 화학과 <sup>1</sup>KIST 생체과학연구본부

Efficient and enantioselective total synthesis of L-783277, a naturally occurring resorcylic 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.



**L-783277**

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일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-958

발표분야: 유기화학

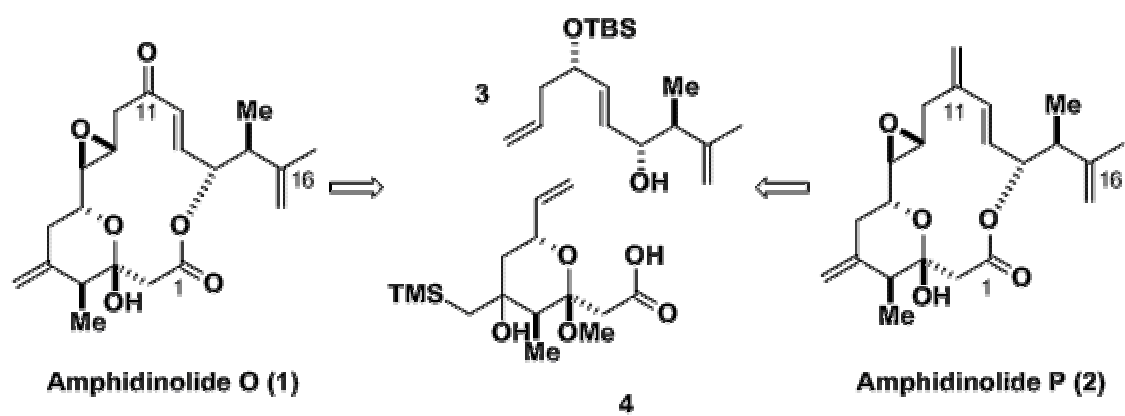
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Towards the Total Synthesis of Amphidinolide O and P: Convergent Approach

황민호 이덕형

서강대 화학과

Okinawan marine dinoflagellate *Amphidinium* sp. contains series of cytotoxic macrolides, named amphidinolide. Two novel 15-membered macrolides, amphidinolides O (1) and P (2), which contains cytotoxicity against murine lymphoma L1210 and human epidermoid carcinoma KB cells in vitro ( $IC_{50}$  values: 1, 1.7 and 3.6 mg/ml, respectively; 2, 1.6 and 5.8 mg/ml, respectively). Structures of amphidinolide O and P were related closely; 1 and 2 have seven chiral centers, epoxide, an internal double-bond, two exo-methylenes (C-5, C-16). The C-11 ketone of compound 1 is replaced by an exo-methylene group in compound 2. From the structural similarity, we planned a convergent strategy for the completion of 1 and 2 via compound 3 and 4; protected hydroxide at C-11. This strategy could be total synthesis of two natural products 1 and 2 in the same process.



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장소: 일산KINTEX

발표코드: ORGN.P-959

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Cyclization of Alkynyl Hydrogen Phosphates Catalyzed by Gold

강동진 엄다한 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 terminal 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 regioselectivity of the cyclization but also to utilize the cyclic phosphate products as coupling partners in transition-metal-catalyzed cross coupling reaction. Herein, we reported an efficient gold-catalyzed cyclization of alkynyl hydrogen phosphates. The cyclization underwent *6-endo-dig*, *6-exo-dig*, or *7-exo-*

*dig* ring closure, depending on the number of carbon atoms present ( $n=1, 2, 3$ ) between the alkyne and phosphoryl group.





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발표코드: ORGN.P-960

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthetic study of modified deoxynucleotides for DNA sequencing technology

김은선 조용서<sup>1</sup> 민선준

KIST 뇌의약연구단 <sup>1</sup>KIST 생체과학연구본부

DNA sequencing technology is a fundamental tool for biological research and medical diagnostics. In the early years, the majority of DNA sequencing has relied on some version of the Sanger sequencing method. However, over the past decade, many next generation sequencing (NGS) methods have been developed for dealing with massively parallel DNA sequencing in inexpensive cost. DNA sequencing by synthesis (SBS) using cleavable fluorophore functional groups as terminators is an efficient approach to compensate the limitations of current DNA sequencing techniques. Thus, it is very important to develop new fluorogenic dNTPs, which are applicable to commercial DNA SBS platforms such as Illumina. Herein, we report design and synthesis of new modified nucleotide analogues having a reversible terminator at the 3'-OH position. We are expecting that these new nucleotides derived from azidoether play a dual role as a fluorescent signal reporter as well as a protective group to block polymerase reaction for SBS. The fluorophore on the DNA extension products is able to determine a type of the incorporated

base and will be easily removed under DNA compatible conditions to regenerate a free 3'-OH group to reinitiate the polymerase reaction.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ORGN.P-961

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and recognition properties of I<sub>2</sub> selective chmosensor

장호 주재운 김기백 장우식 장승현

대구대 화학과

New kinds of host compounds were synthesized by pyrene and anthracene functionalized. Pyrene and anthracene have a lot of  $\pi$  electrons is known as a good fluorescent materials. In this study, we synthesized new host compounds containing pyrene , anthracene, crown ether. Binding interaction of the new host compound with metal cations were studied through absorption spectroscopy and emission spectroscopy. This complex could act as highly sensitive and selective fluorescent probe for I<sup>+</sup>.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of Biocompatible Materials for siRNA Delivery Systems



박정우 박유진 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 the most interesting siRNA delivery systems are peptide-based gene delivery systems. In general, peptide-based delivery exhibits no or low toxicity toward cells or tissues because peptides are common in our bodies and rarely induce immune responses. To overcome the obstacles of siRNA therapy, we used two types of delivery systems. One is peptide-siRNA conjugation method. In this method, various peptides are introduced to the 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.

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발표코드: ORGN.P-963

발표분야: 유기화학

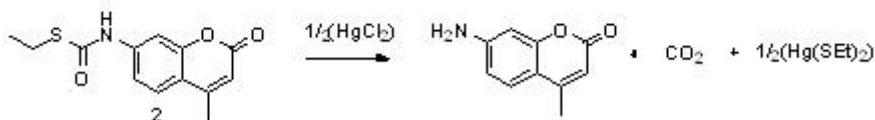
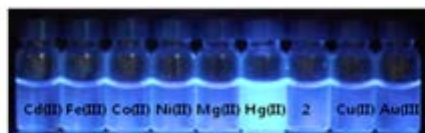
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Hg(II) Selective Fluorescent Indicator: One Step Synthesis

김슬비 조동규

인하대 화학과

Fluorescent indicator 2 was synthesized by a single step reaction. The indicator underwent a Hg(II) specific reaction (hydrolysis- decarboxylation sequence) in the presence of Hg(II), which was verified using LC-MS and nuclear magnetic resonance techniques.



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발표분야: 유기화학

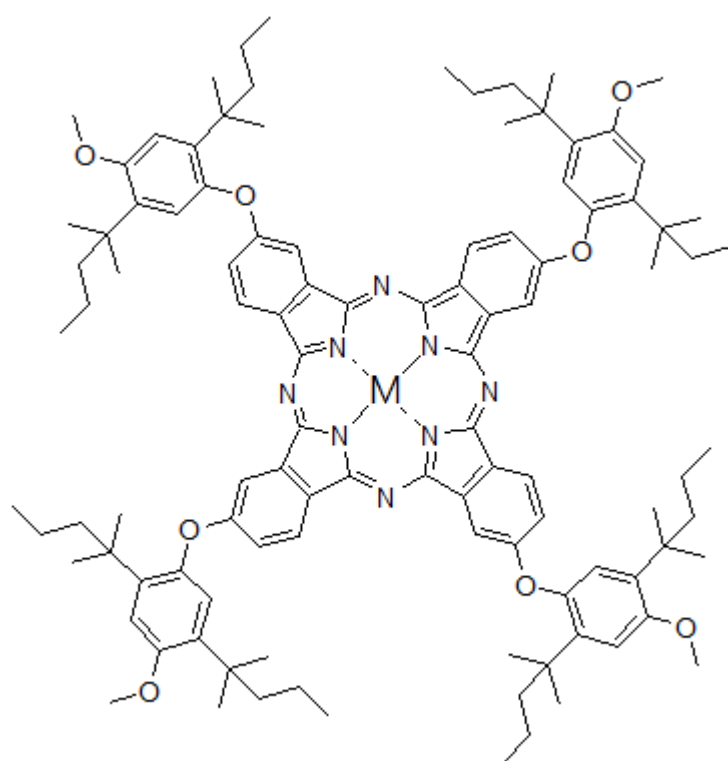
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical and Optical Characterization of Cobalt, Copper and Zinc Phthalocyanine Complexes

이재현 박종욱

가톨릭대 화학과

New phthalocyanine(Pc) derivatives that include the alkyl group in ligand were synthesized based on three core metals such as zinc (Zn), copper (Cu), and cobalt (Co). Electrochemical behaviors and optical properties of the new phthalocyanine derivatives with ligand and different core metal were investigated by using cyclic voltammetry, UV-Visible (UV-Vis.) spectroscopy and photoluminescence (PL) spectroscopy. In UV-Vis. data, maximum values of 2H, Co, Cu, and Zn complexes were 708 nm and 677 nm, 686 nm, 684 nm, respectively.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of triazole and pyrimidine-based chemical library

임동현 박승범<sup>1</sup>

서울대 생물물리 및 화학생물학과<sup>1</sup> 서울대 화학부

The synthesis of fused-triazole scaffolds that are connected with pyrimidine, pyrazole, or pyrazolopyrimidine through carbohydrate-derived linkers is reported here. Pyrimidine, pyrazole, or pyrazolopyrimidine moiety was constructed through the regioselective condensation of the key intermediate, 2-C-formyl glycals, with guanidine, hydrazine, or aminopyrazole. Fused-triazole scaffolds were constructed through the intramolecular azide-alkyne cycloaddition after functionalization of the hydroxyl group from the carbohydrates with azide and alkyne using the  $S_N2$ -type alkylation or Mitsunobu reaction. Overall, the synthetic method described here afforded two privileged structures in a molecule, conserving the stereogenic centers of the carbohydrates.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

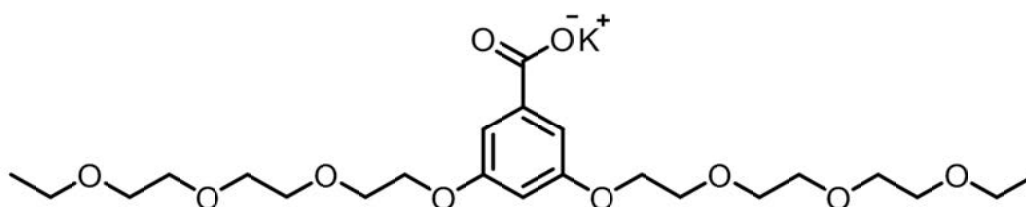
## **Ionic Surfactant-Coated *Burkholderia Cepacia* Lipase as the Highly Active Catalyst in Organic Solvent**

오연옥 이은경 김만주

포항공과대 화학과

Biocatalysis is useful for organic synthesis. For example, lipase is a useful tool for the synthesis of optically active compounds such as chiral alcohols, acids, and their esters. However, lipase catalysis in organic solvent often suffers from reduced activity, selectivity, or stability of enzyme. Therefore, it is important to develop a strategy to improve the reaction performance of lipase in organic solvent. We have developed a highly active enzyme in organic solvent by coating *Burkholderia cepacia* lipase(BCL) with an ionic surfactant. Commercially available BCL(crude BCL) exhibits significantly lower activity than *Candida antarctica* lipase B(CALB; Novozym 435) for acylation of 1-phenylethanol in toluene. Fortunately, we have developed a practical approach for enhancing its activity dramatically. We have discovered that ionic-surfactant-coated *Burkholderia cepacia* lipase(ISCBCL) has great potential as such an excellent enzyme. It is “1000-fold more active” than crude BCL and “2-fold more active” than

Novozym 435. The results indicate that ISCBCL is more efficient than Novozym 435 as the catalyst for the enzymatic reaction in organic solvent.



**ionic surfactant**



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발표코드: ORGN.P-967

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Discovery of ERRgamma Inverse Agonist Eryvarin H and its SAR Study

구자영 박승범

서울대 화학부

Nuclear receptors are one of the important targets for various intracellular functions via regulating gene transcription. Orphan nuclear receptor has no identified ligands while it has similar structure with other identified receptors. Estrogen related receptor gamma is a third subtype receptor of ERRs and one of the orphan receptors. ERR gamma has various biological functions, which have been reported such as oxidative metabolism, suppressing cell proliferation and tumor growth of prostate cancer cells, and modulating cell proliferation and estrogen signaling in breast cancer. We found a inverse agonist, Eryvarin H, of ERR gamma from a number of natural compounds based on docking simulation. Eryvarin H is a known natural compound, which is one of the Eryvarin series isolated from the roots of plant *Erythrina variegata*. Then we synthesized Eryvarin H and its derivatives by our own methods via Suzuki-Miyaura cross-coupling reaction. Change of aryl groups by using different kinds of boronic acids gave us 12 different Eryvarin H derivatives. After synthesis of those compounds, we analyzed their inverse

agonistic effect by using Gal4-fused ERRgamma LBD system embedded on reporter gene assay. We discovered not only Eryvarin H but also its derivatives are inverse agonists of ERRgamma with comparable activity. Moreover, we could analyze the SAR pattern from the structural informations of 12 derivatives and their cell-based assay data. From this research, which is a natural compound based SAR approach assisted by protein-ligand docking, we can conclude that this work is a quite useful way to discover lead compounds for modulating selected target.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mild Opening of Tetrahydrofuranyl Subunits in Steroids Using TFAT (trifluoroacetyl trifluoromethanesulfonate): Application to Synthesis of C17-OH Rockogenin Acetate

신준호 이희승<sup>1</sup> 이종석<sup>2</sup>

한양대 응용화학과 <sup>1</sup>한국해양연구원 해양천연물연구실 <sup>2</sup>한국해양연구원 해양바이오연구센터

An efficient method to open tetrahydrofuranyl ring was developed using highly reactive TFAT (trifluoroacetyl trifluoromethanesulfonate) reagent in the presence of an acid scavenger, 2,6-di-tert-butyl-4-methylpyridine. The above reaction affords an attractive synthesis to introduce a hydroxyl group to highly hindered C17 position in the steroid sapogenin. Thus, this method was successfully applied to the synthesis of C12-?-OBz, C17-?-OH rockogenin acetate (12 steps from hecogenin acetate) where the C17-?-OH group was successfully introduced without excision of the entire F-ring.

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발표코드: ORGN.P-969

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Systematic Study and Bio-Application of 9-aryl-1,2-dihydropyrrolo[3,4-b]indolizin-3-one(Seoul-Fluor)

최은정 박승범<sup>1</sup>

서울대 화학과 <sup>1</sup>서울대 화학부

A novel fluorescent core skeleton, 9-aryl-1,2-dihydropyrrolo[3,4-b]indolizin-3-one, which we named Seoul-Fluor was reported as a tunable and predictable chromophore. In Seoul-Fluor, the electronic characteristics of the substituents have a close correlation with their photophysical properties. The systematic perturbation of electronic densities on the specific positions of Seoul-Fluor allows both emission wavelength tunability covering the full color range and dramatic quantum yield change. On the basis of the computational analysis and experimental observations, we extracted a correlation of photophysical properties including quantum yield and emission wavelength with theoretical calculation. We clearly demonstrate that Seoul-Fluor can provide a powerful gateway for the generation of desired fluorescent probes without trial-and-error process.

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발표코드: ORGN.P-970

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Gradient DBR Porous Silicon Layer for Various Chemical Vapor



Gradient Bragg-structured porous silicon (PSi) were investigated under the exposure of various organic vapors. Gradient DBR PSi whose average pore size decreased as the lateral distance from the Pt electrode increased was generated by using an asymmetric etching configuration. The reflection resonances were measured as a silicon surface. Two types of gradient DBR PSi (H-, and HO-terminated gradient DBR Psi) were used in this study. The detection of volatile organic compounds (VOCs) using the gradient DBR PSi modified with hydrophobic and hydrophobic functionality exhibited different pore adsorption and desorption characteristics.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The efficient construction of 2-oxopiperazine small molecule library via fluoruous tagging strategy in solution phase**

이정애

서울대 생물물리및화학생물학부

Solid-phase strategy for synthesis of small molecules is an efficient library construction method without the need for additional purification step. But there are some disadvantages compared with solution phase reaction such as difficulty of detecting reaction termination and optimizing reaction condition. Thus, fluoruous tag technology that has advantages of solid-phase and solution-phase synthesis has been developed and used for many kinds of small molecules. Therefore, we have developed the synthetic strategy using fluoruous tag for the efficient construction of 2-oxopiperazine small molecule library. Through this strategy, we utilized diverse substrates as 4 diversiting points such as 5 amino acids, 4 grignard reagents, 2 amines that can be attached to fluoruous tag and 5 amines that can be induced after cyclization step. A 200-membered drug like oxopiperazine library has been constructed efficiently through this novel strategy.



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발표분야: 의약화학

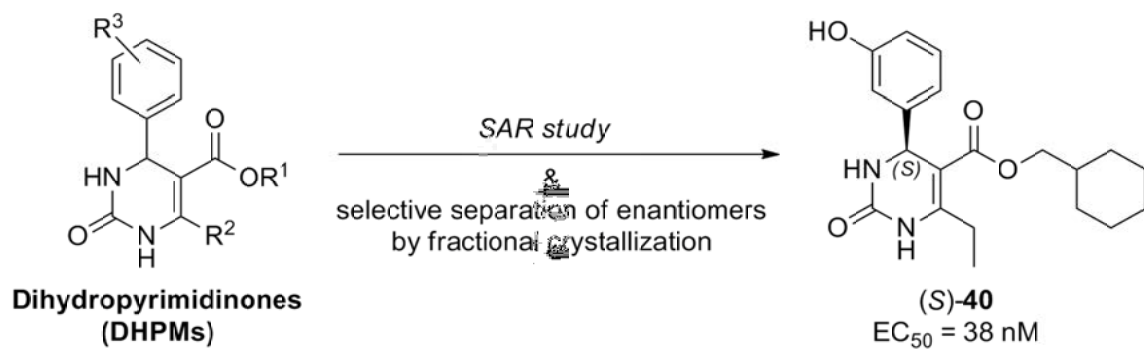
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Discovery of 3,4-dihydropyrimidin-2(1H)-ones with inhibitory activity against HIV-1 replication

김준원 조수연 이두현<sup>1</sup> 권정진<sup>2</sup> 서민정<sup>3</sup> 김영미<sup>3</sup> 박동식<sup>2</sup> 고윤애<sup>3</sup> 최인희<sup>4</sup> 황종연<sup>1</sup> 최지현<sup>1</sup> 박은정<sup>5</sup> 노재성<sup>2</sup> 이진화<sup>6</sup>

한국파스퇴르연구소 의약화학팀 <sup>1</sup>한국파스퇴르연구소 의약화학 <sup>2</sup>한국파스퇴르연구소 <sup>3</sup>한국파스퇴르연구소 의약화학그룹 <sup>4</sup>한국파스퇴르연구소 의약화학부 <sup>5</sup>한국파스퇴르연구소 nano bio chemistry <sup>6</sup>한국파스퇴르연구소 late discovery program(LDP)

3,4-Dihydropyrimidin-2(1H)-ones (DHPMs) were selected and derivatized through a HIV-1 replication assay based on GFP reporter cells. Compounds 14, 25, 31 and 36 exhibited significant inhibition of HIV-1 replication with a good safety profile. Chiral separation of each enantiomer by fractional crystallization showed that only the S enantiomer retained anti-HIV activity. Compound (S)-40, a novel and potent DHPM analog, could serve as an advanced lead for further development and the determination of the mechanism of action.



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발표코드: MEDLP-973

발표분야: 의약화학

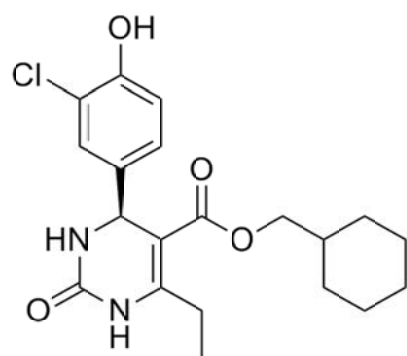
발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A novel 3,4-dihydropyrimidin-2(1H)-one: HIV-1 replication inhibitors with improved metabolic stability**

**김준원 김영미<sup>1</sup> 서민정<sup>1</sup> 조수연 이두현<sup>2</sup> 권정진<sup>3</sup> 박동식<sup>3</sup> 최지현<sup>2</sup> 황종연<sup>2</sup> 고윤애<sup>1</sup> 최  
인희<sup>4</sup> 노재성<sup>3</sup> 이진화<sup>5</sup>**

한국파스퇴르연구소 의약화학팀 <sup>1</sup>한국파스퇴르연구소 의약화학그룹 <sup>2</sup>한국파스퇴르연구소 의  
약화학 <sup>3</sup>한국파스퇴르연구소 <sup>4</sup>한국파스퇴르연구소 의약화학부 <sup>5</sup>한국파스퇴르연구소 late  
discovery program(LDP)

Following the previous SAR of a novel dihydropyrimidinone scaffold as HIV-1 replication inhibitors a detailed study directed towards optimizing the metabolic stability of the ester functional group in the dihydropyrimidinone (DHPM) scaffold is described. Replacement of the ester moiety by thiazole ring significantly improved the metabolic stability while retaining antiviral activity against HIV-1 replication. These novel and potent DHPMs with bioisosteres could serve as advanced leads for further optimization.



**2**

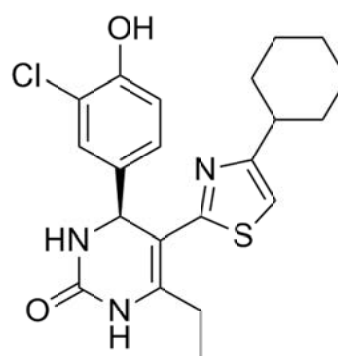
HLM  $t_{1/2}$  = 36 min

RLM  $t_{1/2}$  = 7 min

Low metabolic stability

\*Human (HLM) and rat (RLM) liver microsomes

*bioisostere approach*



**26b**

HLM  $t_{1/2}$  = 682 min

RLM  $t_{1/2}$  = 30 min



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발표코드: MEDLP-974

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Binding mode analysis of novel HIV-1 NNRTI scaffold

고윤애 최인희<sup>1</sup> 이두현<sup>2</sup> 권정진<sup>3</sup> 공선주<sup>4</sup> 조수연<sup>5</sup> 김영미 최지현<sup>2</sup> 김준원<sup>5</sup> 노재성<sup>3</sup> 이  
진화<sup>6</sup>

한국파스퇴르연구소 의약화학그룹 <sup>1</sup>한국파스퇴르연구소 의약화학부 <sup>2</sup>한국파스퇴르연구소 의  
약화학 <sup>3</sup>한국파스퇴르연구소 <sup>4</sup>한국파스퇴르연구소 의약화학실 <sup>5</sup>한국파스퇴르연구소 의약화학  
팀 <sup>6</sup>한국파스퇴르연구소 late discovery program(LDP)

Reverse transcriptase (RT) is one of the promising therapeutic targets for the treatment of HIV-1 infection. There are two types of RT targeting drugs: one is nucleoside reverse transcriptase inhibitors (NRTIs) which bind to the active site of RT, another one is non-nucleoside reverse transcriptase inhibitors (NNRTIs) binding to the allosteric binding site in p66 subunit of RT. There are NNRTI drugs in the market but still need to develop novel NNRTIs because of the drug resistances like K103N, one of the most frequently occurring drug resistances. Our lead optimization strategy focused on overcoming this mutation. We used a clinically used HIV-1 NNRTI, Etravirine (TMC-125), x-ray crystals for docking

study and modification. Our group has synthesized series of pyrazolo amino pyridine (PAP) compounds and found compounds with comparable activities in both wild type and mutant.



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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Protein-ligand docking of known 5-lipoxygenase inhibitors

최인희 고윤애 강선희 김영미 이세연 이수미 박혜영 서정제 서민정 서무영 김재승

이진화<sup>1</sup>

한국파스퇴르연구소 의약화학그룹<sup>1</sup> 한국파스퇴르연구소 late discovery program(LDP)

5-lipoxygenase (5-LO) is an important factor in immune and inflammatory responses, and allergic and inflammatory disorders and also possibly atherosclerosis can be intervened by inhibition of 5-LO. Despite many years of discovery for 5-LO inhibitors, only one clinically approved 5-LO inhibitor is available which is Zileuton. However, Zileuton has shown a variety of adverse effects related to hepatic toxicities. With recent discovery of human 5-LO x-ray crystal structure (3O8Y.pdb), we have applied in silico protein-ligand docking method to analyze how known iron-chelator, redox and non-redox 5-LO inhibitors would bind in the active site. CDocker program in Discovery Studio suite (Accelrys, Inc.) was used for docking. Binding site for docking included all the residues coordinating the ferric iron (H367, H372, H550, N554, I673) and those of the active site. Two iron chelator 5-LO inhibitors, Zileuton and CGS-23885 were docked into the active site. The hydroxyurea group of both compounds docked near the ferric

atom suggesting iron chelation. In addition, this group of Zileuton, and the oxygen atom in the chromene group of CGS-23885 formed hydrogen bonds (H-bonds) with H367. The aromatic rings of CGS-23885 were well positioned and surrounded by active site hydrophobic residues. This may be the reason for lower docked energy than Zileuton. A redox inhibitor, R-68151, has a phenolic group in the structure. The hydroxyl moiety of the phenolic group formed H-bond with I673. The long elongated shape with four rings of R-68151 filled up the tubular shape active site by having hydrophobic and van der Waals interactions with the active site residues. As a comparison, a non-redox inhibitor, CJ-13610, was also docked into the active site of 5-LO. It didn't form any H-bond with either iron coordinating or active site residues. In conclusion, compounds forming H-bonds with at least one of the five iron coordinating residues had redox or iron chelating properties. Also, docking results showed how the chemical functional groups interact with the active site residues. This structure-activity relationship information from docking results could be the basis for developing 5-LO inhibitors with improved efficacy and toxicity profiles.





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장소: 일산KINTEX

발표코드: MEDLP-976

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Biphenyl derivatives as 5-HT<sub>7</sub> receptor antagonists

김지연 추현아<sup>1</sup> 김영재<sup>2</sup> 염미영<sup>3</sup>

동덕여대 응용화학과 <sup>1</sup>KIST 생명보건본부 <sup>2</sup>과학기술연합대학원대 의약및약품화학 <sup>3</sup>KIST 뇌  
의약연구단

5-HT<sub>7</sub> receptor, the most recently added receptor to the 5-HT receptor family, is discretely localized within CNS such as thalamus, hypothalamus, limbic and cortical regions. Although biological functions of this receptor are poorly understood, recent reports suggest that 5-HT<sub>7</sub> receptor is involved in the regulation of body temperature, circadian rhythms, learning and memory, as well as neuronal excitability, inflammatory processes and smooth muscle relaxation of cerebral arteries. Knockout animal studies have provided demonstrative proofs that 5-HT<sub>7</sub> receptor is engaged in the pathomechanism of depression. Thus, 5-HT<sub>7</sub> receptor is potentially a good target for treatment of depression. Based on the known 5-HT<sub>7</sub> receptor ligands, biphenyl derivatives was designed, synthesized and biologically evaluated against 5-HT<sub>7</sub> receptor. The synthesis and biological activity will be discussed in detail.

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장소: 일산KINTEX

발표코드: MEDLP-977

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Biological evaluation of Peripheral benzodiazepine receptor( PBR) ligands for the treatment of Alzheimer's disease

양하연 배애님<sup>1</sup> 태진성 이지연<sup>2</sup> 박병건<sup>3</sup>

연세대 화학과 <sup>1</sup>KIST 생체과학연구본부 <sup>2</sup>성신여대 글로벌의과학과 <sup>3</sup>고려대 생명공학과

The benzodiazepine receptors can be divided, from the point of view of their cellular localization, into two groups: central benzodiazepine receptors (CBR) and peripheral ones (PBR). A peripheral benzodiazepine receptor is localized in many types of tissues, on the surface of the mitochondrial membranes (IMM-OMM). This receptor mediates various mitochondrial functions, including cholesterol transport and steroid hormone synthesis, mitochondrial respiration, mitochondrial permeability transition (mPT) pore opening and cell proliferation and apoptosis. Initial clinical trials have indicated that PBR ligands might be valuable in the treatment of psychiatric disorders and neurological disease such as alzheimer's disease. Therefore, the PBR is targeted to develop alzheimer's disease drug. As part of discovering novel PBR ligands, we designed and synthesized 38 compounds. The synthesized compounds were biologically evaluated against PBR. The detailed design, synthesis and biological evaluation of PBR ligands as alzheimer's disease drugs will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-978

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Water Soluble Ionic Liquid Type Photosensitizers and Its Gold Nanoparticles for Photodynamic Therapy

윤일 심영기<sup>1</sup>

인제대 PDT 연구소 <sup>1</sup>인제대 나노공학부

Water soluble ionic liquid type photosensitizers and its gold nanoparticles have been synthesized and were characterized by IR, UV-vis spectroscopic analyses and transition electron microscopy. And their photodynamic effect has been evaluated by in vitro test for photodynamic therapy.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-979

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Discovery of an Orally Available PAR-1 Antagonists as a Novel Antiplatelet Agent

김진석 최정환<sup>1</sup> 이선경<sup>2</sup>

성균관대 화학과 <sup>1</sup>고려대 화학과 <sup>2</sup>한국화학연구원 의약화학연구센터

We discovered a novel series of orally available potent PAR-1 (protease activated receptor) antagonist, octahydroindene derivatives. The representative compound showed an IC<sub>50</sub> of 0.021  $\mu$ M in a PAR-1 binding assay. It inhibited platelet aggregation in human platelet rich plasma (PRP) with an IC<sub>50</sub> of 0.44  $\mu$ M. In the ex vivo PRP assay in cynomolgus monkeys after oral administration, it inhibited the aggregation dose dependently and showed an almost complete inhibition at 30 mg/kg for 24 h. In addition, the pharmacokinetic and toxicological profile of this series of compounds were evaluated.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-980

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Anti-oxidative and Anti-inflammatory Constituents from the Branches of *Malus sieboldii*

양인정 오태현 김정은 변상희 김수영 이남호

제주대 화학과

This study was designed to analyze the chemical constituents in the extract of *Malus sieboldii* branches and to evaluate their biological activities. Phytochemical investigation of the ethanol extract from *M. sieboldii* branches by using repeated column chromatography with normal-phase silica gel and Sephadex LH-20 resulted in the isolation of six compounds;  $\beta$ -sitosterol (1), epi-catechin (2), 3-*O*- $\alpha$ -L-arabinofuranosyl-8-methoxyquercetin (3), phlorizin (4), avicularin (5), and chrysin-7-*O*- $\beta$ -D-glucopyranoside (6). 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 2, 3 and 5 showed strong DPPH radical scavenging activities with  $SC_{50}$  of 15.7, 25.4 and 17.2  $\mu$ g/mL respectively, whose activities were comparable to a positive control vitamin C ( $SC_{50}$  8.7  $\mu$ g/mL). On the screening of anti-inflammatory activities, the compounds 2 and 6 showed the considerable inhibition on the production of nitric oxide for

the RAW 264.7 cell without any cell toxicities. Based on these results, *M. sieboldii* branches extract could be potentially applicable as anti-oxidant and anti-inflammatory agent in cosmeceutical and/or pharmaceutical preparations.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-981

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and biological evaluation of thieno[3,2-b]pyridine derivatives as urotensin II receptor (UT) antagonists

임채조 이가은<sup>1</sup> 김지영 김낙정 이규양

한국화학연구원 대사증후군치료제연구센터<sup>1</sup> 과학기술연합대학원대 의약및약품화학

Urotensin-II as a cystein-linked cyclic undcapeptide, plays a important role in cardiovascular homeostasis and is known to be one of the most potent mammalian vasoconstrictor. It is a natural ligand of the urotensin II receptor (UT), which is a member of the family of G-protein coupled receptors. In addition, UT is considered to be involved in the regulation of cardiorenal function and have been implicated in the numerous cardiorenal diseases including hypertension, heart failure, atherosclerosis and renal failure. In continuing our efforts to search for novel and potent scaffolds of UT antagonists, we have identified a series of thieno[3,2-b]pyridine derivatives and examined the effects of various substituents around thieno[3,2-b]pyridine core to the UT binding activity. The details of synthesis and SAR results will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDIP-982

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and biological evaluation of pyrrolo[3,2-b]pyridine derivatives as urotensin $\text{II}$ receptor (UT) antagonist

임채조 김정영<sup>1</sup> 김수희<sup>2</sup> 이은경 이규양

한국화학연구원 대사증후군치료제연구센터 <sup>1</sup>과학기술연합대학원대 의약 및 약품화학부 <sup>2</sup>과학기술연합대학원대 의약및약품화학

The urotensin  $\text{II}$  receptor (UT) is a member of the G-protein-coupled receptor superfamily and is expressed in a wide range of tissues. Furthermore, it is known to be involved in the regulation of cardorenal function and is one of the the most promising targets in treatment of cardiorenal diseases. As part of our drug discovery project in the development of potent UT antagonists, we have identified a series of pyrrolo[3,2-b]pyridine derivatives and investigated the effects of various substituents of N-position around pyrrolo[3,2-b]pyridine core to UT binding activity. The details of synthesis and structure-activity relationships (SAR) results will be discussed.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-983

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **$^{18}\text{F}$ -Radiolabeling of RGD-monomer/dimer by Strain-Promoted Alkyne-Azide Click Reaction for Positron Emission Tomography (PET)**

**장승호 JADHAV VINOD HANMANT<sup>1</sup> kalme sachin<sup>1</sup> 이상봉<sup>1</sup> 김혜란<sup>1</sup> 박신혜<sup>1</sup> 김동욱<sup>1</sup>**

전북대 의과대학 핵의학과 <sup>1</sup>전북대 핵의학과

Peptides involving the RGD motive (arginine-glycine-aspartic acid) recognize members of the integrin receptor family. Since the receptors are located mainly on the surface of endothelial cells. Structural modifications of cRGD including mono or dimers of were recently found to improve the binding affinity towards  $\alpha_v\beta_3$  integrin significantly. Strain-Promoted "Click" reaction give high yield, and the bio-orthogonality of the azide-cycloalkyne reaction. We synthesized dibenzo-cyclooctyne conjugated cRGDyk monomer and dimer followed by  $^{18}\text{F}$ -labeling by SPAAC (strain-promoted azide-alkyne click) reaction for PET.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-984

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Construction of a Unique Drug-like 2,4,5-trisubstituted Thiazole Libraries Using BAL Resin on Solid-phase

배미선 김용상 유서현 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. In this regard, owing to the fact that thiazole derivatives exhibit a wide range of important biological activities, they serve as attractive targets for combinatorial library construction via solid-phase synthesis. For example, thiazoles exhibits the activities against cyclin-dependent kinase (CDK) and glycogen synthase kinase-3 (GSK-3). Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of 2,4,5-trisubstituted thiazole derivatives through resin-bound BAL linker. We had previously report a useful method for the solid-phase synthesis of 2,4,5-trisubstituted thiazole derivatives using a sulfone traceless linker. However, the developed method some limitation which were couldn't introduce efficiently various substituents such as amine, amides, sulfone amides, and urea on the 2-position of thiazole core skeleton by nucleophilic substitution reaction at last cleavage step. We are

studying cleavage condition on solid-support under TFA. Therefore, we believe our efficient approach is suitable for the construction of drug-like 2,4,5-trisubstituted thiazole libraries in a high throughput manner.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-985

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Optimization Process of a Novel 3-Arylethynyl-substituted Thieno[2,4-b]pyrazine Derivatives as a Wnt/ $\beta$ -catenin Pathway Inhibitors

김나연 곽세훈 이은실<sup>1</sup> 공영대

동국대 화학과 <sup>1</sup> 동국대 의약화학연구실

The Wnt signaling is one of the key signaling pathways that regulate cell proliferation, differentiation, and morphogenesis. Wnt proteins constitute a family of highly conserved secreted glycoproteins that play multiple roles in the development and progression of diseases. Small-molecule inhibitors of this pathway are desired because it is believed their clinical use would suppress cancer cell growth. As a result, there has been an interest in identifying small molecule inhibitors of Wnt signaling as tool compounds for research or as precursors to new generations of anticancer drugs. Several potent small-molecule inhibitors have been reported; however, the development of therapies to specifically target the Wnt pathway in cancer cells is still in its infancy. To identify small molecule inhibitors of Wnt/ $\beta$ -catenin pathway, we are screening 3-arylethynyl-substituted thieno[2,4-b]pyrazine derivatives

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-986

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Solid-phase Synthesis of 2-Amino/Amido/Sulfonamido Substituted-1H-benzo[d]imidazole Derivatives via Thiourea Linker on BAL Resin**

이지형 정세린 양정원 공영대

동국대 화학과

Combinatorial chemistry of small organic molecules in solution phase or on solid support has a significant impact on the drug discovery. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. In this regard, because 2-amino/amido/sulfonamido substituted benzo[d]imidazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO and various receptor antagonistic, they serve as attractive targets for combinatorial library construction via solid-phase synthesis. Therefore we have been exploring the potential of resin-bound benzo[d]imidazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of benzo[d]imidazole based library through resin-bound BAL linker. Especially, we will discuss about solid-phase synthetic route to a unique substituted

benzo[d]imidazole derivatives based on diversity oriented synthesis concept. The final compounds were obtained in good yields and high purities upon cleavage from the resins.



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장소: 일산KINTEX

발표코드: MEDLP-987

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Solid-phase Parallel Synthesis of a Novel N-[Alkylsulfonamido-spiro(2H-1-benzopyran-2,4-piperidine)-6-yl] substituted Amide and Amine Drug-like Libraries**

김지혜 이지형 김슬기 공영대

동국대 화학과

Over several years, we have investigated many structural classes of 5-LO inhibitors with the aim of identifying orally active 5-LO (5-lipoxygenase) target as anti-inflammatory inhibitors. As the results, we found out a novel 6-amino-2,2-dimethyl-3,4,6-trisubstituted-2H-1-benzopyran hit compound (one representative lead compound is KRH-102140 with the 6-amino-2,2-dimethyl-3,4,6-trisubstituted-2H-1-benzopyran and showed good in vitro activity at 0.16  $\mu$ M IC<sub>50</sub> value)<sup>4a</sup> toward 5-LO target.<sup>4</sup> However, we didn't find out much improved hit compound by optimization process of KRH-102140 core skeleton derivatives. Therefore, our concern focused on the development of a spiro-benzopyran core skeleton to improve more active benzopyran derivatives than the KRH-2140. As the results, we report a solid-phase parallel synthesis of a novel N-[alkylsulfonamido-spiro(2H-1-benzopyran-2,4-piperidine)-6-yl]

substituted amide 1A and amine 1B derivatives that relies on BAL linker and present an chemical properties using a in silico screening.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-988

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Solid-phase Synthesis of N-Substituted-2-Aminobenzothiazole Derivatives via Cyclization Reactions of Thiourea Resin

김슬기 이은실<sup>1</sup> 곽현정 공영대

동국대 화학과 <sup>1</sup> 동국대 의약화학연구실

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Especially Compounds containing the benzothiazole moiety are special interest because they have an even broad biological activity. Also solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient 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 2-Amino/Amido/Sulfonamido substituted benzo[d] thiazole based library through resin-bound BAL linker. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-989

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Construction of a Novel drug-like 2-Thioxoimidazolidin-4-one  
Derivatives using Various Amino acids via Isothiocyanate linker on  
Solid-phase**

이재민 배미선 김용상 공영대

동국대 화학과

The factor of success in innovative drug search depends on how many we have the various and creative drug like library. The compounds equipped with the molecular diversity, there are also more probability to find the new drug. The solid phase synthesis of heterocyclic combinatorial libraries is a strategy to have drug discovery process. And Solid-phase synthesis of heterocyclic core skeleton serve as the core components of a large number of substance that process a wide range of interesting biological activities. 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 present a convenient solid-phase synthetic method for combinatorial generation of 2-thioxoimidazolidine-4-one derivatives through resin-bound benzyl thiocyanate linker on BAL resin. The 2-thioxo imidazolidine derivatives have attracted much attention since it have been

reported to be responsible for interesting biological activities such as Hif $\alpha$  and Wnt signal path way, and various receptor antagonist. Through making the various substituted aromatic building blocks, we can obtain linear compound. The final compounds were obtained in good yield and high purities from solution-phase synthetic process.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-990

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Solid-phase Parallel Synthesis of 2-Amino/Amido/Sulfonamido Substituted Benzo[d]oxazole Derivatives Using BAL Resin

정세린 양정원 양승주 공영대

동국대 화학과

Heterocyclic skeletons serve as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. Solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound-2-amino/amido/sulfonamido substituted benzo[d]oxazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. A general method is described for the solid-phase synthesis of 2-amino/amido/sulfonamido substituted benzo[d]oxazole derivatives. The sequence developed for this purpose is based on cyclization reactions of resin-bound thioureas. N-alkylation, N-acylation and N-sulfonylation reactions of 2-amino/amido/sulfonamido substituted benzo[d]oxazole resins yield the desired variously functionalized benzo[d]oxazole resins. Finally, 2-amino/amido/sulfonamido substituted benzo[d]oxazole are then generated in good yields and high purities by cleavage of the respective 2-amino/amido/sulfonamido

substituted benzo[d]oxazole resins. 2-amino/amido/sulfonamido substituted benzo[d]oxazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO and various receptor antagonists, they serve as attractive targets for combinatorial library construction via solid-phase synthesis.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-991

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Solid-phase Synthesis and Cyclization Reactions of Novel Pyrazole Derivatives via Hydrazine Linker on AMEBA Resin

곽현정 김나연 이원주 공영대

동국대 화학과

Solid-phase synthesis of combinatorial chemistry has emerged as a powerful methodology for the preparation of libraries of small organic compounds in order to accelerate the drug discovery process. And heterocyclic compounds serve as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. As a part of an ongoing drug discovery program, we have been exploring the potential of new and highly efficient synthetic methods for various resin-bound pyrazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present novel solid-phase synthesis for combinatorial generation of pyrazole-based libraries through resin-bound hydrazine linker on AMEBA resin. During the past decade, 1,3,4,5-substituted pyrazole derivatives of five-member ring heterocyclic compounds have attracted much attention for their interesting biological activities such as COX- II inhibitors, 5-LO inhibitors, and various receptor antagonists. The progress of reactions could be monitored as resin-

boundintermediates by ATR-FTIR spectroscopy. The final compounds were obtained in good yields andhigh purities upon cleavage from the AMEBA resin.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-992

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Solid-phase Synthesis of Drug-like 5-Phenyl-(2-amino and 2-amido substituted)1,3,4-Oxadiazole Library via Reagent-based Cyclization of Thiosemicarbazide**

양승주 이석형 곽세훈 공영대

동국대 화학과

Solid-phase organic synthesis(SPOS) is now routinely used to prepare druglike, small organic molecules in medical chemistry programs. This procedure enables the generation of massive numbers of hit and lead compounds as part of high-throughput screening technologies. Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of a large number of substances that possess a wide range of interesting biological activities. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound 1,3,4-oxadiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. The 2-amino 2-amido substituted 1,3,4-oxadiazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistic. Herein we would like to



present a novel solid-phase synthetic method for combinatorial generation of 1,3,4-oxadiazole library via reagent-based cyclization of thiosemicarbazide. The final compounds were obtained in good yields and high purities upon cleavage from the resins.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-993

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of thioflavin-T analogues as a potential amyloid imaging agents

정순재 박정훈<sup>1</sup> 양승대<sup>1</sup> 허민구<sup>1</sup> 유국현

동국대 화학과 <sup>1</sup>한국원자력연구원 방사선기기연구부

Alzheimer's disease (AD) is the most common form of dementia, involves accumulation of amyloid plaques. Amyloid beta (A $\beta$ ) is the main component of amyloid plaques, and thioflavin-T (ThT) is widely used to visualize and quantify the presence of A $\beta$ . In this study, we synthesized the ThT analogues for detection of A $\beta$ 40 fibrils in vitro. 2-(2'-Methoxy-4'-aminophenyl)benzoxazole (1) was synthesized by the condensation of 2-aminophenol and 4-amino-2-methoxybenzoic acid at 200°C in polyphosphoric acid. 2-(2'-Methoxy-4'-methylaminophenyl)benzoxazole (2) was monomethylated using the deprotonation 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 deprotonating 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 A $\beta$ 40 aggregates for their fluorescence response. Among tested 6 compounds, compound 2 has two critical requirements for fluorescence imaging probe; high fluorescence responsiveness and strong binding affinity.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-994

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and IKK-2 inhibitory activity of Thiadiazole and Thiazolidinone derivatives

신민재 김정현<sup>1</sup> 남길수<sup>2</sup> 추현아<sup>3</sup> 노은주<sup>4</sup>

연세대 화학과 <sup>1</sup>KIST 생체과학연구본부 <sup>2</sup>KIST 뇌과학연구소 <sup>3</sup>KIST 생명보건본부 <sup>4</sup>KIST 생체  
과학연구부

The modification of IKB proteins depends on the IKK (IKB Kinase) complex (IKK1 and IKK2). IKK2 is a vital for translating proinflammatory stimuli (TNF- $\alpha$ , IL-6, IL1- $\beta$ ) into the activation of NF- $\kappa$ B. An inhibitor of IKK 2 could be effective in treatment of proinflammatory related disease such as rheumatoid arthritis, inflammatory bowel disease, lupus, and multiple sclerosis. The discovery of orally active small molecules IKK inhibitors as therapeutic agent for the treatment of autoimmune disease and inflammatory disorder has been reported. Here, based on previous our IKK-2 inhibitors, the new thiadiazole and thiazolidinone derivatives. were synthesized and biological results are described. Sixteen compounds based on thiadiazole and thiazolidinone moiety were synthesized and evaluated for the inhibitory potency of IKK-2 by TR-FRET method. Compound KNS0073 (% inhibition 85.5%, IC<sub>50</sub>= 0.94 $\mu$ M) showed good IKK-2 Inhibitory Activity.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-995

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Hydrophilic Photosensitizer of Purpurinimide Oligomer Ethyleneimine Conjugates Encapsulated in Biodegradable Polymer

김정화 윤일<sup>1</sup> 심영기<sup>2</sup>

인제대 나노시스템공학과 <sup>1</sup>인제대 PDT 연구소 <sup>2</sup>인제대 나노공학부

Hydrophobic agents have a good cellular invasion. But on the other hand, a major disadvantage of hydrophobic agents is that time of absolutely removal of the materials from the body is so slow. Hydrophilic agents are quick to out of body, but it cannot penetrate cell wall unlike hydrophobic ones. purpurinimide derivative conjugated with polyethylimine(PEI) was synthesized from hydrophilic polymer for reinforced hydrophilicity. These materials were encapsulated into poly lactic-co-glycolic acid (PLGA) nanoparticles together. Size of this nanoparticle is less than 230 nm. The PLGA outer layer, hydrophobic biological polymer, facilitated cellular invasion causing endocytosis. And then, PLGA layer disintegrated through the acidity of tumor cell. So the hydrophilic photosensitizers could be delivered into the tumor cell.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-996

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of New Derivatives of Purpurinimide and Chlorin Amide Encapsulated in Biodegradable Polymer

김정화 윤일<sup>1</sup> 심영기<sup>2</sup>

인제대 나노시스템공학과 <sup>1</sup>인제대 PDT 연구소 <sup>2</sup>인제대 나노공학부

Hydrophobic agents have a good cellular invasion. But on the other hand, a major disadvantage of hydrophobic agents is that time of absolutely removal of the materials from the body is so slow. Hydrophilic agents are quick to out of body, but it cannot penetrate cell wall unlike hydrophobic ones. For the purpose of the effect, we had an idea as follows. First step, we made two hydrophilic photosensitizers. Chlorine e6 13(1)-N,N-dibutylamide was synthesized by dibutyl amine group and carboxylic group. These materials were encapsulated into poly lactic-co-glycolic acid (PLGA) nanoparticles together. Size of this nanoparticle is less than 230 nm. The PLGA outer layer, hydrophobic biological polymer, facilitated cellular invasion causing endocytosis. And then, PLGA layer disintegrated through the acidity of tumor cell. So the hydrophilic photosensitizers could be delivered into the tumor cell.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-997

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **N-Heteroaryl-3-Phenylsulfonyl-2-Hydroxy-2-Methylpropionamide Derivatives ; as Androgen Receptor Antagonists**

김낙정 이규양 강정모 김성환<sup>1</sup> 강남숙<sup>2</sup>

한국화학연구원 대사증후군치료제연구센터 <sup>1</sup>한국화학연구원 화학유전체 연구실 <sup>2</sup>충남대

The androgen receptor(AR) is a ligand binding transcription factor in the nuclear hormone receptor super family. The AR antagonists is a key molecular target in the etiology and progression of prostate cancer. A series of N-Heteroaryl-3-phenylsulfonyl propionamide derivatives has been synthesized and biological evaluated using cell based assay (LNCap/PC-3 cells). The synthetic method and structure-activity relationships will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-998

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Identification of Anti-oxidative and Anti-inflammatory Constituents from the Branches of *Carpinus turczaninowii*

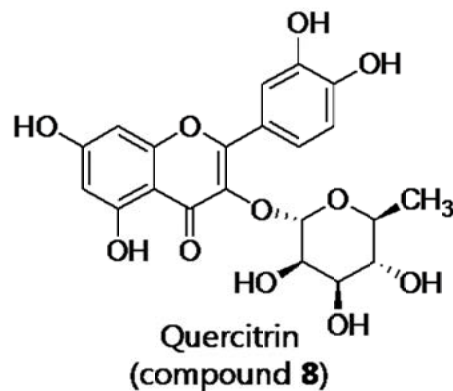
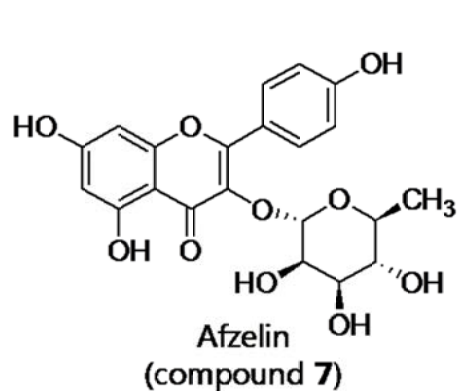
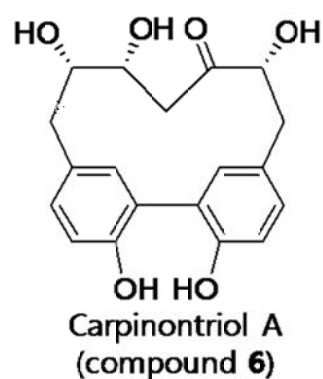
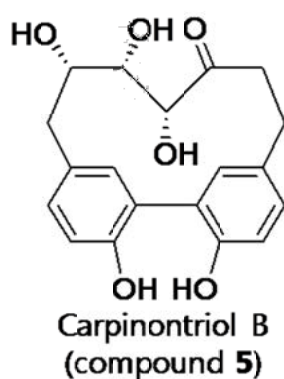
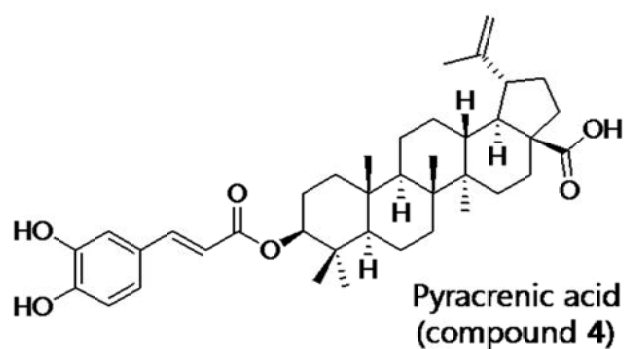
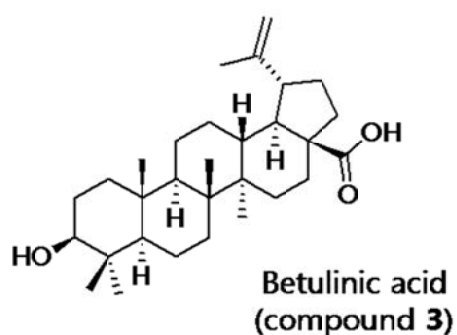
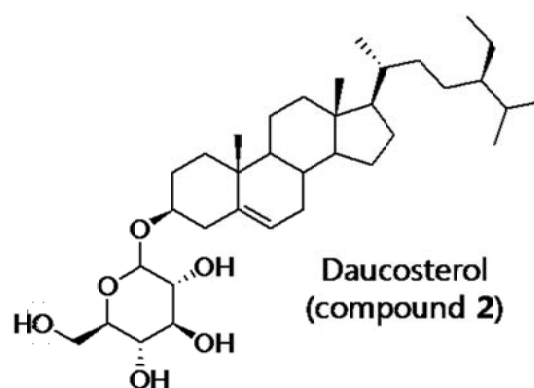
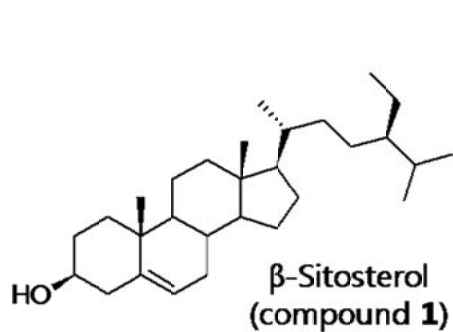
고하나 김상숙<sup>1</sup> 김성천 한정환 강지미 이라겸 이남호

제주대 화학과 <sup>1</sup>국립원예특작과학원 감귤시험장

*Carpinus turczaninowii* is a tree belonging to Betulaceae family. Phytochemical investigation of the ethanol extract from branches of *C. turczaninowii* by using repeated column chromatography resulted in the isolation of eight compounds;  $\beta$ -sitosterol (1), daucosterol (2), betulinic acid (3), pyracrenic acid (4), carpinontriol B (5), carpinontriol A (6), afzelin (7) and quercitrin (8). The structures of these compounds were identified by spectroscopic methods and by comparing their data to those in the literature. As far as we know, all of the compounds except quercitrin (8) were isolated for the first time from this plant. The isolated compounds were also subjected to the activity screenings on anti-oxidation and anti-inflammation. For the anti-oxidation tests, the compounds 4 and 8 showed strong DPPH radical scavenging activities with  $SC_{50}$  of 55.2 and 62.4  $\mu$ M respectively, whose activities were comparable to a positive control vitamin C ( $SC_{50}$  43.5  $\mu$ M). In addition, compounds 4, 5, 6 and 8 showed strong ABTS<sup>+</sup> radical scavenging activities with  $SC_{50}$  of 34.1, 42.1 45.8 and 29.6  $\mu$ M respectively, indicating comparable



activity to vitamin C ( $SC_{50}$  31.6  $\mu$ M). On the screening of anti-inflammatory activities, the compounds 5 and 6 showed the considerable inhibition on the production of nitric oxide for the RAW 264.7 cell without exhibiting cell toxicities. Based on these results, *C. turczaninowii* branch extract could be potentially applicable as anti-oxidant and anti-inflammatory agents in cosmeceutical and/or pharmaceutical preparations.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-999

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthetic studies on new 2-nitroimidazole derivatives with isoxazole and oxime structures for imaging tumor hypoxia

최정화 이해황 고훈영

인하대 화학과

Tumor hypoxia is the biological situation where tumor cells have been deprived of oxygen. The detection of hypoxia cell is important for treatment planning, such as in cases of cancer or myocardial ischemia. A number of isotopically labeled 2-nitroimidazole derivatives have been investigated as potential hypoxia markers. The nitro-aromatic classes of bio reductive derivatives were developed on the basis that the nitro functionality of the compound is able to be reduced under hypoxic conditions. Since 2-nitroimidazole heterocycles is the key structure in the field of imaging of hypoxia, it is important to introduce this 2-nitroimidazole ring for the discovery of new compounds. As part of discovering new imaging ligands, new 2-nitroimidazole with isoxazole and oxime isomers containing fluorine and primary alcohol functionality were designed and synthesized. The basic concept, design and synthetic efforts of the target structures as possible hypoxia imaging ligands will be presented.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1000

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Biological Evaluation of the Mitochondrial Permeability Transition Pore Inhibitors for the Treatment of Alzheimer's Disease

김태훈 박병건<sup>1</sup> 이지연<sup>2</sup> 배애님<sup>3</sup>

과학기술연합대학원대 의약 및 약품화학 <sup>1</sup>고려대 생명공학과 <sup>2</sup>성신여대 글로벌의과학과

<sup>3</sup>KIST 생체과학연구본부

$\beta$ -Amyloid peptide(A $\beta$ ) is produced from transmembrane amyloid precursor protein(APP) by sequential actions of  $\beta$ - and  $\gamma$ -secretase. A $\beta$  is implicated in the pathogenesis of Alzheimer's disease(AD) by interaction of A $\beta$  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 A $\beta$  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 numerous novel scaffolds, and the synthesis and

biological evaluations of those compounds were performed. The detailed synthesis and biological evaluation of mPTP inhibitors as Alzheimer's disease drugs will be presented.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1001

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of $^{18}\text{F}$ -Labeled Quinoxaline derivative as a Potent PET Radiopharmaceutical

김희정 김동연 박정훈<sup>1</sup> 양승대<sup>1</sup> 허민구<sup>1</sup> 유국현

동국대 화학과 <sup>1</sup>한국원자력연구원 방사선기기연구부

Wnt/ $\beta$ -catenin signaling is over expressed in colon cancers and lung cancers. Quinoxaline derivatives are a class of compounds that have shown selective and effective inhibition of Wnt/ $\beta$ -catenin signaling. This work is aimed at the development of  $^{18}\text{F}$ -labeled quinoxaline derivatives for cancer imaging through Wnt/ $\beta$ -catenin signaling. 2-fluoro-*N*-methyl-*N*-(2-(3-(phenylethynyl)quinoxalin-2-yloxy)ethyl)ethanamine was synthesized in seven chemical steps and obtained in a 15% overall yield. 2- $^{18}\text{F}$ -fluoro-*N*-methyl-*N*-(2-(3-(phenylethynyl)quinoxalin-2-yloxy)ethyl)ethanamine was prepared in a 40% radiochemical yield.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1002

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and antiOXIDATIVE activity of GALLIC ACID DERIVATIVES

박가영 이진호

계명대 화학과

The catechins present in Green tea have been reported to have antioxidative activity. Green tea contains four main catechin substances: EC, ECG, EGC and EGCG. EGCG is the most powerful of these catechins. EGCG as an antioxidant is about 25-100 times more potent than vitamins C and E. However, the difficulty of synthesis and purification of (—)-epicatechin gallate (ECG) and (—)-epigallocatechin gallate (EGCG), makes it hard to be optimized further and developed as to be drug. Based on structural character that both ECG and EGCG have galloyl group, the modification of gallic acid was performed to obtain antioxidant which could be obtained easily. Simple modification of gallic acid provided potent antioxidants which are better than Vitamin C.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1003

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 2-(Aminopyrimidine-4-yl)phenol derivatives with anti-cancer effects

김진아 이진호

계명대 화학과

Protein kinases, as cell function regulators, mediate most of the signal transduction pathways that control such activities as cell growth, metabolism, differentiation and apoptosis. More than 400 human disease have been linked to aberrant protein kinase signaling, which has made protein kinases important drug targets. Pyrimidines have been widely used as a scaffold for small molecular drug and many of them have been reported to exhibit potent inhibition against human cancer cell line as a kinase inhibitor. Based on the previous study, a series of novel 2-(2-aminopyrimidine-4-yl)phenol derivatives were designed and synthesized. The modification was done mainly on substituent at 4-position of phenol. Antiproliferative activities of compounds against human cancer cell lines were studied by MTT assay. Structure activity relationship will be discussed.

일시: 2012년 4월 25~27일(수~금) 3일간

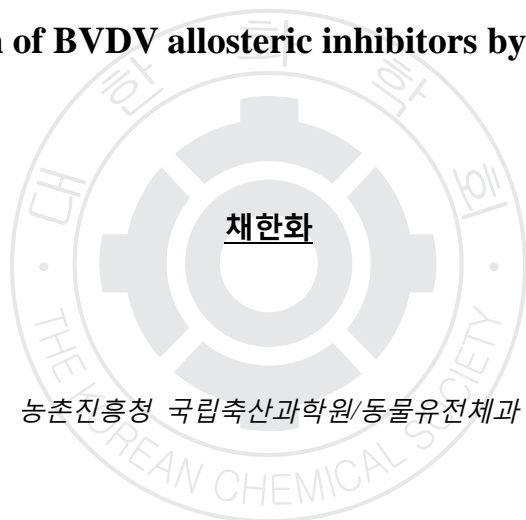
장소: 일산KINTEX

발표코드: MEDLP-1004

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Classification of BVDV allosteric inhibitors by decision trees



The Flaviviridae pestivirus genus includes animal pathogens of major economic impact for the livestock industry such as Bovine Viral Diarrhoea virus (BVDV), Border disease and Classical Swine fever viruses. The allosteric inhibitors would share structurally common features and physical properties originated from conserved residues of binding site of the RNA-dependent RNA polymerase (RdRP) in the family. The classification of known BVDV allosteric inhibitors focused on the binding site can be useful in the designing of effective inhibitors. Data set containing 1200 inhibitors was collected from the published literatures. The nature of the descriptors employed in classification trees can reveal structural requirements that make a molecule inhibitory activity against BVDV. Classification methods including genetic function approximation (GFA), recursive partitioning (RP) were applied to analyze the structure-activity relationship using 2D/3D molecular structural descriptors. To guide splitting criteria and optimize decision tree, the predictabilities of our classification models were validated using external test sets that were selected randomly. The decision tree classifying BVDV inhibitors gave the key descriptors and



these descriptors to represent structure pattern providing useful additional insight into what the common features to inhibitors would enhance activity. The classification models could be used to the screening protocols for new inhibitor molecules against BVDV RdRp.



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1005

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Antiangiogenic Activity of Artemisinin-Glycolipid Hybrids on Chorioallantoic Membranes

민동국 임은영 김민규 정만길

연세대 화학과

Artemisinin, a sesquiterpene isolated from *Artemisia annua* L., and its derivatives have been used clinically to treat drug-resistant malaria. Recently, artemisinin and its derivatives have been demonstrated to exert antitumor activity by in vitro and in vivo studies, suggesting that it may be used in anticancer strategies. Novel hybrids of non acetal and acetal-type derivatives at C-12 of artemisinin and glycolipids were synthesized via efficient coupling reactions. Some of these hybrids showed potent in vivo antiangiogenic activity on the chorioallantoic membrane (CAM) that was higher than or comparable to those of fumagillin and thalidomide at a concentration of 2.5 nmol.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1006

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of a Dual-Labeled Probe of Dimethyl Lithospermate B with Photochemical and Fluorescent Properties

임은영 민동국<sup>1</sup> 김민규<sup>2</sup> ricci jeremy michel 정만길

연세대 화학과 <sup>1</sup>연세대 이과대학 <sup>2</sup>연세대 화학과

Dimethyl lithospermate B (DLB) is a highly potent natural antioxidant and antidiabetic polyphenol with unknown mode of action. To determine its cellular targets, a photochemical and fluorescent dimethyl lithospermate B probe was designed and efficiently synthesized. The dual-labeled chemical probe for biological application was evaluated by UV and fluorescence to determine its electrochemical absorption and emission properties. This probe could be valuable for investigating ligand-protein interactions and subcellular localization.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MEDLP-1007

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Discovery of Artemisinin-Glycolipid Hybrids as Anti-oral Cancer Agents

박용서 김민규 민동국<sup>1</sup> 임은영 ricci jeremy michel 정만길

연세대 화학과 <sup>1</sup>연세대 이과대학

Novel artemisinin-glycolipid hybrids were directly synthesized from 12b (C?-C)-type deoxyartemisinin and glycolipid and exhibited exceptional in vitro anticancer activity, particularly against the oral carcinoma cancer cell lines, respectively. The artemisinin-glycolipid hybrids, with effective concentrations under 20uM, demonstrated better anticancer activity than either artemisinin or glycolipid alone and showed five times more anti-oral cancer activity than either cisplatin or paclitaxel.

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발표코드: MEDLP-1008

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Molecular modeling of 3-(4,5,6,7-tetrahydro-3H-imidazo[4,5-c]pyridin-2-yl)-1H-quinolin-2-ones as VEGFR-2 kinase inhibitors

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A series of 3-(4,5,6,7-tetrahydro-3H-imidazo[4,5-c]pyridin-2-yl)-1H-quinolin-2-ones have been identified as a new class of VEGFR-2 kinase inhibitors. To provide a rationale for the experimental in vitro activities of the quinolinone derivatives, docking and 3D-QSAR analysis on their structure and VEGFR-2 inhibitory activity was performed. A representative high active compound was predicted by this QSAR modeling and verified by experimental data. Described herein are the SAR of the compounds on VEGFR-2 kinase activity.

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발표코드: MEDLP-1009

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and in vitro Antibacterial Activity of Novel 3-Azabicyclo[3.3.0]octanyl Oxazolidinones

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케모인포메틱스연구센터

The increasing use of antimicrobials has resulted in many pathogens developing resistance to the existing powerful drugs. Consequently, there is a pressing need to develop new antibiotics to keep place with bacterial resistance. The introduction of linezolid (marketed under the trade name Zyvox) gave a new chemical class of oxazolidinone-containing antibacterial. Linezolid binds to 50S ribosomal subunit and inhibits the formation of 70S complex leading to the inhibition of protein synthesis. To date, numerous new derivatives with varied structural modifications have been reported in various patent reviews and scientific literature but none of these have led to the development of a new drug belonging to the oxazolidinone class. We synthesized series of oxazolidinone-type antibiotics in which the C-ring has been modified by substituted azabicyclic ring. Acetamide or triazoles heterocycle was used as C-5 side chain of oxazolidinone. The resulting series of compounds was then screened in-vitro against panel of

susceptible and resistance Gram-positive, Gram-negative bacteria and *Mycobacterium tuberculosis* (Mtb) H37Rv. Almost derivatives of this series exhibited good activity against the tested bacteria. Three of these compounds showed better activity over the reference compound linezolid. Four of these compounds were more active than linezolid against Mtb and another four are more active against *Haemophilus influenzae* (Hi).



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발표코드: MEDLP-1010

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and Pharmacological Evaluation of New Pyrazole and Isoxazole Derivatives for the Treatment of Neuropathic Pain

이주현 염수연<sup>1</sup> 강순방<sup>2</sup> 금교창<sup>3</sup>

고려대 화학과 <sup>1</sup>고려대 화학 <sup>2</sup>KIST 뇌의약연구단 <sup>3</sup>KIST 케모인포메틱스연구센터

Neuropathic pain is a debilitating chronic syndrome that often arises from injuries to central and peripheral nerves. Such pain has been hypothesized to be the result of an aberrant expression and function of calcium channels at the site of injury. In particular, the expression and modulation of the T-type calcium channel plays a key role in the pathogenesis of neuropathic pain, and blocking this channel is well known to be therapeutically important.



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발표코드: MEDLP-1011

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Discovery of aminopyridine derivatives substituted with benzoxazole as c-Met kinase inhibitors

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c-Met is a receptor tyrosine kinase that is expressed in endothelial and epithelial cells. In normal cells, c-Met is activated by its ligand, hepatocyte growth factor (HGF)/scatter factor (SF). When HGF binds to c-Met, causes receptor dimerisation and autophosphorylation of tyrosines 1234 and 1235, and phosphorylated c-Met subsequently triggers the activation of downstream signaling pathway. According to the role of c-Met signaling in cancer progression and metastases, the c-Met receptor is considered a potential target for cancer therapy. The c-Met kinase inhibitors are able to block autophosphorylation of the c-Met kinase, thereby interrupting its downstream signaling pathways. We have performed docking of aminopyridine derivatives substituted with benzoxazole complexed with c-Met kinase to study the orientations and preferred active conformations of these inhibitors. Docking helped to analyze the molecular features which contribute to a high inhibitory activity for the studied compounds. In addition, the predicted biological activities of the c-Met kinase inhibitors, measured as IC<sub>50</sub> values were obtained

by using quantitative structure?activity relationship (QSAR) methods: Comparative molecular field analysis (CoMFA) and comparative molecular similarity analysis (CoMSIA).



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발표코드: MEDLP-1012

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Role of Korea Chemical Bank in Hit Evaluation after HTS using Diversity Chemical Library

황순희 김선우 김선호

한국화학연구원 한국화합물은행

한국화합물은행은 산.학.연 등에서 기탁한 22 만여 종의 화합물을 관리하고 있으며, 현재까지 430 개 작용점에 대한 고효율약효시험(HTS) 활용과 도출된 100 개 작용점에 대한 Hit 를 대상으로 한 선도물질화 연구를 지원하며 다양성이 확보된 화합물로 구성된 독창적인 라이브러리를 운영하여 신물질개발 분야에서 선진국과의 격차를 극복하려 한다. 또한, HTS 후 도출된 Hit 평가 과정에서 Hit 화합물의 순도 및 유도체 검색을 통한 SAR 자료, Pre-ADME 검색을 통한 선도물질성 결과 등을 관련기관에 제공하고 있다. 아울러 Hit 발생 빈도가 높은 화합물 골격에 대한 조사를 통하여 false positive 에 대한 일반적 정보를 제공하여 선도물질개발을 위한 Hit 평가를 좀 더 효율적으로 진행할 수 있도록 하고 있다, 그 결과 독창적인 골격을 지닌 Hit 가 다량 도출되고 있으며, 그 중 항암제, 당뇨병 및 난치성 질환과 관련된 Hit 화합물로 후속연구가 진행 중에 있다.

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장소: 일산KINTEX

발표코드: MEDLP-1013

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Docking-based 3D-QSAR and pharmacophore modeling study for c-Met inhibitor

송인식 이주연<sup>1</sup> 조성윤<sup>2</sup> 이광호<sup>3</sup> 채종학<sup>4</sup> 이성광

한남대 화학과 <sup>1</sup>충북대 화학과 <sup>2</sup>한국화학연구원 난치성질환치료제연구센터 <sup>3</sup>한국화학연구원  
신물질본부/난치성 <sup>4</sup>한국화학연구원 신물질연구본부/신약플랫폼기술팀

On binding to the cell surface receptor tyrosine kinase (TK) known as mesenchymal epithelial transition factor (c-Met), hepatocyte growth factor (HGF) contribute to oncogenesis and tumor progression in several human cancers and promotes aggressive cellular invasiveness that is strongly linked to tumor metastasis. 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 79 compounds (in-house data), with comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). 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 the active site to further elucidate the accuracy of the models.

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발표코드: MEDLP-1014

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Antimycobacterial Activity of 1,3,4-thiadiazoles

이일영 강민서<sup>1</sup> 김필호<sup>2</sup> 김종승<sup>1</sup> Helena Boshoff<sup>3</sup> Clifton E. Barry<sup>3</sup>

한국화학연구원 감염증치료물질연구팀 <sup>1</sup>고려대 화학과 <sup>2</sup>한국화학연구원 난치성질환치료제연구센터 <sup>3</sup>National Institutes of Health

Approximately one third of the world's population is infected with Mycobacterium tuberculosis. 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 against this disease. The emerging serious problem both in terms of TB control and clinical management prompted us to synthesize derivatives of 2,5-disubstituted 1,3,4-thiadiazoles. All synthesized compounds were assayed in vitro for antimycobacterial activity against the H37 Rv strain of Mycobacterium tuberculosis. The synthesis and activity as well as the structure-activity relationships of these compounds will be discussed.

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장소: 일산KINTEX

발표코드: MEDLP-1015

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Evaluation of (3,5-dimethyl)-pyrazole derivatives as GPR109A agonists

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한국화학연구원 <sup>1</sup> 한국화학연구원 의약화학연구센터

3,5-Dimethylpyrazole derivatives were synthesized and biologically evaluated as full agonists for the high affinity niacin receptor GPR109A. The (3,5-dimethyl)pyrazole ring was formed by the condensation reaction of various 3-substituted pentane-2,4-dione and hydrazine hydrate. The 1-position of pyrazole was further diversified with (pyridine-3-yl) carbonyl or (pyrazine-3-yl) carbonyl derivatives to elucidate the structure activity relationships. The activation activity of the synthesized compounds on GPR109A was evaluated using the GPR109A overexpressed cell lines.

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발표코드: MEDLP-1016

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design, synthesis and biological evaluation of protease-activated receptor 2 (PAR2) antagonists for the treatment of arthritis

차지현 조남철<sup>1</sup> 고훈영 배애님<sup>2</sup>

인하대 화학과 <sup>1</sup>연세대 생명공학과 <sup>2</sup>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  $\beta$ -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 quinazoline derivatives was 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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발표코드: MEDLP-1017

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Biological Evaluation of Serotonin Receptor Agonist as Antiobesity

서용완 배애님<sup>1</sup>

인하대 자연과학대학 화학과 <sup>1</sup>KIST 생체과학연구본부

The 5-HT<sub>2C</sub> receptors appear to be restricted to the central nervous system (CNS) where it demonstrates a wide distribution. The receptors have been considered as therapeutic targets for the treatment of various central nervous system disorders such as depression, anxiety, epilepsy, schizophrenia, and sleep disorders. Also, 5-HT<sub>2C</sub> receptors have been considered as target receptor for anti-obesity. However, the limit to the development of up to the present does not possess good selectivity and specificity of drug candidates to the receptors. They also activate 5-HT<sub>2A</sub> and 5-HT<sub>2B</sub> receptors, resulting in various side effects associating to these receptors, hallucination and valvular hypertrophy respectively. Therefore, anti-obesity drug candidates are greatly focused on developing more selective and specific 5-HT<sub>2C</sub> agonists. As part of discovering novel 5-HT<sub>2C</sub> agonists, we designed and synthesized 40 compounds. The synthesized compounds were biologically evaluated against 5-HT<sub>2C</sub>. The detailed design, synthesis and biological evaluation of 5-HT<sub>2C</sub> agonists as anti-obesity drugs will be presented.

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발표코드: MEDLP-1018

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Identification of a novel Protease-Activated Receptor 2 antagonist using a virtual screening approach

조남철 차지현<sup>1</sup> 노경태 배애님<sup>2</sup>

연세대 생명공학과 <sup>1</sup>인하대 화학과 <sup>2</sup>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. The inhibition of PAR2 activation by small molecule antagonists may provide a pharmacological basis for interfering with these acute processes. In the present work, we have generated a pharmacophore model for PAR2 antagonist to identify novel compounds. The pharmacophore model was comprised of 4 hydrophobic feature, one hydrogen bond acceptor and one hydrogen bond donor. This model was virtually screened to the databases of 2.1 million compounds and hits subsequently were filtered by 8 criteria such as fitvalue, drug properties and *in silico* ADMET tests. Consequently, two compounds were found by cell-based PAR2 assay and anti-inflammatory test as specific PAR2 antagonist. Moreover, these compounds can be raised into a potential anti-inflammatory drug candidate after optimizing and passing several phases of clinical trials.

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발표코드: MEDLP-1019

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design, Synthesis and Biological Evaluation of Substitued Antofine Analogues

권용석 김상희

서울대 약학대학/약학과

Phenanthroindolizidine alkaloids are pentacyclic natural products isolated mainly from *Cynachum*, *Pergularia*, *Tylophora*, and some genera of the *Asclepiadaceae* family. These pentacyclic natural products exhibit a variety of biological effects including antiamebic, antibacterial, antitumor, antifungal, and antiviral activities. Especially, (-)-antofine has received significant attention as a potential anticancer agent, due to the profound cytotoxic activity against various cancer cell lines. However, this class of natural products has not yet been developed for clinical use, because of the serious central nervous system toxicity. To overcome these unsuitable properties, structural modifications are deemed necessary. In an attempt to reduce drawbacks of phenanthroindolizidine alkaloids, we designed the analogues in which the hydrogen atom of antofine was replaced with a hydrophilic group such as hydroxymethyl or carboxylic group. We envisioned that this modification would add hydrophilic character to the molecule, thus lowering the BBB permeability and increasing the water solubility. Herein, we reported the efficient

synthesis of the designed polar antofine analogues in chiral forms as well as in racemic forms and their in vitro anticancer activity.



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발표코드: MEDLP-1020

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis, Urease Inhibition, Antioxidant and Antibacterial Studies of Some 4-Amino-5-aryl-3*H*-1,2,4-triazole-3-thiones and their 3,6-Disubstituted 1,2,4-Triazolo[3,4-*b*]1,3,4-thiadiazole Derivatives

Muhammad Hanif Muhammad Saleem Muhammad T. Hussain<sup>1</sup> Nasim H. Rama Sumera Zaib<sup>2</sup> Muhammad Adil M. Aslam<sup>2</sup> Peter G. Jones<sup>d2</sup> Jamshed Iqbal<sup>2</sup>

*Department of Chemistry, Quaid-i-Azam University*<sup>1</sup>*Department of Applied Sciences, National Textile University*<sup>2</sup>*Department of Pharmaceutical Sciences, COMSATS Institute of Information Technology*

A new series of 4-amino-5-aryl-3*H*-1,2,4-triazole-3-thiones, bearing various methoxybenzyl and methoxyphenethyl groups, was synthesized by refluxing potassium hydrazinecarbodithioate salts in dilute aqueous solution of hydrazine hydrate. These salts were formed by the reaction of acid hydrazides and carbon disulfide in methanolic potassium hydroxide solution at 0-5 °C. 4-Amino-5-aryl-3*H*-1,2,4-triazole-3-thiones were condensed with different substituted aromatic acids to yield 3,6-disubstituted-1,2,4 triazolo[3,4-*b*]1,3,4-thiadiazoles. The structures of the newly synthesized compounds were characterized by infrared (IR), <sup>1</sup>H and <sup>13</sup>C nuclear magnetic resonance (NMR) spectroscopies, elemental analysis and mass spectrometric (MS) studies. Structure of one of the compounds was further confirmed by single crystal X-ray diffractometry (XRD). All the synthesized compounds were screened for their

urease inhibition, antioxidant and antibacterial activities. Some compounds showed excellent urease inhibition activity, more than the standard drug. Others exhibited potent antioxidant activity. All the compounds showed significant antibacterial activities as compared to standard drug.



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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Design and synthesis of triazole-based inhibitors of influenza virus Neuraminidase

정강연 김태우 Tasneem Islam<sup>1</sup>

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Influenza is a major cause of mortality, particularly in children and the elderly. The global impact of influenza epidemics is estimated to be 3.5 million cases of severe illness and 300,000 to 500,000 deaths annually. Protection through vaccination is limited due to the antigenic variation of the influenza virus. Antiviral agents, thus far remain an important approach to epidemic influenza. Rational drug design has led to the discovery of the two anti-influenza drugs currently being used to treat infected patients (oseltamivir, Tamiflu<sup>TM</sup> and zanamivir, Relenza<sup>TM</sup>). Reports of the emergence of drug resistance make the development of new anti-influenza molecules a priority. Two sialic acid recognizing proteins, hemagglutinin and sialidase, on the viral surface have been shown to be crucial in invasion and have provided many exciting opportunities for rational structure-based drug discovery of anti-influenza agents. To date the most successful structure-based anti-influenza drug discovery has arisen from targeting the

sialidase function. In order to study important recognition features required in the inhibition of sialidase, we synthesized a range of sialyl nucleoside mimetics based on very inexpensive carbohydrate. D-Fructose was used as a substrate for the efficient preparation of 1,2,3-triazole derivatives using the copper-catalyzed azide-alkyne Huisgen cycloaddition ("click chemistry"). As a preliminary study, a small library of 1,2,3-triazole-linked D-fructose derivatives has been synthesized in good yield which will be screened for its influence on influenza neuraminidase inhibitory activity.





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발표코드: MEDLP-1022

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of prenylated hydroquinone, quinone, and chromene natural products and their biological activity

이석준 오상태 지정희

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Because more than 70% of the Earth's surface is covered by oceans, many marine plants are used for food, a source of minerals, dietary fiber, nutrition, and medicine. Numerous marine natural products and their unique constituents have been found to be useful for pharmacological studies to treat various diseases. Diverse hydroquinones, quinones, and chromenes with prenyl units originated from marine sources show various biological activities such as cytotoxicity against cancer cells, vasodilatation effect on basilar artery, cholinesterase inhibition effect for Alzheimer's disease, lipid peroxidation inhibitory effect, and antioxidation effect. Recently, we efficiently synthesized several prenylated hydroquinones, quinones, and chromenes compounds and obtained interesting biological activities of synthetic and natural products. In this presentation, we will show the results.

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## Synthesis of Artemisinin with Substituted Sulfidyl or Sulfonyl Moiety and Their Anti-angiogenesis Activity

이석준 오상태 지정희

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Artemisinin, a natural endoperoxide sesquiterpene isolated from *Artemisia annua* L. and its synthetic derivatives are popular antimalarial agents and are recently being considered as potential lead compounds in the discovery of drug for various human diseases. Although Chen et al. had previously reported that artemisinin, dihydroartemisinin, and artesunate have a weak antiangiogenesis effect; we were the first to discover that the addition of substituted sulfide or sulfone functionality to the C-10 position of artemisinin enhances the inhibitory effect of artemisinin against angiogenesis. Based on our preliminary results, we constructed a novel series of anti-angiogenesis agents for a potential anticancer drug using an acid-catalyzed substitution reaction of 3 with various thiols as a key reaction and reported the anti-angiogenesis effect.

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## Synthesis and preliminary evaluation of activity of potential inhibitors of Nitric Oxide Synthase (NOS)

Ashrafuzzaman MD 정찬성<sup>1</sup>

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NOSs (Nitric Oxide Synthases) are the only enzymes known to simultaneously require five bound cofactors/prosthetic groups; FAD, FMN, Haem, tetrahydrobiopterin (BH<sub>4</sub>) and Ca<sup>2+</sup>-calmodulin (CaM). NO (Nitric Oxide) is an important cellular signaling molecule, having a vital role in many diverse biological processes. NOS catalyzes the synthesis of Nitric Oxide (NO) from the terminal nitrogen atom of L-arginine (L-Arg) in the presence of NADPH and dioxygen (O<sub>2</sub>). In mammals, three distinct genes encode NOS isozymes: neuronal (nNOS or NOS<sub>1</sub>), cytokine-inducible (iNOS or NOS<sub>2</sub>), and endothelial (eNOS or NOS<sub>3</sub>). NOSs are usually existed as dimer in their active form, required BH<sub>4</sub>((6R))-5,6,7,8-tetrahydrobiopterin) by cofactor. Recently, Bacterial NOS (bNOS) has been shown to protect bacteria against oxidative stress, diverse antibiotics, and host immune response. Although NO mediates several physiological functions, its overproduction has been reported in a number of clinical disorders, including neurodegenerative disorders (Parkinson's disease, Alzheimer's disease). Our designed pyrimidine

derivatives were synthesized by Vilsmeier-Haack reaction and cyclization. Block the  $\text{BH}_4$  binding site using our designed compounds induce instabilization of NOS, as a result, overproduction of NO is expected to be reduced, which could therefore be a useful intervention in the treatment of various diseases.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Structure-based Virtual Screening and Biological Assay for Matrix Metalloproteinase-1 inhibitors

정종영 노경태<sup>1</sup>

(사)분자설계연구소 신약개발팀<sup>1</sup> 연세대 생명공학과

Skin photoaging is a complex process involving a number of intrinsic and exogenous causes. Exogenous aging is caused by extrinsic harmful environments, which activate the decline of many physiological processes such as elasticity and melanogenesis control. The signal pathway activated by UV expresses MMP-1 to disrupt collagen structure in the skin tissue to culminate skin wrinkle and laxity. Generally MMP isozymes have multiple subsites near catalytic Zinc ion in Catalytic domain. These subsites determine substrates specificity of MMP isozymes. One MMP-1 structure have a large hydrophobic pocket of S1-prime subsite, which is the significant subsites near catalytic Zinc ion to determine substrate specificity in MMP family. The Pharmacophore query was designed based on this MMP-1 structure with a large S1-prime subsite. The pre-built chemical library with over 3.5 million compounds was filtered with several Zinc binding group substructures before virtual screening. This focused library was screened with pharmacophore query to select hit compounds, which insert substructures into the large S1-prime

substitute. Finally 20 hit compounds were selected as candidates of MMP-1 inhibitor and its inhibitory activity was evaluated on MMP-1 enzyme assay.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Isolation and biological activities of psammaplycin analogs from the tropical marine sponge

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Psammaplysin, known to exhibit potent antimalarial activities, are nonterpenoid secondary metabolites derived from bromotyrosine. In the course of our search for bioactive substances from the tropical marine sponges, eight psammaplysin analogs have been isolated. They exhibited moderate to high inhibition activities against the growth of cancer cell lines.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Isolation and biological activities of irciniastatins from the tropical marine sponge *Ircinia ramosa*

유수정 이희승<sup>1</sup> 이연주<sup>2</sup>

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Irciniastatins (also known as psymberin) reported to exhibit selective cancer cell growth inhibition at nanomolar level concentrations, have been isolated from the tropical marine sponge *Ircinia ramosa* collected from Chuuk, Micronesia. Further investigations are underway to discover other irciniastatin analogs.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## A potent chondrogenic small molecule in hBM-MSC

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서울대 화학과 <sup>1</sup>서울대 화학부

Mesencymal stem cells (MSCs), which are multipotent cells that can differentiate into cartilage, bone and adipose et al, can synthesize cartilage specific extracellular matrix (ECM) abundant in collagen type II and glycosaminoglycan (GAG) as the result of chondrogenesis in chemically defined medium including dexamethasone and transforming growth factor- $\beta$  (TGF- $\beta$ ) superfamily such as TGF- $\beta$ 1, TGF- $\beta$ 3 and bone morphogenetic protein (BMP). For this reason, the cell-based repair of articular cartilage defects using chondrocytes formed by the differentiation of MSCs should be expected to improve clinical outcome. However, it is a considerable factor that high doses TGF- $\beta$  is able to generate undesired side effects such as synovitis, pannus formation, cartilage erosion or joint effusion and TGF- $\beta$  levels are considered as a potential marker in cancer patients. Furthermore, TGF- $\beta$  and dexamethasone are not specific chondrogenic differentiation factor. In recent, small molecules that can selectively control proliferation and differentiation of stem cells through the temporal perturbation of target biological materials have been emerging as alternative to nonspecific differentiation methods. Thus, the

identification of potent and specific small molecule modulators credible alternative to TGF- $\beta$  for inducing chondrogenesis should gain insight into the developmental mechanisms of MSCs and improve the efficiency of clinical trials. To address this issue, we report the novel synthetic small molecules 5a, which can selectively differentiate human bone marrow derived MSCs (hBM-MSCs) into chondrocyte.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Protective effects of cleavage agents on INS-1 cells against h-IAPP-induced apoptosis

조민하 배형은 최원석 한슬기 박두한 정근홍<sup>1</sup>

삼육대 화학과 <sup>1</sup>육군사관학교학교 화학과

Recently, the properties and its apoptosis of amyloid proteins have been the topic of many investigations. We have been trying to synthesize cleavage agents which showed cleavage yields as much as 9~14%, which does not sufficiently support the agents' protection of beta-cells from the cytotoxicity of h-IAPP. In vivo tests of INS-1 cells were carried out to better understand the potential of using these cleavage agents as drug candidates.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Kinetic Study of Artificial Metalloprotease Using Metal-Organic Ligand Complex

오윤탁 배형은<sup>1</sup> 김경진<sup>1</sup> 박두한<sup>1</sup> 정근홍<sup>2</sup>

삼육대 융합과학과 <sup>1</sup>삼육대 화학과 <sup>2</sup>육군사관학교 학교 화학과

Peptide bond hydrolyzing is very challenging in normal condition in terms of its stability. There have been great interests in synthesizing metalloproteases using transition metal ions. Among them, Cu(II) ion has been used as a key catalytic group in developing artificial metalloprotease. In this study, we carried out the researches about the kinetic studies on proteolysis by Cu(II) ion ligand complexes. This will provide another crucial information about that the catalytic drug candidates, which have been uses Cu(II) ion, would not affect significantly on normal proteins in body.

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## Structure Guided Synthesis of Ixoazole Library and Discovery of PPAR $\gamma$ -Selective Agonists

고민설 박종민 구자영 박승범

서울대 화학부

The peroxisome proliferator-activated receptors (PPARs) have been focused due to their roles related to the glucose, lipid, and lipoprotein homeostasis. There are three PPAR subtypes (termed PPAR alpha, PPAR delta, and PPAR gamma) according to their distinct genetic profiles. Among them, PPAR gamma activation via small molecule ligands has important pharmaceutical meaning for the control of metabolic disorders, cancer and inflammation. We designed ligand library based on the crystal structures of ligand binding domain of the PPARs. Because conventional PPAR ligand has common molecular framework, (1) an acidic head part, (2) a linker part, (3) a hydrophobic tail part, we designed our molecular library mainly based on those characters. Especially, we focused on the linker part and hydrophobic tail part. The key moiety of the ligand is isoxazole and N-carbamoylated urethane, which can give the additional hydrogen bonding and enhances hydrophobic interaction. Primary round of moiety selection was performed using the transactivation reporter assay result of simple carbamate library. We concluded that the PPAR gamma can

be a selective target out of the other subtypes and the ethyl substituent is the best option for fitting to the middle region of the PPAR gamma active site and subsequent activation. Next, we introduced carbamoyl moiety to the tail part for make enhanced fitting. Finally, we discovered PPAR gamma selective agonist with single digit nanomolar activity. This discovery demonstrated that computational chemistry combined with rational design and combinatorial chemistry is a powerful tool to decipher the complex structure-activity relationship.



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## Heteroaromatic Moieties in the Sphingosine Backbone of $\alpha$ -Galactosylceramides for Noncovalent Interactions with CD1d

송희범

서울대 자연과학대학 화학부

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- $\gamma$ , TNF- $\alpha$ ) or immunomodulatory response (e.g., IL-4, IL-10), respectively. Disruption of the balance between Th1 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 describe synthesis of a new galactosylceramides containing new ceramide skeleton as KRN7000 analogues.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile one-pot synthesis of thiol-functionalized hollow silica microspheres

박지훈 김정민 최인성

KAIST 화학과

Hollow silica microspheres have attracted much attention due to their versatile applications to catalysis, drug delivery, and biosensor. In the conventional synthetic method, polymer particles, such as polystyrene (PS) particles, were chosen as a template of the silica wall. The selected dissolution step of polymer core was performed, at last, to form hollow silica microspheres. Although this method was able to generate mono-dispersed hollow silica microspheres, these multiple steps seemed to be time consuming. Moreover, it is formidable to select appropriate dissolution solvent and calcination temperature in varied conditions. In this context, the novel synthetic method should be presented to meet the growing interest of biological applications. Herein, we present the one-pot synthetic method of thiol-functionalized hollow silica microspheres. Our synthetic method is simple and highly applicable to biological applications because we adopted cysteamine, which could direct the hydrolysis of silicon alkoxides, as a catalyst.



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## Size- and shape-controlled synthesis of Ag nanomaterials via proton beam irradiation

송재희

순천대 화학과

We present a facile one-pot synthetic route for the preparation of silver nanocrystals via a simple proton beam irradiation process at room temperature. Size- and shape-controlled silver nanostructures were prepared in an aqueous phase-based solution without the addition of any harsh reductants. Morphologies of the prepared nanostructures were controlled just by changing the stabilizer and by controlling the molar concentration ratios of surfactants to metal precursors. It was observed that the size of the resulting Ag nanocrystals was easily varied by changing the stabilizer from hexadecyltrimethylammonium bromide to sodium dodecyl sulfate. We also found that the size of the prepared silver nanocrystals was decreased as the molar ratio of hexadecyltrimethylammonium bromide to silver ion was increased.

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## Surface modification of MWCNT and preparation of MWCNT-Ag-NPs hybrids via proton beam irradiation

송재희

순천대 화학과

Hybrids of multi-walled carbon nanotubes with metal nanomaterials are attractive candidates for the use in catalysis, energy storage, and nanotechnology. Among them, CNT-Ag nanocomposites drew significant attention due to their potential applications in advanced materials. In this study, we report a new synthetic route to decorate carbon nanotube (MWCNT) with silver nanoparticles (Ag-NPs) via a simple proton beam irradiation process at room temperature. The surfaces of MWCNTs were functionalized with thiol groups through several steps including oxidation. Shape of the prepared silver on the surface- modified MWCNT was spherical and the diameter of the silver was in the range of ~4 nm. The characterization has been done by using FE-TEM, and EDS analysis.

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## Synthesis and Luminescence Characteristics of Nanosized $\alpha'$ - and $\beta$ -Sr<sub>2</sub>SiO<sub>4</sub> Phosphors

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Yellow phosphors combined blue emitting semiconductor chips for white light emitting diodes (LEDs) have attracted the considerable interest due to facile fabrication, high brightness and long lifetime. In order to obtain the maximum efficiency, the phosphors should absorb the light from LED emission as much as possible. In this work, nanosized Sr<sub>2</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> phosphors were synthesized from nanosized SiO<sub>2</sub> particles prepared by a sol-gel method. Morphology, crystal structure, and optical properties Sr<sub>2</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> were examined by a scanning electron microscope (SEM), a powder X-ray diffractometer (XRD) and a spectrofluorometer. The excitation spectrum of Sr<sub>2</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> exhibited a broad band in the wavelength range from 300 nm to 460 nm, which is mainly due to 4f<sup>7</sup> → 4f<sup>6</sup>5d transition of the Eu<sup>2+</sup> ion. Two emission bands at 490 nm (green) and 560 nm (yellow) with varying intensity were observed in the luminescence spectra. The  $\beta$ -Sr<sub>2</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> phosphor had higher photoluminescence intensities than the

$\alpha'$ - Sr<sub>2</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> phosphor. The emission characteristics of the  $\alpha'$ - and  $\beta$ -Sr<sub>2</sub>SiO<sub>4</sub> Doped with Eu<sup>2+</sup> phosphors were examined and discussed in detail.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Analysis of structure of Spinel $\text{LiMn}_2\text{O}_4$ with different Li content by neutron diffraction analysis

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Spinel  $\text{LiMn}_2\text{O}_4$  became one of the most attractive material for rechargeable Li-ion batteries because of the intrinsic advantages, such as, structural stability, moderate capacity(148mAh/g), high voltage capability, low material cost, and environmentally safety. In the stoichiometric  $\text{LiMn}_2\text{O}_4$ ,  $\text{Li}^+$  ion is occupied 8a site (tetrahedral site).  $\text{Mn}^{3+}$  ion and  $\text{Mn}^{4+}$  ion are occupied 16d site (octahedral site). When small excess amount of Li-ion is added to  $\text{LiMn}_2\text{O}_4$ , the extra Li-ion will occupy other sites, such as 8b site and 16c site in the spinel structure. The Li-ion has a small scattering factor of X-ray. Neutron diffraction analysis can distinguishes between different atomic isotopes, resolve light atoms in material. In this study, spinel  $\text{LiMn}_2\text{O}_4$  of different Li contents, i.e.  $\text{LiMn}_2\text{O}_4$  and  $\text{Li}_{1.07}\text{Mn}_2\text{O}_4$ , were synthesized from the  $\text{Mn}_3\text{O}_4$  precursor. The crystal structure of the materials were examined by X-ray diffraction and neutron diffraction analysis, for in-depth analysis of  $\text{LiMn}_2\text{O}_4$  of different Li content. Coin-type (CR2032)

Li-ion rechargeable batteries with the cathode of the  $\text{LiMn}_2\text{O}_4$  were assembled and tested their electrochemical performance.



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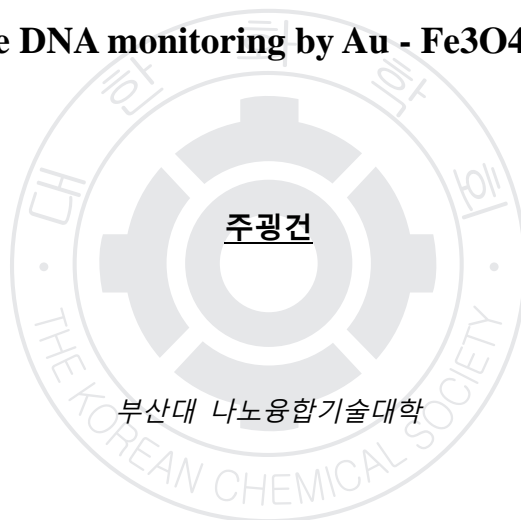
장소: 일산KINTEX

발표코드: MAT.P-1038

발표분야: 재료화학

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## Ultrasensitive DNA monitoring by Au - Fe<sub>3</sub>O<sub>4</sub> nanocomplex



Quantitative detection of biomolecules has become increasingly important in a variety of fields, including medical diagnostics, food safety, and anti-bioterrorism. We report a simple, sensitive, and inexpensive quantitative approach for DNA detection based on the optical properties of gold nanoparticles and gold-coated magnetic nanoparticle hybrids. We employed a simple one-step reaction to synthesize gold-coated iron oxide nanoparticles (Fe<sub>3</sub>O<sub>4</sub>@Au NP). Fe<sub>3</sub>O<sub>4</sub> nanoparticles were used as the central core for preparation of Fe<sub>3</sub>O<sub>4</sub>@Au in an aqueous state without precipitation and aggregation of nanoparticles. Citrate-coated Fe<sub>3</sub>O<sub>4</sub> nanoparticles were prepared and subsequently coated with Au layers through reduction of HAuCl<sub>4</sub> by citrate on the surface Fe<sub>3</sub>O<sub>4</sub>. The resulting Fe<sub>3</sub>O<sub>4</sub>@Au nanoparticles showed good paramagnetic properties and were coated with thin layers of gold atoms (~10 nm) having an average diameter of ca. 20 nm. These magnetic nanoparticles were well-dispersed in water and stable at physiological pH without precipitation. Nucleic acid-functionalized Fe<sub>3</sub>O<sub>4</sub>@Au nanoparticles were then hybridized with complementary target DNA molecules. The Au-Fe<sub>3</sub>O<sub>4</sub>@Au nanocomplex remains in

solution at a concentration proportional to the concentration of the target DNA and its optical properties allow it to be easily quantified using UV/Vis absorption spectroscopy. The limit of detection for this method was as low as 0.1fM. This selectable detection system is easy to operate, inexpensive, and versatile, making it a candidate for future use in predicting the seafood safety risks through detection of different DNA sequences and any related genetic mutations.





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## Mechanical Properties of Multilayered Chitosan/CNT Nanocomposite Films

Sun Fangfang

부산대 나노융합기술학과

A multi-performance MWCNT-reinforced chitosan nanocomposite was fabricated by unique methods: a freeze-drying process associated with the sublimation and compression (SAC) method, and the casting-evaporation (CE) method. We obtained ordered and multilayered structures with limited porosity, and well-dispersed MWCNT structures of the chitosan nanocomposite, especially when the SAC method was used. In the case of the nanocomposite films prepared by the CE method, the mechanical strength and elongation were significantly increased by up to about 40% compared with the pure chitosan films. On the other hand, the ordered and porous multilayered pure chitosan films prepared by the SAC method showed significantly lower tensile strength and elongation compared to the pure solid chitosan films. However, the relative enhancement of the mechanical properties of multilayered MWCNT/chitosan nanocomposites with some porosity was higher, especially in terms of the elongation, which showed a twofold improvement in strain. The relaxed bond, which could be a relatively strong hydrogen bond, between the functional groups in the chitosan chains and the functionalized surface of the MWCNTs

might be stretched under stress, thereby improving the ductility of the multilayered nanocomposite films. In addition, the viscoplastic behavior of the films by the EC method could become more active with increasing strain rate. Interestingly, ordered and porous pure chitosan films did not reveal the viscoplastic behavior; it rather presented strain softening and viscoelastic characteristics. However, the interaction between the chitosan chains and the surface-modified MWCNTs could regenerate viscoplasticity of the chitosan films.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Topochemical Oxidation of Transition Metals in Layered Double Hydroxides by Anthraquinone-2-sulfonate

이종현 나정운<sup>1</sup> Dermot OHare<sup>2</sup> 정덕영<sup>3</sup>

가톨릭대 화학과 <sup>1</sup>가톨릭대 화학 <sup>2</sup>University of Oxford <sup>3</sup>성균관대 화학과

A novel synthetic approach to highly crystalline hydrotalcite-like  $\text{Co}^{2+}$  (or  $\text{Ni}^{2+}$ )- $\text{Fe}^{3+}$ -layered double hydroxides (LDHs) has been developed using a one-pot topochemical oxidation reaction by anthraquinone-2-sulfonate (AQS2) anions. The  $\text{Fe}^{3+}$ -bearing LDHs were synthesized through in situ redox reaction between  $\text{Fe}^{2+}$  ions and intercalative anions, AQS2, where the quinone groups in AQS2 anions induced a sole oxidation of  $\text{Fe}^{2+}$  into  $\text{Fe}^{3+}$  to form the LDH phase during the slow precipitation by using hydrolysis of hexamethylenetetramine. The LDH phases were confirmed and the refined lattice parameters were  $c = 60.0 \text{ \AA}$  and  $a = 3.12 \text{ \AA}$  ( $a = 2d(110)$ ) for the Co-Fe-LDH, and  $c = 60.3 \text{ \AA}$  and  $a = 3.08 \text{ \AA}$  for the Ni-Fe-LDH, respectively. The basal spacing of  $20.1 \text{ \AA}$  for the Co-Fe-LDH gave an effective separation of  $15.4 \text{ \AA}$  to accommodate the AQS2 anions with an antiparallel arrangement in the interlayer spaces of LDH. We found that the AQS2 anions played a key role in the oxidative intercalation process to minimize the structural deformation of the hydroxide layers during the topochemical oxidation of  $\text{Fe}^{2+}$ .

ions because of a strong intermolecular interaction between the AQS2 anions being self-assembled into the interlayer spaces of LDH. This unique topochemical oxidation procedure suggested in this study can be extended to prepare other important series of transition-metal LDHs in various  $M^{2+}/Fe^{3+}$  ratios for pure spinel ferrites.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Metal Ion-Enriched Polyelectrolyte Complexes and Their Utilization for Multilayer Assembly and Catalytic Nanocomposite Films

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Mixing of Ag<sup>+</sup> doped polyethyleneimine (PEI) and polyacrylic acid (PAA) produced polyelectrolyte complex particles (PECs) in solution. Positively charged Ag<sup>+</sup> doped PECs (PECs-Ag<sup>+</sup>) with spherical shape were deposited alternatively with PAA for multilayer assembly. The multilayered film involving PECs-Ag<sup>+</sup> was reduced to generate a composite nanostructure. Metal NP-enriched nanocomposite films were formed by additional post-adsorption of precursors on PECs within the films, which resulted in enhancing catalytic and electrical properties of the composite films. Since the films contain PECs which can response to pH changes and most of NPs are embedded in the PECs, interesting catalytic properties which are not expected in particle-typed catalyst were observed upon pH changes. Owing to reversibly structural changes of the films and tight immobilization of NPs within the films, film-typed catalysts showed enhanced performance and stability during the catalytic reaction under various pH conditions, compared to particle-typed catalysts.

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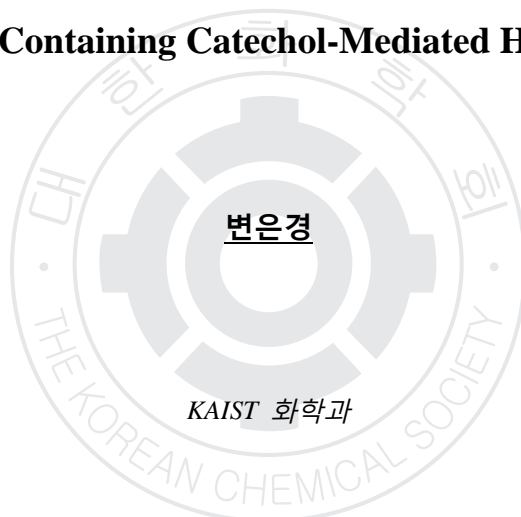
장소: 일산KINTEX

발표코드: MAT.P-1042

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Graphene-Containing Catechol-Mediated HA Hydrogel



Hydrogel has been widely investigated as a carrier for drug delivery. For example, hydrogel consisted of biocompatible polymers has been successfully used to encapsulate a variety of pharmaceuticals, such as peptides and proteins. The kinetically controlled released drugs from hydrogels can treat tissue-specific diseases. Recently, carbon material/hydrogel hybrid system has been of interest as a new hydrogel system, because it has advantages of the attractive structural reinforcement in biomedical applications. In particular, graphene that has unique physical, electrical, and thermal properties has been recognized as a novel biomaterial. Graphene-based materials offer not only an enormous potential but also wide applications. Among the various applications, many research groups are intensively exploring biomedical applications of graphene. In this study, we propose a novel graphene-based platform for anticancer drug delivery. Graphene oxide (GO) was chosen as a drug depot due to its excellent drug-loading efficiency originated from its lateral 2D shape and hydrophobic nature that are ubiquitous interactions between the drug and GO. GO was functionalized with 6arm-PEG-amine, and incubated with doxorubicin(DOX),

anticancer drug. After that, the resulting GO/DOX hybrids were mixed with catechol-conjugated hyaluronic acid, and the formation of hydrogel was immediately occurred after the addition of oxidizing agent,  $\text{NaIO}_4$ , into the solution. The prepared hydrogel showed relatively rigid mechanical property, and the controlled release of drug from the hydrogel was observed for 5 days under physiological conditions. We believe that the graphene-based hydrogel system is widely applicable for biological sensing, cancer therapies and potentially biomedical imaging.



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발표코드: MAT.P-1043

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A new host material based on Carbazole for blue phosphorescent organic light-emitting diode**

**빈종관 홍종인**

서울대 화학부

We have synthesized a new blue light-emitting material based on carbazole for use in phosphorescent organic light-emitting diodes (PhOLEDs). A new host material, 9'-triphenylsilanyl-9'H-[9,3',6',9'']tercarbazole (SitCz), has a higher T<sub>g</sub> value (168 °C) compared to mCP or SimCP. The device with the optimized structure shows high blue EL performance with a current efficiency of 46.3 cd/A, a power efficiency of 36.5 lm/W, an external quantum efficiency of 27.2 %, and CIE coordinates of (0.13, 0.29) at 100 cd/m<sup>2</sup>. These results are comparable with the previously reported highest values for the Firpic-doped blue PhOLEDs.



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발표코드: MAT.P-1044

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Small Modular Dye-Sensitized Solar Cells on Flexible Substrate

윤용태 권도훈 김영일

부경대 화학과

1X5 cm<sup>2</sup> of strip cells were connected in series, known as a Z-connected type on PEN/ITO. Owing to properties of flexible substrate, low temperature process is essential for flexible DSCs. Low temperature process is good for mass production or energy saving but this makes weak inter-particles or particle-substrate connection. In this experiment, small particle assisted TiO<sub>2</sub> coating sol was made to overcome a demerit of low temperature process. Small size of anatase was hydrothermally synthesized and mixed with commercially available. Filling pores between large particles with smaller one enhance inter-particles and particle-substrate connection. This helps make much thicker TiO<sub>2</sub> film than usual. The film was easily peeled off during drying after coated with two layers of magic tape, but it is not after mixing. Simultaneously, improvement of inter-particle connection makes increase of photovoltaic performance of DSC.

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발표코드: MAT.P-1045

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Pd-decorated carbon nanotubes for electrochemical  
oxidation of oxalic and oxamic acids**

**김유현 최현철**

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT.P-1046

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Electrocatalytic oxidation of hydrazine on Pd-decorated  
graphene**

**김지당 최현철**

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

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장소: 일산KINTEX

발표코드: MAT.P-1047

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Preparation & electrochemical characteristic of Pt-decorated graphene**

김지당 최현철

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT.P-1048

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of transition metal inserted Lithium adsorbent by Solid State Method

김양수 나강문 박병규 이상로<sup>1</sup>

한국기초과학지원연구원 순천센터 <sup>1</sup>목포대 신소재공학과

Because manganese oxides exhibit excellent cation exchange and molecule adsorptive properties, they can be used as nano-ion-sieves, molecular-sieves and catalysts. Advanced separation and sensing technologies have been developed by application of the nano-ion-sieve materials. In this trusted research it is proposed the lithium adsorbent(spinel type  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ ) which has a new absorption efficiency. And to manufacture adsorbent it was made the safe and stable conditions through the conditional establishment of solid state method (the departure material, heat treatment temperature and atmosphere condition).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 은 알킬 카바메이트 복합체를 이용한 은 나노 입자의 제조

**김경아 공명선**

단국대 나노바이오의과학과

은 나노입자는 항균효과, 광학적 활성을 가지며 산화 촉매, 전자파 차폐, 광 반사막 및 도전성 회로 등 많은 분야에서 응용되고 있다. 특히 전기전자 부품의 회로에서 미세 금속패턴을 형성에 매우 유용하기 때문에 이에 대한 관심이 증가하고 있다. 종래의 액상 환원법을 이용해 금속 나노입자를 제조하는 방법들은 나노 입자의 제조의 공정이 복잡하고 금속의 농도가 낮아서 대량 생산하기에는 부적합하며, 안정성이 떨어지거나 소성온도가 높아 다양한 종류의 기관 사용에 제한이 있는 등의 여러 문제점을 안고 있다. 본 연구에서는 은 나노 입자 제조의 전구체로써 은 알킬 카바메이트를, 환원제로써 히드라진 또는 피페라진 유도체를 이용하여 은 나노입자를 제조하였다. 은 나노입자의 응집이 일어나지 않도록 올레 산과 알킬 암모늄 카바메이트를 안정제로 사용하였고, 은 나노입자의 분포 및 크기를 제어할 수 있도록 환원제와 안정제를 이용한 간단한 제조공정으로 다양한 형태의 은 나노입자를 만들었다. 이렇게 제조한 은 나노입자의 모양과 크기를 TEM,

SEM 으로, 은 입자 형성을 XRD 로 확인하였고, TGA 로 두 안정제의 함량 및 분해 온도를 확인하였다.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## H<sub>2</sub> bubbling 환원기법을 이용한 은 나노 입자의 제조

김경영 공명선

단국대 나노바이오횢과학과

금속 나노 입자의 제조는 그들의 잠재적인 특성 때문에 최근에 많은 연구의 관심이 집중되고 있다. 특히 은(Ag)은 전자재료의 전극, 전자파 차폐, 반사판의 재료뿐만 아니라 아주 적은 양으로도 강력한 항균성을 가지고 있기 때문에 수술용품, 창상피복재 및 화장품 등의 향미생물/항균 기능을 필요로 원료나 전자파 차폐, 반사막 및 도전성 전극 등 전자재료 널리 활용되고 있다. 본 연구에서는 안정한 은 나노 입자를 제조하기 위하여 전구체로서 은 알킬 카바메이트 복합체(silver alkylcarbamate complex)를 사용하고 환원제로서 수소를 이용하였다. 나노입자의 안정제로 PVP(polyvinylpyrrolidone)를 사용하였으며 은 알킬카바메이트 복합체 농도, 안정제의 농도, 수소의 양 등과 같이 다양한 인자들을 달리하여 은 나노 입자의 분포 및 크기를 제어하였다. 이렇게 제조한 은 나노 입자의 성질을 TGA, TEM, SEM 및 XRD 등을 이용하여 확인하였으며 그 입자로서 은 페이스트를 제조하여 그 물폴로지와 전극의 성능을 평가하였다.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study of core-extended perylene imide dye for a dye-sensitized solar cell

장병권 박동원<sup>1</sup> 도정윤<sup>2</sup>

부산대 첨단정보및디스플레이소재협동과정 <sup>1</sup>광주과학기술원 솔라에너지연구소 <sup>2</sup>부산대 화학  
교육과

Ruthenium complex dyes have been studied for high photovoltaic performance of dye-sensitized solar cells (DSSCs). Expensive price and rarity of ruthenium complexes make us to give attention to organic sensitizers. They are prospective to improve the performance with high molar absorptivity and wide absorption bands. Perylenes have rigid and flat structures and photochemical/thermal stability. Many perylene derivatives have been reported as electron acceptor or electron transfer material. In the research, the core-extended perylene imide dye was developed for DSSC. Thermal adduct of asymmetric perylene anhydride imide and 1,2,4-triazoline-3,5-dione is spontaneously oxidized to yield fully pi-conjugated fused polybenzenes. It absorbs light from visible to NIR of up to 900nm. PV performances of the new perylene dye will be discussed by fabricating DSSC with several metal oxides and electrolytes.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nonionic Brij Surfactant-Mediated Synthesis of Au Nanomaterials with High Surface Area

장민훈 유효종

한림대 자연과학대학 화학과

A variety of mesoporous metallic nanoparticles have been synthesized in the lyotropic liquid crystalline phases of nonionic surfactants.<sup>1)</sup> In general The nonionic surfactants are not only serving as mild reducing agents, but also likely acting as capping or structure-directing agents. Here, we present unique shape controls of anisotropic Au nanomaterials in nonionic surfactant brij solution<sup>2)</sup>. In particular, we successfully synthesized hexagonal multi-layered gold spirangles through a simple process in aqueous brij 700 solution. The growth of single- and multi-layered gold crystals was controllably changed through the change of reaction temperature. Raspberry-like gold nanoparticles (Au RLNPs) were synthesized in high yield through the reduction of  $\text{HAuCl}_4$  by Brij 35 surfactant in basic condition. The synthesized Au RLNPs possess high surface area, which is possibly useful structural factor for the applications. The highly-red shifted surface plasmon resonances (SPRs) of Au RLNPs originate from the rough, raspberry-like surface of Au RLNPs. The size of Au RLNPs can be controlled by varying the amount of NaOH and

HAuCl<sub>4</sub>.

- 1) (a) G. S. Attard, C. G. Goltner, J. M. Corker, S. Henke, R. H. Templer, *Angew. Chem. Int. Ed.*, 1997, 36, 1315-1317; (b) T. Kijima, T. Yoshimura, M. Uota, T. Ikeda, D. Fujikawa, S. Mouri, S. Uoyama, *Angew. Chem. Int. Ed.* 2004, 43, 228-232; (c) Y. Yamauchi, T. Momma, T. Yokoshima, K. Kuroda, T. Osaka *J. Mater. Chem.* 2005, 15, 1987-1994.
- 2) (a) M. H. Jang, J. K. Kim, H. Tak and H. Yoo\*, *J. Mater. Chem.*, 2011, 21, 17606 (b) M. H. Jang, J. K. Kim, and H. Yoo\*, *J. Nanosci Nanotechnol*, accepted



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Role of Graphene as a Template for 2D Sheet-like Ordering of Anatase TiO<sub>2</sub> nanoparticles

이장미 김인영<sup>1</sup> 황성주<sup>1</sup>

이화여대 화학나노과학부 <sup>1</sup>이화여대 화학·나노과학과

Exfoliated graphene nanosheets are applied as a template for the 2D sheet-like ordering of anatase TiO<sub>2</sub> nanoparticles. The heat-treatment of the uniformly hybridized nanocomposite of layered titanate-reduced graphene oxide (RGO) at higher than 600°C induces the phase transition of layered titanate to anatase TiO<sub>2</sub> as well as the elimination of RGO component, leading to the formation of the sheet-shaped porous aggregates of RGO-free TiO<sub>2</sub> nanoparticles. The nanocomposites calcined at 500-700°C display promising functionality as negative electrode for lithium ion batteries. Among the present calcined derivatives, the 2D-shaped aggregate of TiO<sub>2</sub> nanoparticles obtained from calcination at 600°C delivers the largest specific discharge capacity. Such a superior electrode performance of the 600°C-calcined nanocomposite is attributable both to the improved stability of the crystal structure and crystal morphology of titania and to the enhancement of Li<sup>+</sup> ion transport in the porously aggregated titania via the enlargement of mesopores. The present findings clearly demonstrate the usefulness of RGO

nanosheets as a template for 2D ordered superstructures of metal oxide nanoparticles with the improvement of electrode performance.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Phase Transition Route to Electrochemically Active $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$ Nanoparticles using Layered $\text{MnO}_2$ Nanosheets

오승미 황성주<sup>1</sup>

이화여대 화학·나노과학과 <sup>1</sup>이화여대 화학·나노과학과

Spinel-structured  $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$  nanoparticles can be synthesized by a phase transition of the  $\text{Co}^{2+}$ -layered  $\text{MnO}_2$  nanocomposites at elevated temperatures. The precursor nanocomposites of  $\text{Co}^{2+}$ -layered  $\text{MnO}_2$  are prepared by an electrostatically-derived self-assembly between negatively charged  $\text{MnO}_2$  nanosheets and  $\text{Co}^{2+}$  cations. The heat-treatment of the as-prepared  $\text{Co}^{2+}$ -layered  $\text{MnO}_2$  nanocomposites at 600-800 °C yields binary  $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$  nanoparticles with tunable particle sizes. According to X-ray diffraction and field emission-scanning electron microscopic analyses, the binary  $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$  particles show cubic spinel structure and spherical morphology with the particle size of ~20-30 nm. The chemical composition of the  $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$  nanoparticles is easily tunable by changing the reactant ratio between  $\text{Co}^{2+}$  ions and layered  $\text{MnO}_2$  nanosheets. The obtained  $\text{Co}_x\text{Mn}_{3-x}\text{O}_4$  nanoparticles display promising functionality as a negative electrode for lithium rechargeable batteries.

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발표분야: 재료화학

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## Synthesis of Fluorescent Silica Nanoparticles in a Reverse Microemulsion through Double-Layered Doping of Fluorescein

박준성 한응태 유효종<sup>1</sup>

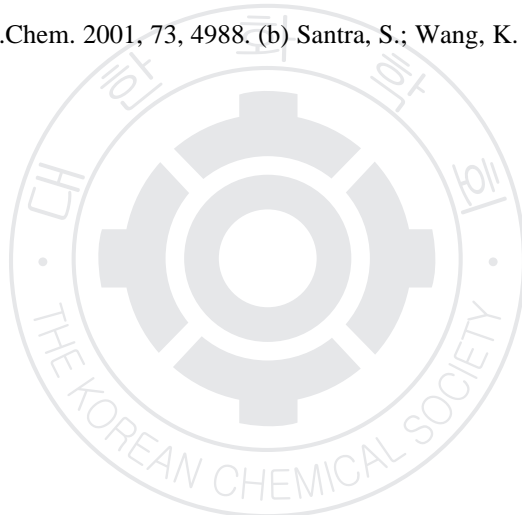
한림대 화학과 <sup>1</sup>한림대 자연과학대학 화학과

Nano-sized fluorescent silica materials have been extensively studied and applied to a variety of areas including biomedical and biosensing technologies. One of the well-known methods for the synthesis of fluorescent silica nanoparticles is a reverse microemulsion method, which have been useful and efficient for the preparation of narrow-size distributed silica nanoparticles doped with fluorophores.<sup>1</sup> However, it is comparably difficult to prepare organic dye doped silica nanoparticles since most of organic dyes are highly hydrophobic, therefore, the incorporation into the hydrophilic silica matrix is not easy. In addition, relatively small organic dyes are easily washed out while the fluorescent silica nanoparticles are purified. To synthesize the fluorescent silica nanoparticles with organic dyes, we have developed a simple but novel approach based on the repeated and double-layered condensation of TEOS (Tetraethylorthosilicate) and APTS (3-Aminopropyltriethoxysilane). Water-soluble, highly fluorescent double-layered silica nanoparticles (FL-DLSN) have been successfully synthesized using a reverse

microemulsion method. The microemulsion was prepared by mixing of surfactant (Brij35), co-surfactant, organic solvent, water, and an aqueous solution of excess fluorescein dye. Initially, TEOS (Tetraethylorthosilicate) was hydrolyzed by the addition of  $\text{NH}_4\text{OH}$  as a catalyst, and then polymerized to generate core silica nanoparticles. Although the fluorescein is hydrophobic, this organic dye is believed to be incorporated within the hydrophilic silica matrix, mainly due to the effect of high fluorescein concentration. For the preparation of FL-DLSN, APTS (3-Aminopropyltriethoxysilane) was sequentially added into the reaction mixture, and reacted on the surface of pre-generated core silica nanoparticles to form the second layer as a shell. The second silica layer from the condensation of APTS can protect the fluorescein dye within the core silica matrix as well as act as a support for the binding with fluorescein through the amide bond formations, which makes silica nanoparticles more highly fluorescent. Here, we are presenting the synthetic details for the FL-DLSN, fluorescence data, microscopy images, and how this noble particle can be applied to biosensing technologies.

#### References

1. (a) West, R.; Fink, M. J.; Michl, J. *Science* 1981, 214, 1343-1344. Santra, S.; Zhang, P.; Wang, K. M.; Tapeç, R.; Tan, W. H. *Anal.Chem.* 2001, 73, 4988. (b) Santra, S.; Wang, K. M.; Tapeç, R.; Tan, W. H. *J. Biomed. Opt.* 2001, 6, 160.





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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of [(dcbpy)M(dmit)] (M=Ni (II), Pd (II), Pt (II)) Organometallic Complexes for Dye-Sensitized Solar Cells (DSSCs)

박수나 정혜인 장연임 안병관

가톨릭대 화학과

A series of  $d^8$  transition metal-based organometallic dye complexes, (dcpy)Ni(dmit), (dcpy)Pd(dmit) and (dcpy)Pt(dmit), with a dithiolato ligand were synthesized (dcpy = 4,4'-dicarboxy-2,2'-bipyridine; dmit = 2-thioxo-1,3-dithiole-4,5-dithiolate) and their chemical structures were characterized. The optical and electrochemical properties of these metal complexes were also investigated and compared in detail.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile Synthesis Method of Mesoporous Gallium Oxide Thin Films

홍정은 권영욱

성균관대 화학과

We report the synthesis of the mesoporous gallium oxide ( $\text{Ga}_2\text{O}_3$ ) thin films by using a non ionic surfactant (F-127) as a structure directing agent. None of the previously reported the mesoporous  $\text{Ga}_2\text{O}_3$  has a thin film structure. The mesoporous  $\text{Ga}_2\text{O}_3$  thin films are expected to utilize as acid-catalysts or other functional materials. Furthermore the mesoporous  $\text{Ga}_2\text{O}_3$  thin films can be converted to  $\text{Ga}_2\text{S}_3$  films which are semiconductor materials by supercritical fluid reaction. All films have wormlike structure and about 10nm pore sizes. Also we can control the film thickness in the range of 40 - 340nm depending on the composition of gallium source ( $\text{GaN}_3\text{O}_9$ ) and F127 of the coating solution. X-ray diffraction (XRD), transmission electron microscopy (TEM) and scanning electron microscopy (SEM) were used for structural analysis. The elemental ratio of Ga/S was determined by an energy dispersive spectrometer (EDS).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Bimetallic Pt-Mn nanoparticles with highly improved activity for oxygen reduction and methanol oxidation reaction**

**Matin Md Abdul 권영욱**

성균관대 화학과

Pt-based catalysts have been well known to exhibit improved electrocatalytic activities due to particularly modulated surface structures favorable for anode and cathode catalysts for fuel cells. We synthesized bimetallic Pt-Mn catalysts with different molar ratios using a modified ethylene-glycol reduction method via sonochemistry. A variety of analytical techniques such as X-ray Diffraction, Inductively Couple Plasma-Absorption Emission Spectroscopy and Cyclic Voltammetry was used to determine average particle size, composition and electrocatalytic properties. Bimetallic Pt-Mn nanoparticles sized with 1.75-2.50 nm evidenced by Transmission Electron Microscopy were narrowly dispersed supported on carbon. The electrocatalytic activity was investigated in terms of saturated-oxygen and methanol in an electrolyte of 0.1M HClO<sub>4</sub> at a room temperature. All Pt-Mn catalysts demonstrated superior electrocatalytic activity in oxygen reduction and methanol oxidation reduction compared to that of typical commercial Pt catalyst. Our synthesis method is very simple and rapid.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Plasmonic-Coupling-Based Colorimetric Detection of Glutathione

**장유진 김종승<sup>1</sup> 김동하**

이화여대 화학나노과학과 <sup>1</sup>고려대 화학과

The rapid and sensitive recognition of thiol-containing amino acids including cysteine (Cys), homocysteine (Hcy) and glutathione (GSH) in disease diagnosis such as AIDS, Alzheimer's and Parkinson's diseases is highly relevant since the level of the amino acids in human physiology can be an indicator of a certain disease. Meanwhile, gold nanoparticles (Au NPs) have been widely investigated due to their unique surface plasmon resonance (SPR) property, which accompanies color changes by the formation of aggregates between neighboring nanoparticles. Thus, they can be applied as a colorimetric sensor based on the optical properties when the target molecules form a bridging network on the surface of Au NPs. To date, the functionalized Au NPs have been used as colorimetric probes in DNA, proteins and metal ions detection. Herein, we present an addressable colorimetric sensing system composed of bisindole compound tethered onto the surface of Au NPs, especially for the selective determination of GSH over Cys and Hcy. It displayed a selective colorimetric change in the presence of GSH from red to purple/blue but it showed no response when Cys or Hcy were introduced. The aggregation induced by

complexation between bisindole derivatives tagged Au NPs and amino acids is monitored by transmission electron microscopy (TEM) and UV-vis spectroscopy. The mechanism is also suggested based on the result of photoluminescence (PL) spectrum.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Controllable wall thickness of Ruthenium Oxides Nanotubes by Cyclic Voltammetric Deposition

조상현 김상민 유상훈<sup>1</sup> 박성호<sup>1</sup>

성균관대 에너지과학과 <sup>1</sup>성균관대 화학과

Ruthenium oxide (RuO<sub>2</sub>) nanotube arrays were prepared by electrochemical cyclic voltammetric deposition method using aqueous ruthenium chloride and with assistance of anodic alumina oxide (AAO) templates. We found that the wall thickness and length of RuO<sub>2</sub> nanotubes could be controlled by cyclic voltammetric deposition and varying potential range. The synthetic controllability on RuO<sub>2</sub> nanotubes was attributed to the ionic diffusion rate in different deposition conditions. As-prepared RuO<sub>2</sub> nanotubes were applied as electrochemical supercapacitor electrodes to study the relationship between performance and synthetic methods. This work is significant in understanding how to controlled synthesis of RuO<sub>2</sub> nanotubes and how to maximize materials usage as supercapacitors

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Observation on the peak shifting of quadrupole modes when binding dopamine in multi-block Nanorods modified with Human-IgG

최윤정 장호영<sup>1</sup> 박성호

성균관대 화학과 <sup>1</sup>성균관대 에너지과학과

We have synthesized Au single-component nanorods(NRs), Ag single-component NRs, and Au-Ag-Au tri-block and multi-block NRs by the porous alumina template deposition process and observed their peak-shifting of quadrupole modes after adsorbing Human-IgG as dopamine(DA) antibodies on the surfaces of Au and Ag blocks and adding DA molecules interacting with antibodies. It could be verified that DA antibodies could be adsorbed on both Au and Ag surfaces through the optical and fluorescence images. Compared with three different NRs, the magnitude of peak-shifting changed according to the length of Ag block and the number of repeating units of Au and Ag in NRs. The experimental observation of optical properties of these NRs was compared with the theoretical simulation using DDA calculation.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fabrication of Pt-coated Au Nanoplates for Shape-controlled Pt Nanoframes

장희정 홍순창 LIULICHUN<sup>1</sup> 이지혜 박성호

성균관대 화학과 <sup>1</sup>성균관대 화학

Au nanomaterials can be fabricated with a variety of morphologies and commonly used as a template. In this report, we demonstrated the formation of shape-controlled Pt nanoframes from gold etching process. It is hard to grow Pt shell onto the surfaces of Au nanoplates due to the lattice mismatch between Au and Pt and the interfacial energy. To solve this problem, we added a little amount of additional Ag ion in the growth solution. Ag ions affect the growth mode and provoke galvanic replacement. This experiment makes it possible to control the growth of Pt on Au templates in detail. We also controlled the thickness of nanoframes by changing the ratio of  $[Ag^+]$  to  $[Pt^{4+}]$ , and the morphology with Au nanoplates having different shapes, such as prism and disk. Pt nanoframes can be generated because Pt layers would be deposited relatively thicker in the edge of Au nanoplates than in the terrace. This tendency follows typically galvanic replacement reactions in that deposition of growth materials preferred on the edge to on the terrace.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Size-controlled synthesis of palladium nanoparticles using Proton Beam Irradiation

이임균 송재희<sup>1</sup>

순천대 기초의화학부 <sup>1</sup>순천대 화학과

최근 환경 친화적 산업이 요구되는 시대에 손쉽고 안정적인 팔라듐 나노입자를 만들 수 있다면, 환경과 산업에 크게 이바지 할 것이다. 본 실험에서는 양성자 빔을 환원제처럼 이용하여 수용액 상태의 팔라듐 이온에 조사하여 실온에서 팔라듐 나노 입자를 합성 할 수 있었다. 더 나아가, 계면활성제의 종류, 계면활성제와 팔라듐의 몰 비를 바꾸어 가며 팔라듐 나노입자의 크기를 조절 할 수 있었다. 계면활성제는 cetyltrimethyl ammonium bromide(CTAB)과 sodium dodecyl sulfate(SDS)를 사용하였다. 합성된 Pd 나노입자는 UV-Vis absorption spectroscopy 와 Transmission Electron Microscopy (TEM) 분석으로 확인하였다. 계면활성제 대 팔라듐 이온의 몰 비가 증가 할수록 팔라듐 나노입자의 크기가 증가 하는 것을 확인 할 수 있었다.

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## Preparation of Goethite Nanoparticle for Inorgnaic Template Applications

한양수 윤주영

(주)나노스페이스

Nanocrystalline goethite ( $\alpha$ -FeOOH) particles with spindle-type particle morphology are prepared by chemical hydrolysis using ferrous salt. In the chemical hydrolysis reaction route, ferrous sulfate,  $\text{Fe}(\text{SO}_4)_2$ , is forced hydrolyzed by the addition of  $\text{NaOH}/\text{Na}_2\text{CO}_3$  aqueous solution to obtain ferrous hydroxide precipitate, followed by the aeration with air bubbling for the transformation to goethite particles. The hydrolysis and aeration conditions are systematically controlled to optimize the preparation of monodispersed spindle shaped goethite particle with the particle size of 100~200 nm and the aspect ratio of 10~20. The resulting goethite powders are evaluated by powder X-ray diffraction analysis, scanning electron microscopy, nitrogen adsorption - desorption isotherm, zeta-potential, and particle size analysis method. Furthermore, thus prepared monodispersed goethite nanoparticles are utilized as inorganic templates for the preparation of ceramic membranes with controlled pore morphology and size.

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## Preparation of Solvent-Free Inorganic-Organic Nanohybrid Coating Dispersions

한양수 윤주영

(주)나노스페이스

A series of novel waterborne inorganic-organic hybrid dispersions are prepared by an intercalation and interlayer hydrolysis reaction. Intercalation of melamine and urethane dispersions into layered silicates resulted in synthetic resin-layer silicates nanohybrids with ordered stacking structures. Subsequent hydrolysis of silane compounds such as tetraethoxysilane, (TEOS), vinyltrimethoxysilane (VTMS) and polysiloxane in the presence of the synthetic resin-silicate hybrid dispersions produces novel waterborne inorganic-organic hybrid dispersions. The novel hybrid dispersions are solvent-free and easily formulated into coatings which are low in volatile organic content, and fit the need for the environmental regulations. It is also found that the coated films using hybrid dispersions possess superior performances in pencil hardness, scratch resistance, film adherence and optical transparency.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Essential Oil Containing Nanocomposite for the Treatment of Fish Parasitic Disease

한양수 윤주영 이남호<sup>1</sup>

(주)나노스페이스<sup>1</sup> 제주대 화학과

Layered nanocomposites between organically modified montmorillonite and d-Limonene ( $C_{10}H_{16}$ ) were prepared by novel solid-solid reaction at room temperature. Cetyltrimethylammonium cation was used as interlayer modifier for adsorption of hydrophobic limonene molecules. The hydrophobic interactions between alkylammonium and the aromatic compound are thought to be the driving force for the solid-state intercalation. Thus prepared limonene containing intercalative nanocomposite exhibits a sustained-releasing property, which can be utilized in the treatment of fish parasitic disease, Scuticocilliosis in the cultured Olive Flounder. The intercalative nanocomposite confers the advantages such as reducing volatile loss, improving solubility, reducing toxicity, controlled releasing, and facilitating the formulation of liquids into solid granules or powders, and providing for ease of handling, leading to the improvement of insecticidal activity of d-limonene.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study on the Optical Property of Gold Nanorods as a Function of Their Aspect Ratio

안지아 정현

동국대 화학과

Recently, gold nanoparticle has attracted considerable attention due to their unique physicochemical, electronic and optical properties and their chemical stabilities in biological field such as chemical sensing, biological imaging, drug delivery and phototherapeutics. Particularly, nanosized gold particles have mainly been studied because of their unique optical properties that are size and shape dependent. The phenomenon is known as surface Plasmon resonance (SPR), whose frequency strongly depends on the aspect ratio of gold nanorod. In order to control aspect ratio of gold nanorods, two-step seed-mediated growth method was used. First, gold seed nanoparticles of which size is about 2 ~ 4 nm were prepared and further gold ion source was reduced in solution containing gold seed particles by reducing agent such as sodium borohydride and ascorbic acid. The aspect ratio of obtained gold nanorods has been successfully controlled by changing of addition amount of  $\text{AgNO}_3$  during rod growth process. The

Plasmon absorption maxima for the obtained gold nanorods varied as a function of the aspect ratio, from 687 nm (aspect ratio is 2.4) to beyond 815 nm (aspect ratio is 4.3).



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study on Intracellular Uptake of $\text{Fe}_3\text{O}_4$ Magnetic Nanoparticles Depending upon Surface Modification

이동현 정현

동국대 화학과

Magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles are emerging as ideal candidates for drug delivery and biomedical applications due to their ultra-fine sizes, biocompatibility and superparamagnetic properties. However, the as-prepared magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles are easily aggregated and can be attacked by immune system and removed from the body. Therefore, surface modification is necessary to make them hydrophilic and stable against aggregation and non-specific uptake in a biological system. We used the silica ( $\text{SiO}_2$ ) and polyethyleneglycol (PEG) derivatized phospholipid ligands to improve their intracellular uptake. In this study, oleate and oleylamine stabilized magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles were prepared by the high temperature organic phase synthesis. The resulting magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles were then encapsulated by silica ( $\text{SiO}_2$ ) and PEG-phospholipids shell to endow them with biocompatibility. The as-synthesized magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles were characterized by measurements of X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM), and Fourier transform infrared

spectroscopy (FT-IR). Further, silica ( $\text{SiO}_2$ ) and PEG-phospholipid encapsulated magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles were followed with measurements of X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM) and dynamic light scattering (DLS), and Fourier transform infrared spectroscopy (FT-IR). The cytotoxicity of silica ( $\text{SiO}_2$ ) and PEG coated magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles was measured by MTT assay (cell viability test). After that, these surface modified nanoparticles were treated bone marrow mesenchymal stem cells (BM-MSCs) and measured Fe concentrations within cells after the incubation by inductively coupled plasma-atomic emission spectrometry (ICP-AES) analysis for uptake efficiency in cell lines depending upon the nature of coated materials and surface properties.





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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Cobalt Hydroxide Nanosheets by Exfoliation of Dodecyl Sulfate Ions intercalated Cobalt Hydroxide

권민재 정현

동국대 화학과

The nanosheet cobalt hydroxide was prepared by exfoliation of cobalt hydroxide intercalated with dodecyl sulfate ions under the formamide media. The dodecyl sulfate ions intercalated layered cobalt hydroxide was obtained by co-precipitation of an aqueous solution of cobalt nitrate hexahydrate and sodium dodecyl sulfate (SDS) through hexamethylenetetramine (HMT) hydrolysis methods. The thickness of cobalt hydroxide nanosheets is in the molecular range, while their lateral size ranges from several hundred nanometers to several micrometers. The physicochemical characterizations of the obtained cobalt hydroxide nanosheets was performed by, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), ultraviolet-visible spectroscopy (UV), atomic forced microscopy (AFM), scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (TEM).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of europium complexes intercalated clay nanohybrid

김아란 정현

동국대 화학과

Complexes of europium(III) with 1,10-phenanthroline were intercalated into Na-montmorillonite and laponite XLG clay minerals by ion exchange reactions. The guest lanthanide complex was obtained by simple complexation reaction between europium chloride ( $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$ ) and 1,10-phenanthroline (phen) as a function of molar ratio of  $\text{Eu}^{3+}$  ion and ligand molecule. The precursor complexes were 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, scanning electron microscopy, Fourier transform infrared, UV-vis, and fluorescence spectra, and their properties and structure were determined. The intercalated complex exhibits luminescence where both the 1,10-

phenanthroline “antenna” effect and the intensity maxima (a characteristic red  $^5D_0$ - $^7F_2$  emission) are comparable to the free complex.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermal behavior study of manganese oxide nanoparticles on graphene layer

강명구 정현

동국대 화학과

In this study, we report thermal behavior of manganese oxide nanoparticles decorating on monolayer graphene. The monolayer graphene was made by “peeling off” method on the  $\text{SiO}_2/\text{Si}$  substrate (200 nm) and monodispersed and nonaggregated manganese oxide ( $\text{Mn}_3\text{O}_4$ ) nanoparticle (about 5.5 nm sized) was synthesized through the thermal decomposition of manganese(II) acetate tetrahydrate in the presence of surfactant such as oleic acid and oleylamine. Nanohybrid film was obtained by simple Langmuir-Blodgett self-assembly of nanoparticles on graphene film as a function of concentration of nanoparticles. The obtained graphene/ $\text{Mn}_3\text{O}_4$  nanohybrid has only one-layer of nanoparticles in order to minimized surface potential of nanohybrid. After heat treatment, the decorated nanoparticles became epitaxial growth and made island structure. The prepared  $\text{Mn}_3\text{O}_4$  nanoparticle was confirmed by Fourier transform infrared spectroscopy (FT-IR) and powder X-ray diffraction (XRD). Morphology of nanoparticle was characterized by high resolution transmission electron microscopy (HR-TEM). The thermal behavior of

nanoparticle was studied by thermogravimetric (TG) and differential thermal analysis (DTA). Morphological change of nanohybrid after thermal treatment was determined by Atomic force microscope (AFM) measurements.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Crystal Structure and Dielectric Behavior of Pseudo-Cubic Perovskite Oxides

박나영 김영일

영남대 화학과

Preparations of complex perovskites  $\text{BaM}_{0.9}\text{M}'_{0.1}\text{O}_{3+y}$  ( $M = \text{Ti, Zr}$ ;  $c = \text{Nb, Ta}$ ) were studied by solid state ceramic methods at 1350-1550 °C. As revealed by high-resolution synchrotron X-ray powder diffraction, samples with  $M' = \text{Ta}$  could be formed in single phase, which was not the case of  $M' = \text{Nb}$ . Both  $\text{BaM}_{0.9}\text{M}'_{0.1}\text{O}_{3+y}$  samples exhibited an insulating behavior with a band gap wider than 3 eV. It implied that the defects generated by the aliovalent substitutions of Ta/Ti(Zr) were compensated by cation vacancies instead of the reduction. Therefore it is proper to describe the products as  $(\text{BaM}_{0.9}\text{Ta}_{0.1})_{3/3.05}\text{O}_3$  or  $(\text{BaM}_{0.9}\text{Ta}_{0.1})_{0.984}\text{O}_3$ . In contrast to the tetragonal and polar  $\text{BaTiO}_3$ , its derivative  $(\text{BaTi}_{0.9}\text{Ta}_{0.1})_{0.984}\text{O}_3$  was stabilized in a simple cubic average structure (space group,  $pm-3m$ ). However,  $(\text{BaZr}_{0.9}\text{Ta}_{0.1})_{0.984}\text{O}_3$  maintained the isostructural relation to  $\text{BaZrO}_3$ . Above structural and compositional modifications of  $\text{BaTiO}_3$  and  $\text{BaZrO}_3$  caused considerable-dependent phase transitions for the titanate, and the substantial increase of dielectric constants for the zirconate.

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발표코드: MAT.P-1073

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of New Blue Light Emitting Iridium Complexes Containing Trimethylsilyl group

김철영 권순기<sup>1</sup> 김장주<sup>2</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학부 <sup>2</sup>서울대 재료공학부

Organic light-emitting diodes(OLEDs) have attracted great attention in the past decades, because they show a number of attractive in flexible, high efficiency, low power light sources, cost competitive and full color flat panel displays. Phosphorescence materials are generally based on heavy metal complexes in OLEDs. Phosphorescence materials can emit light from both singlet and triplet excitations, enabling the fabrication with close to 100% internal quantum efficiency. Thus, a lot of effort has been spent investigating the third row transition-metal complexes to develop highly efficient phosphors that can emit all three primary colors.[3] Especially, iridium complexes show the most effective emitter because of their high photoluminescent efficiency and relatively short excited state lifetime. In this research, we designed new iridium complex using combination of dppe ligand and trimethylsilyl group as bulky electron donating group for OLEDs. We provide syntheses and characterization of two new blue Ir(III) complexes containing perfluoropropyl ancillary ligand and trimethylsilyl group.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

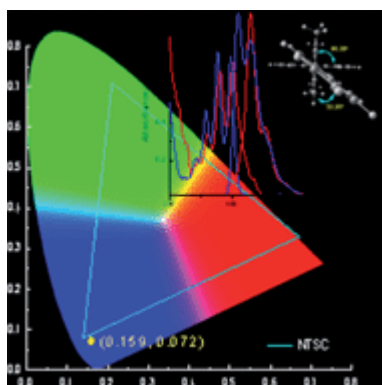
## Highly rigid and twisted anthracene derivatives: a strategy for deep blue OLED materials with theoretical limit efficiency

김란 권순기<sup>1</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학부

New highly twisted and rigid blue materials composed of anthracene with xylene as the core unit and either naphthalene or phenyl end units were synthesized. Non-doped devices using BDNA displayed 5.26% maximum external quantum efficiency with CIE color coordinates (x, y: 0.159, 0.072).





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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Manufacturing new catalyst on synthesis bio fuel by using ordered mesoporous carbon

김순근 김지만<sup>1</sup>

경기과학고 영재교육지원부 <sup>1</sup>성균관대 화학과

As petroleum is running out, bio fuel is the important alternative energy. Therefore, nowadays, synthesizing bio fuel is very important. To be economically, manufacturing effective catalyst on synthesizing bio fuel is important. Synthesizing bio fuel is kind of esterification, whose reactants is oleic acid, methanol and the production is methyl oleate(oleic acid methyl ester). The study used OMC(ordered mesoporous carbon) as a catalyst on synthesis. However, there are lots of kind in OMC so that many kinds of OMC was compared. The precursor of used OMC is sucrose and p-TSA. To make OMC, OMS which usually use in treating petroleum business have to be treated. There is step of treating OMS. The order is carbonization, postprocessing, and removing silica cover. Carbonization temperature is 500 °C, 700 °C, 900 °C. The postprocessing temperature is 160 °C. Hydrofluoric Acid is used to remove silica cover. To investigate the conversion efficiency of catalyst, the experiment was carried out in 110 °C, ratio of methanol and oleic acid is 9:1(w/w). To identify conversion efficiency into reaction time, liquid was

extracted at 10, 30 60, 90, 120, 180, 240, 300 minutes after reaction started. To analyse the density of methyl oleate in liquid, GC-MS was used. The column of GC-MS is omegawax 250.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Formation of DNA-silica complexes using the oligodeoxynucleotide as a catalytic template

정영환 박지훈<sup>1</sup>

한국폴리텍바이오대학 바이오생명정보과 <sup>1</sup>KAIST 화학과

DNA is the fundamental genetic material for the storage and transfer of information from one generation to another. Moreover, it has the bio-specific binding ability to proteins, enzymes, small organic molecules. With growing interest of organic/inorganic hybrid, DNA which has unique biological characteristics would be combined with inorganic materials. In this context, it would have significant meaning to synthesize DNA-silica complexes under physiologically favorable conditions (i. e., ambient pressure, room temperature or below, and near neutral pH values). Here, we formed DNA-silica complexes using the oligodeoxynucleotide as a catalytic template for biomimetic silicification.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## new synthesis method of carbon sphere using household microwave oven

연주랑 친구<sup>1</sup>

세종대 무기화학<sup>1</sup> 세종대 화학과

Carbon sphere (solid carbon sphere, hollow carbon sphere, carbon nano scroll etc) because of its unique properties (low weight, thermal insulation, high compressive strength) have attracted interest of science communities. We have synthesized carbon sphere in two steps. First of all, we have carried out intercalation of potassium into graphite sheet by irradiating microwave using household microwave oven. Finally, decomposition of intercalated graphite sheet was carried out at 800°C to obtain carbon sphere. We have confirmed the formation of solid carbon spheres of 2~5μm by utilizing scanning electron microscopy (SEM), and Transmission electron microscopy (TEM).

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Control of gallium composition and densification of Cu-In-Ga-Se thin films

노세진 이연수 차지현 정덕영

성균관대 화학과

Sonochemically synthesized  $\text{Cu}(\text{In}_{1-x}\text{Ga}_x)\text{Se}_2$  (CIGS) colloidal solutions with variety gallium composition were prepared. Gallium composition was controlled by amount of Ga precursor in synthesis step of CIGS nanoparticles. The CIGS ink was casted by spin coating on Mo coated soda lime glass and annealed 450~550 °C with Ar atmosphere in a rapid thermal annealing system. Morphology of CIGS films were changed by Ga composition and small amount of antimony impurity incorporation in the CIGS film assisted film grain growth. Cadmium sulfide layer (n-type) was deposited on CIGS films by using the chemical solution deposition to prepare p-n junction. The structural properties, morphologies, compositions, electrical properties of CIGS films were investigated by X-ray diffraction, Raman spectroscopy, scanning electron microscopy, X-ray fluorescence spectroscopy and Hall effect measurement.

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발표코드: MAT.P-1079

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Cobalt Layered Double Hydroxide Films in Aqueous Solution via Ammonia Gas Transfer

김하나 정덕영

성균관대 화학과

Cobalt layered double hydroxide (Co-LDH) films were successfully synthesized on glass substrates in aqueous metal salt solution by ammonia gas transfer method. When glass substrates were dipped in metal precursor solution and placed with a dilute solution of  $\text{NH}_4\text{OH}$  in an enclosed chamber, Co-LDH films with two separated regions were formed. Bottom layers of Co-LDH films were grown perpendicular to the substrate with thickness of  $2\mu\text{m}$ . Ball-like structures of Co-LDHs were stacked on the bottom layer and it could be removed by ultrasonication. On the other hand, when glass substrates were fixed to touch with the surface of an aqueous metal salt solution, we could obtain the bottom layers only. Co-LDH films were characterized by scanning electron microscopy (SEM), high resolution- transmission electron microscopy (HR-TEM), X-ray diffraction (XRD) pattern, and thermogravimetric-differential thermal analysis (TG-DTA). The SEM images show clearly that Co-LDHs were grown homogeneously all over

the surface of the glass substrate. The formation of Co-LDH films could be kinetically adjusted by changing temperature, concentration of  $\text{NH}_4\text{OH}$  solution, and reaction time.





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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthetic Polydopamine as a Photosensitizer for Polymer-Sensitized Solar Cells

남혜진 김명실<sup>1</sup> 김지만<sup>1</sup> 정덕영<sup>1</sup>

성균관대 기초과학연구소 <sup>1</sup>성균관대 화학과

An efficient electron injection by direct dye-to-TiO<sub>2</sub> charge transfer of new synthetic polydopamine (PDA) as a photosensitizer was demonstrated. Spontaneous self-polymerization using dip-coating (DC) and cyclic voltammetry (CV) were applied to TiO<sub>2</sub> layers under a nitrogen atmosphere, which offers a facile and reliable synthetic pathway to make the solar cells. Both synthetic methods led to excellent photovoltaic results and the PDA-DC exhibited larger current density and efficiency values than those for the PDA-CV. The PDA showed strong adhesion to the nanocrystalline TiO<sub>2</sub> electrodes and the interface were studied through the control of the coating methods, reaction times and solution concentration in order to maximize the conversion efficiency. The solvent and the electrolyte were critical to the energy conversion.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Chemical Composition of Electrochemically deposited $\text{Cu}_2\text{ZnSnS}_4$ thin films

김지현 정덕영

성균관대 화학과

Preparation of  $\text{Cu}_2\text{ZnSnS}_4$ (CZTS), a thin film solar cell absorber layer in terms of low-cost and abundant material source, by using single step electrochemical method was investigated. The CZTS thin films on Mo substrate were successfully synthesized by electro-deposition using ternary metal salt solution, tartaric acid and tri-sodium citrate at room temperature. The thin films were heated in elemental sulfur vapor ambient for 1 hour. Stoichiometry and morphology of the as-deposited films and samples after heat treatment were characterized by scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray fluorescence and X-ray diffraction. The thickness and metal ratio of the optimized CZTS absorber layers was 1 micrometer and  $\text{Cu} : \text{Zn} : \text{Sn} = 2 : 1 : 1$ . The chemical composition could be controlled by changing variables such as temperature, applied voltage and metal concentration in precursor solution. We investigated electrical characteristic by Mott-Schottky plot with impedance measurement and the I-V measurement showed the p-type semiconductor.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Cu-In and Cu-Ga Binary Metallic Precursors for CuInS<sub>2</sub> and CuGaS<sub>2</sub> Thin Films**

이연수 노세진 차지현 정덕영

성균관대 화학과

I -III-IV<sub>2</sub> chalcopyrite compounds are the most promising light-absorbing materials for highly efficient thin film solar cells. Among them, CuInS<sub>2</sub> and CuGaS<sub>2</sub> are attractive candidates for photovoltaic applications because they have wide direct band gap and high absorption coefficient. In order to overcome the cost limitation, non-vacuum-based process is required. We synthesized novel Cu-In and Cu-Ga metallic precursors by chemical reduction methods in liquid media. As-prepared metallic precursors were casted onto Mo substrates and heated for sulfur atmosphere to prepare CuInS<sub>2</sub> and CuGaS<sub>2</sub> thin films. The precursors and thin film samples were characterized by X-ray diffraction, scanning electron microscopy, Raman scattering, and elemental analyses. The metallic precursors were successfully transformed into Cu-M-S<sub>2</sub> (M=In or Ga) compounds and no other impurity phase was observed. Optical and electrical properties of these films were studied. We opened a new cost-effective way to fabricate large-area thin film solar cells.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mixed Colloidal Suspension and Hybrid Paper of Layered Titanate- Graphene: Flexible, Mechanically Strong, and Antibacterial Membrane

김인영 박수혜 김태우 황성주

이화여대 화학·나노과학과

Homogeneously mixed colloidal suspensions of reduced graphene oxide (RGO) and layered titanate nanosheets are synthesized and applied as precursors for the fabrication of freestanding hybrid films. The obtained mixture colloidal suspensions show a high colloidal stability and good dispersion ability because of an electrostatic repulsion between negative-charged nanosheets of RGO and layered titanate. The composition of hybrid paper is readily tuneable by controlling the volume ratio of RGO/layered titanate in the precursor colloidal suspension. The vacuum-assisted filtration of these mixture colloidal suspensions yields well-aligned hybrid papers of RGO—layered titanate. X-ray diffraction and scanning electron microscopic analyses clearly demonstrate the layered structure and 2D morphology of the resulting hybrid papers. According to X-ray absorption, Fourier transform-infrared, and micro-Raman spectroscopy, there is no significant change in the chemical bonding nature of layered titanate and RGO nanosheets before

and after the formation of hybrid paper. Of prime interest is that the mechanical properties of hybrid papers are much better in terms of flexibility and stiffness than the pure paper of layered titanate or RGO nanosheet. All of the obtained hybrid papers of RGO-layered titanate display a high antibacterial activity for the deactivation of *E. Coli O157*. The present experimental findings clearly demonstrate that the mixture colloidal suspensions of layered titanate and RGO nanosheets are fairly useful as precursors for the synthesis of various graphene—metal oxide hybrid papers with improved functionality.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Crystal structure and photoelectrochemical properties of trirutile-type $\text{ASb}_2\text{O}_6$ (A = Zn, Mg) for dye-sensitized solar cells

장지연 배지희 김승주

아주대 에너지시스템학부

Dye-sensitized solar cells (DSSC) are based on the dye sensitization of wide band gap semiconductors used in the form of mesoporous nanocrystalline films. Many attempts have been made to prepare and characterize the oxide semiconductors such as  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{SnO}_2$  and  $\text{Nb}_2\text{O}_5$  for application to DSSC. Antimony compounds,  $\text{ASb}_2\text{O}_6$  (A = Zn, Mg) also have a wide band gap. However it has never been reported yet as an electrode material for DSSC. In this work, We have prepared zinc antimony oxide ( $\text{ZnSb}_2\text{O}_6$ ) and magnesium antimony oxide ( $\text{MgSb}_2\text{O}_6$ ) by solid state method. The change in crystal structure of  $\text{ASb}_2\text{O}_6$  were monitored by means of powder X-ray diffraction. When the compounds were heated up of 500°C, the structure changed to trirutile-type from rutile in which Mg or Zn ion and Sb ion are ordered with 1:2 ratio. Each energy band gap was estimated from UV-Vis diffuse reflectance data. The particles were deposited onto F-doped  $\text{SnO}_2$  glass and subsequently heated at 500°C. Dye adsorption was carried out by immersing the antimony compound films in an ethanol solution of the conventional

ruthenium dye (N719).  $\text{MgSb}_2\text{O}_6$  and  $\text{ZnSb}_2\text{O}_6$ -based solar cell exhibited good conversion efficiency respectively under AM 1.5,  $100\text{mW}/\text{cm}^2$  illumination. This result shows a possibility of using the antimony compounds as a photoelectrode material for DSSCs



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and application of silver nanoparticles with short-length surfactant for SERS probe

이계행 배두리<sup>1</sup>

한국기초과학지원연구원<sup>1</sup> 한국기초과학지원연구원 물성과학연구부

Silver nanoparticles(NPs) with short-length surfactant was synthesized by adding NaBH<sub>4</sub> into in an aqueous solution of AgNO<sub>3</sub> and trisodium citrate. The size, shape, and optical property of the fabricated Ag NPs were investigated by transmission electron microscopy (TEM), UV-vis spectroscopy. These particles could be successfully applied in the field of surface enhanced Raman spectroscopy (SERS). SERS activity of silver NPs was checked using 4-mercaptobenzoic acid as a probe molecule. In addition, silver NPs with short-length surfactant compared with other silver NPs with long-length surfactant for SERS activity. Also, hollow gold NPs were synthesized through galvanic exchange of HAuCl<sub>4</sub> with silver NPs. Surface roughness of the hollow Au NPs could be controlled by reaction temperature for galvanic exchange. The surface roughness influenced SERS activity of the particles.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Large-scale synthesis of InP/ZnS quantum dot through continuous flow reactor and their application

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We report the massive synthetic method of InP/ZnS core/shell quantum dots (QDs) by using a continuous flow reactor. This reactor is formed based on successive combination of the batched mixer and the tube furnace with flowing solution. This reactor were connected with steel tubes with 3.2 mm diameter for flowing the solution, and InP core and InP/ZnS core-shell were successively synthesized at this reactor in one step. The flow rate of this reactor was typically 100 times larger than conventional microfluidics reactors. In order to synthesize high quality InP/ZnS QDs, we controlled the flow rate and the growing temperature. As the result, we obtained InP/ZnS QDs from bluish green to red which is adaptable for a white LED device.

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발표코드: MAT.P-1087

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New Synthetic Routes to $\text{Ag}_3\text{PO}_4$ Nanoparticles and Their Self-Assembled Nanocomposites with Visible Light Photocatalytic Activity

조윤경 김태우<sup>1</sup> 황성주<sup>2</sup>

이화여대 화학·나노과학과 <sup>1</sup>이화여대 지능형 나노바이오소재 연구센터 <sup>2</sup>이화여대 화학·나노과학과

Silver orthophosphate  $\text{Ag}_3\text{PO}_4$  nanoparticles with the particle size of ~30—40 nm can be successfully synthesized by adopting PVP polymer as capping agent. The formation of silver orthophosphate nanoparticles with a body-centered cubic structure and a negative surface charge is confirmed by powder X-ray diffraction and zeta potential measurement. The electrostatically-derived assembly between anionic  $\text{Ag}_3\text{PO}_4$  nanoparticles and cationic amine-anchored CdS nanoparticles yields intimately coupled nanocomposite of  $\text{Ag}_3\text{PO}_4$ —CdS. The resulting nanocomposites display the Bragg reflections of hexagonal cadmium sulfide and silver orthophosphate phases. The homogeneous hybridization of CdS and  $\text{Ag}_3\text{PO}_4$  nanoparticles is clearly evidenced by field emission-scanning electron microscopy and energy dispersive spectrometry analysis. Diffuse reflectance UV-vis spectroscopy measurement clearly demonstrates that both of the  $\text{Ag}_3\text{PO}_4$  nanoparticle and its nanocomposite with CdS nanoparticles show

visible light absorbing ability. Both of these materials are fairly active for the photoinduced generation of  $O_2$  gas and the photodegradation of organic molecules.



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발표코드: MAT.P-1088

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Experimental relative binding energies of various carbon nanotube surfactants using flavin-carbon nanotube templates

오현규 심진숙<sup>1</sup> 주상용<sup>1</sup>

연세대 화학<sup>1</sup> 연세대 화학과

Development of Monodisperse single-walled carbon nanotubes (SWNTs) are an important step to understand basic properties of carbon nanotubes and apply them in fundamental and industrial applications. Combination of more than two nanotube surfactants has been implemented for separation of carbon nanotubes according to chirality (i.e.,  $(n,m)$ ), handedness of tubes<sup>1</sup>. However, the underlying mechanism of such dual surfactant separation is still unknown. Here, we showed that flavin mononucleotide (FMN)-wrapped SWNTs can be an excellent platform for measuring relative binding energy of various surfactants such as sodium cholate, sodium dodecyl sulfate, sodium dodecylbenzenesulfonate, and DNA, due to the relatively high redshift ( $\Delta E_{11}^s$  and  $E_{22}^s$  are 15-51 and 23-71 meV, respectively) of FMN-carbon nanotube transitions<sup>2</sup>. The binding energy of each surfactant has been determined by Hill equation, where its coefficient was resolved by UV-Vis-NIR absorbance and photoluminescence. Based on this experimental binding energy, we calculated various thermodynamic

parameters such as enthalpy and Gibb's free energy. The result enables us to understand the underlying mechanism of separation of semiconducting SWNTs with specific chirality and paves a venue to study the physical properties of single chirality carbon nanotubes.

[1] B. Weisman et al., *Nat. Nanotech.*, **5**, 443~450 (2010).

[2] S.-Y. Ju et al., *Nat. Nanotech.*, **3**, 356 (2008).



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장소: 일산KINTEX

발표코드: MAT.P-1089

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Selective Synthesis of Azines by Solid State Reactivity Between Solid Hydrazine and Solid Aldehydes

이규형 이병노 최종명 유효진 장혜령 허남희

서강대 화학과

We have synthesized conjugated azines through simple solid state grinding of solid hydrazine and carbonyl compounds such as aldehydes and ketones using a mortar and a pestle. The solid hydrazine ( $\text{H}_3\text{N}^+\text{NHCO}_2^-$ ) isolated as a crystalline solid in supercritical  $\text{CO}_2$  conditions can be considered as a new synthetic alternative to liquid hydrazine ( $\text{NH}_2\text{NH}_2\cdot\text{H}_2\text{O}$ ). A remarkable finding is that the azine derivatives were readily prepared in the absence of solvents simply by grinding. Furthermore, the solid-state reactions show high selectivity, which yield over 97% of the product. The reaction proceeds smoothly at room temperature, producing only  $\text{CO}_2$  and  $\text{H}_2\text{O}$  waste. We will also demonstrate that a wide range of azine products can be obtained from the ground mixture in high yields with excellent selectivity. The solid-state grinding method does not require any solvent and/or additives, which renders a novel, environmentally benign process for preparing various organic and inorganic compounds.

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장소: 일산KINTEX

발표코드: MAT.P-1090

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Tunable Charge Transport in Layer-by-Layer Assembled Graphene Transistors

주필재

울산과학기술대 친환경에너지공학부

We demonstrate a controlled, systematic method to tune the charge transport in graphene field-effect transistors based on alternating layer-by-layer assembly of positively and negatively charged graphene oxide followed by thermal reduction. Surprisingly, tuning the number of bilayers of thermally reduced graphene oxide multilayer films allowed achieving either ambipolar or unipolar (both n- and p-type) transport in graphene transistors. Based on X-ray photoemission spectroscopy, Raman spectroscopy, time-of-flight secondary ion mass spectrometry, and temperature-dependent charge transport measurements, we found that nitrogen atoms from the functional groups of positively charged graphene oxide are incorporated into the reduced graphene oxide films and substitute carbon atoms during the thermal reduction. Such nitrogen doping process occurs in different degrees for graphene multilayers with varying numbers of bilayers and thereby results in the interesting transition in the electrical behavior in graphene multilayer transistors. We believe that such a versatile method to control the charge transport in

graphene multilayers will further promote their applications in solution-processable electronic devices based on graphene.





일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT.P-1091

발표분야: 재료화학

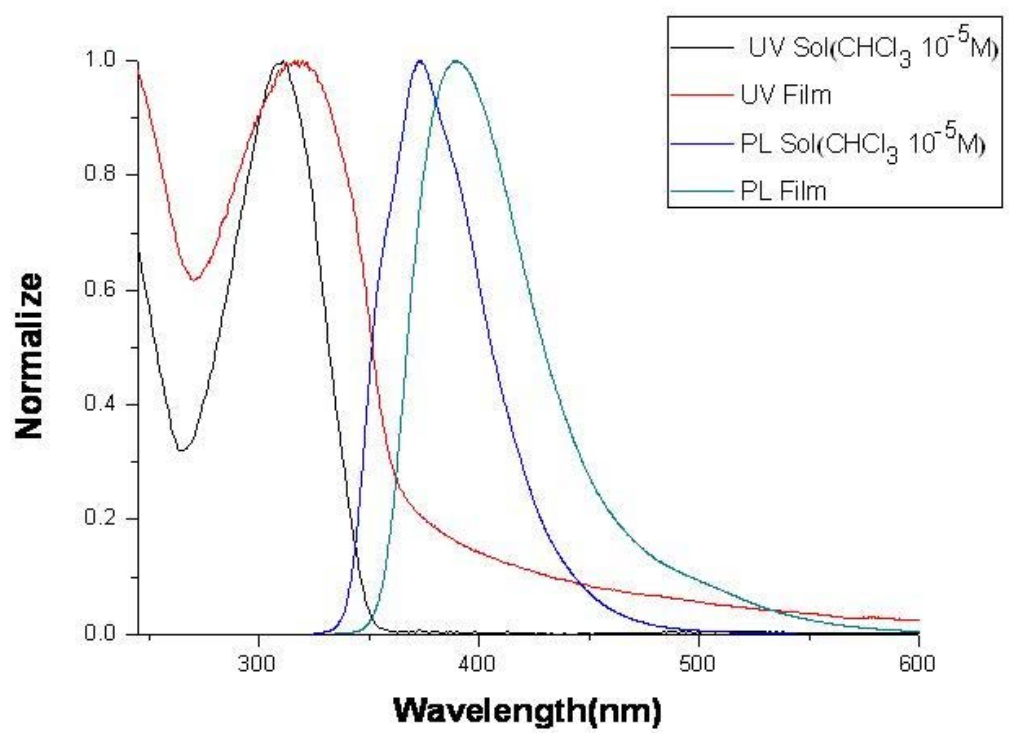
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly Efficient New Electron-Transporting Materials for Organic Light-Emitting Diodes

유승진 김철영 추아현 권순기<sup>1</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학부

New Electron-Transporting Materials were characterized by optical properties(UV-vis, PL), electric properties(cyclic voltametry) , thermal properties (differential scanning calorimetry (DSC) , thermal gravimetric analysis (TGA)).



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장소: 일산KINTEX

발표코드: MAT.P-1092

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Dendritic Developer Materials for Thermal Printing System

장연임 최원호 안병관

가톨릭대 화학과

A series of dendritic developer compounds with phenolic (phenol  $-(OH)_1$ / catechol  $-(OH)_2$ / gallic acid  $-(OH)_3$  groups) units which react with leuco dyes for a coloring process in thermal recording/ printing system were designed, synthesized and characterized. The reaction properties of leuco dye with these developer materials were investigated and compared with bisphenol A. In addition the effect of the number of phenol units on the reaction with leuco dye molecules was studied in detail.

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장소: 일산KINTEX

발표코드: MAT.P-1093

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A New Bulky Trimethylsilylxylylene Substituted Iridium(III) Complex with Picolinic Acid as Ancillary Ligand

한승훈 권순기<sup>1</sup> 김윤희 김철영

경상대 화학과 <sup>1</sup>경상대 나노신소재공학부

We designed and synthesized a new bulky trimethylsilylxylylene substituted iridium(III) complex with picolinic acid as ancillary ligand, bis(5(2,5dimethyl4(trimethylsilyl)phenyl)2phenylpyridine)iridium(III) picolinate [Ir(dmtpy)<sub>2</sub>pic], by Suzuki coupling reaction and confirmed using various spectroscopic studies. The Thermogravimetric analysis shows the 5% weight loss (1T5%) at 356 °C with the glass transition temperature (T<sub>g</sub>) of 198 °C from differential scanning calorimetry studies. The photophysical and electrochemical studies show the photoluminescence emission at 520 nm (in solution) with the band gap energy of 2.59 eV. Ir(dmtpy)<sub>2</sub>pic dopant in phosphorescent organic light emitting diodes exhibits the yellow-green emission at 528 nm with CIE color coordinates of (0.37, 0.58) with higher device current efficiency of 30.2 cd/A, the external quantum efficiency of 10.2% and the power efficiency of 10.1 lm/W.

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장소: 일산KINTEX

발표코드: MAT.P-1094

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient synthesis of nonionic surfactant by flow chemistry

박선영 조원제 유국현

동국대 화학과

The hydroxy-substituted aliphatic amides act as surfactants, synthesized from fatty acids or esters and ethanolamine. It was thought worthwhile to perform their synthesis using a toxic alkaline catalyst. Toxic catalyst enters the environment in significant amounts through wastewater treatment plants or by direct release into watercourses. Its possible chronic effects on sensitive species and their potential environmental impact must be minimized, depending on the biodegradability and toxicity of the surfactants. On this study, we synthesize nonionic surfactant by using microreactor for not using toxic catalyst. Microreactor is a brand-new glassware for micro fluidic chemistry. It has several advantages over accuracy temperature control, high safety, continuous process and easy to scale up.

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장소: 일산KINTEX

발표코드: MAT.P-1095

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## High Efficiency Doped Blue Organic Light Emitting Devices Based on Anthracene Derivatives

추아현 신지수 박종광<sup>1</sup> 권순기<sup>2</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학과 <sup>2</sup>경상대 나노신소재공학부

Organic electroluminescent devices (organic light-emitting diodes, OLEDs) have been widely investigated for their applications in high efficiency, low drive voltage, large display area, full color flat panel displays. The three basic color components (red, green and blue) are needed to obtain a full-color display. While a larger number of exceptional red and green emitters have been developed that satisfy the requirements for OLEDs, efficient and stable organic blue emitters are still rare. As a result, development of high-performance blue-emitting materials is a subject of current interest.

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장소: 일산KINTEX

발표코드: MAT.P-1096

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Supramolecular Velcro Based on Strong Host-Guest Interactions between Cucurbit[7]uril and Ferrocene Derivatives

안영주 장윤정 김기문<sup>1</sup>

포항공과대 화학과 <sup>1</sup>포항공과대 화학과, WCU 첨단재료과학부

Sea mussels, spiders and silk worms inspire scientists to develop new adhesive materials for useful applications. With strong adhesive power, they function well even in wet conditions where commercial adhesive materials usually fail to function. To overcome the limitations of conventional adhesive materials, we have decided to develop a new adhesive system - supramolecular “velcro” - working in the water by taking advantage of the exceptionally strong and specific host-guest interaction between cucurbit[7]uril (CB[7]) and ferrocenemethylammonium (FA) ion ( $K \sim 10^{12}$ ) in aqueous solution. Our approach includes preparation of CB[7]- and FA-functionalized surfaces. The details of preparation, characterization of the surfaces and their adhesive properties will be presented.

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발표코드: MAT.P-1097

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## High Efficiency Nondoped Blue Organic Light Emitting Devices Based on Anthracene

신지수 추아현 박종광<sup>1</sup> 권순기<sup>2</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학과 <sup>2</sup>경상대 나노신소재공학부

Blue organic light-emitting devices (OLEDs) have attracted much attention for their importance in both full color display and solid-state lighting.<sup>1</sup> Given that phosphorescent OLEDs can theoretically achieve 100% internal quantum efficiency, many researchers have reported phosphorescent materials with high efficiency deep-blue emission.<sup>2</sup> However, phosphorescence OLEDs typically have shorter lifetime and sharper efficiency roll-off at high brightness. Thus, phosphorescence and fluorescence OLEDs are often considered to be complementary and suitable for different applications. On the other hand, many high performance OLEDs involve doping of emitters into host materials.<sup>3</sup> However, efficacious doping often requires precise control of doping concentration and inevitably increases manufacturing cost. It has also been pointed out that potential phase separation in the dopant?host system can render energy transfer ineffective.<sup>4</sup> For these reasons, nondoped devices using blue light-emitting fluorescent OLEDs are still attracting considerable attention.



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발표코드: MAT.P-1098

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of Harmless Nanomaterials Disinfectant Including Copper Ions

김순근 김지만<sup>1</sup>

경기과학기술연구원 화학생명과학부 <sup>1</sup>성균관대 화학과

Recently, water pollution problems have become serious problems. According to this, removing microorganisms in water is an important issue. , Copper and silver ions are known to good at sterilization of microorganisms. However, commercial use of these substances are unreasonable due to economic costs and human health hazards of substances. Therefore, we studied about developing a high effective disinfectant for microbiological harmless to humans at low economic cost. We developed spherical nano materials including copper ions in their mesoporous pores. We counted the reduced number of E. coli in sterile conditions to determine sterilization effectiveness. We also used phaeomuriformis which is most dangerous microorganism in our life. In addition, we determined the duration and the possibility of particle use in humidifier or laundry machine. We can determine the excellency compared with existing materials. As a result, developed material has capable of 97.7% showed a sterilization, the same concentration was higher than the general or copper ions.

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장소: 일산KINTEX

발표코드: MAT.P-1099

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of long-range-ordered mesoporous titania thin film and its application

최서영 권영욱

성균관대 화학과

Long-range-ordered mesoporous titania thin film (MTTF) was synthesized by self-assembly mechanism using P123 as a surfactant and titanium butoxide as a metal precursor in 1-butanol with various ratios followed by aging and calcination. The characterization of this film was examined by Small angle X-ray diffraction (XRD), Scanning electron microscope (SEM) and transmission electron microscope (TEM). Well ordered cubic or hexagonal structure was observed in particular ratio and especially, cube pattern could be achieved with relatively high precursor ratio and low acidity.

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발표코드: MAT.P-1100

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New Pyridopyrazine Skeletron-Based Electron-Transporting Materials

노윤기 김란 권순기<sup>1</sup> 김윤희

경상대 화학과 <sup>1</sup>경상대 나노신소재공학부

2,3-Di(pyridine-2-yl)-7-(4-triphenylsilyl)phenylpyrido[2,3-b]pyrazine (DPPP) containing pyridopyrazine was designed and synthesized as a new electron-transporting material for organic light-emitting devices (OLEDs). The obtained material forms homogeneous and stable amorphous film. The new synthesized showed the reversible cathodic reduction for hole blocking material and the low reduction potential for electron transporting material in organic EL devices. The molecule possess excellent thermal stability with glass transition temperature ( $T_g$ ) of 115°C in nitrogen. DNTPD (60 nm)/NPD (30 nm)/CBP:Irppy 6% (40 nm)/Balq (10 nm)/ETL (30 nm)/LiF (0.5 nm)/Al structured device were fabricated using DPPP as electron transport material. The maximum luminance reached at 25000 cd/m<sup>2</sup>. The current efficiency was 10.9 cd/A even high current.

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장소: 일산KINTEX

발표코드: MAT.P-1101

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Possible Rearrangement of Dialkyl-2H-Benzimidazole and Its Implication to Performance of Organic Solar Cells: a Density Functional Theory Study

구자민

광주과학기술원 신소재공학과, PIMS

In low-band-gap copolymer for the bulkheterojunction photovoltaic cells (OPVC), dialkyl-2H-benzimidazoles incorporated with carbazole derivatives are used as an acceptor. Copolymer with 2,2-dimethyl-2H-benzimidazole(ref1) exhibit lower band-gap and more favorable efficiency in OPVC than its derivatives with longer dialkyl side chains. To understand the property change according to the alkyl side chain length, quantum chemical calculation is carried out on the four copolymers with dialkyl-2H-benzimidazoles (dimethyl (MBI), diethyl (EBI), dibutyl (BBI) and dihexyl (HBI)). Then, between the methyl- and others-benzimidazole, no difference is observed in electronic and transition property. So we assumed and investigated the rearrangements such as isomerization and hydrogen transport on benzimidazole. 22BI is less stable than isomerized 12BI that has a N-H or N-R bonding in gas phase and in aqueous solution, and activation energy of MBI is larger than the others (MBI > EBI ? BBI ? HBI). In

this result, we suggest that the rearrangement do not occur in the MBI due to high activation energy relatively, but, longer alkyl side chains on imidazole are rearranged during synthesis process. Quinoid-type 22BI decreases the band-gap in copolymer system and affects the good performance in OPVC. Rearrangement in BI with longer dialkyl side chain, however, results in the loss of good properties of copolymer system in OPVC performance. (1)Song, S.; Jin, Y.; Park, S. H.; Cho, S.; Kim, I.; Lee, K.; Heeger, A. J.; Suh, H. Journal of Materials Chemistry 2010, 20, 6517.



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장소: 일산KINTEX

발표코드: MAT.P-1102

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of lead telluride based heterostructure for thermoelectric application

성은규 한미경<sup>1</sup> 여철현<sup>2</sup> 김성진<sup>3</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학나노과학부 <sup>2</sup>연세대 화학과 <sup>3</sup>이화여대 화학과

Lead telluride (PbTe) is one of the promising thermoelectric materials in temperature range 400-800K. Recent progress in thermoelectric materials has involved decreasing lattice thermal conductivity with nano-scaled morphology and increasing electrical conductivity with doping. Specially, heterostructures (e.g., core/shell) are expected to have boundary-enhanced phonon scattering effect. Therefore, heterostructures with materials that have small lattice mismatch could reduce the thermal conductivity of a thermoelectric material without deteriorating its electric properties, thus enhancing ZT value. Reduction of Bismuth on pre-made PbTe in the presence of surfactants was performed resulting in the formation of surface-modified PbTe nanocubes comprising a PbTe core and a Bi shell. The synthesized core-shell nanostructures are investigated by using HR-TEM and XRD analysis. PbTe based heterostructures are expected to contribute to improvement of the thermoelectric performances.

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발표코드: MAT.P-1103

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Sulfur-doped/adsorbed Highly Exfoliated Graphite for Metal-free Electrocatalyst for Oxygen Reduction in Fuel Cells

박지은 장유진<sup>1</sup> 김동하<sup>1</sup> 김성진<sup>2</sup>

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Fuel cells are clean, sustainable energy conversion devices for power generation, and they commonly use platinum as the electrocatalyst. However, Pt-based catalysts suffer from very limited reserves, high cost, and inactivation by CO poisoning. Thus, exploring nonprecious metal or even metal-free catalysts to rival platinum in activity on fuel-cell technologies has been needed. Recent studies have proven that the carbon materials doped with the elements such as N, P or B atoms have pronounced catalytic activity. Herein, we demonstrate a controlled synthesis of sulfur-doped/adsorbed highly expanded graphite (HEG) by liquid precursor-based chemical vapor deposition (CVD) technique. All the HEGs were characterized by Raman spectroscopy, transmission electron microscopy, X-ray diffraction analysis and X-ray photoemission spectroscopy. We demonstrate the resultant S-doped/adsorbed HEG can act as a metal-free catalyst for oxygen reduction reaction (ORR) in fuel cells with a comparable performance as Pt catalyst. The S-

doped/adsorbed HEGs provide a new approach to carbon-based efficient metal-free ORR catalysts for oxygen reduction in fuel cells.





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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Amine-Modified $\text{Fe}_3\text{O}_4@\text{SiO}_2$ and $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{Porous SiO}_2$ : A promising material for $\text{CO}_2$ removal**

**김경 박지은<sup>1</sup> 김성진<sup>2</sup>**

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학 나노과학과 <sup>2</sup>이화여대 화학과

Removal of carbon dioxide( $\text{CO}_2$ ), “green house gas”, from atmosphere has drawn particular attention because of their link to potential climate change.  $\text{CO}_2$  capture by adsorption on amine functionalized porous solid materials has been one of the promising methods. We have synthesized amine functionalized  $\text{Fe}_3\text{O}_4@\text{SiO}_2$  and  $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{Porous SiO}_2$  core shell materials using 3-aminopropyltriethoxysilane(APTES) under various conditions. The resultant materials were characterized by transmission electron microscopy, infrared spectroscopy and thermogravimetric analysis. We evaluated Brunauer-Emmett-Teller (BET) surface area and  $\text{CO}_2$  adsorption capacity by  $\text{N}_2$ ,  $\text{CO}_2$  adsorption/desorption experiment. Comparing with simple silica nanoparticles, amine modified ones have a higher capacity in  $\text{CO}_2$  adsorption because both physisorption and chemisorption take place on the amine modified surface. As the amount of APTES increase, the BET surface area decreases while maximum adsorption capacity is enhanced.

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발표코드: MAT.P-1105

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nitrogen-Doping and Characterization of Graphene Oxide

김여진 박지은<sup>1</sup> 김성진<sup>2</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학 나노과학과 <sup>2</sup>이화여대 화학과

Graphene exhibits various interesting properties which could be utilized for potential applications. The chemical reduction of graphene oxide is considered to be an efficient method to produce graphene sheets in bulk quantity at relatively low cost. Currently, the chemical doping of graphene is an active area of research. Chemical doping is an effective method to intrinsically modify the properties of graphene. Among them, nitrogen doping plays a significant role in improving some properties of graphene. In this study, graphene oxide sheets were synthesized from graphite powder using a modified Hummers method. Nitrogen-doped graphene sheets were prepared through various methods including hydrothermal method in the presence of hydrazine hydrate and thermal annealing in ammonia. Then, the characteristic of each N-doped graphene sheets were compared to each others. The characteristic were investigated through N<sub>2</sub> adsorption, XRD, HR-TEM, XPS, and elemental analysis.

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발표코드: MAT.P-1106

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study on Controlling Bandgaps and Thermoelectric Properties of Titanium Oxide Nanowires by H<sub>2</sub> Reduction

김소영 김하영<sup>1</sup> 한미경<sup>2</sup> 김성진<sup>1</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학과 <sup>2</sup>이화여대 화학나노과학부

Titanium dioxide has emerged as a thermoelectric material because of its low thermal conductivity, large Seebeck coefficient and stability in high temperature. Single crystalline TiO<sub>2</sub> can have improved thermoelectric properties by introducing oxygen defect sites in TiO<sub>2</sub> by reduction. The thermoelectric properties and bandgap energy of modified titanium oxide have been investigated, aiming at studying for the effect of reduction and morphological change on the properties. Single crystal rutile TiO<sub>2</sub>-x nanowires are synthesized by hydrothermal method followed by hydrogen reduction at high temperature to introduce oxygen deficiency in TiO<sub>2</sub>. The morphological features and structure of modified titanium oxides NWs are characterized by FE-SEM and HR-TEM. The optical bandgaps of TiO<sub>2</sub>-x NWs are determined by UV/Vis spectroscopy. Band gaps of reduced titanium oxides are varied depend on their reduction temperature. The thermoelectric properties also have been significantly improved by degree of

reduction. We find that the electrical conductivity and thermal conductivity of reduced titanium oxide  $\text{TiO}_{2-x}$  are enhanced compared to those of  $\text{TiO}_2$ .



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effects of Cu intercalation on thermoelectric properties of $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$ and $\text{Bi}_2\text{Te}_{2.5}\text{Se}_{0.5}$

유혜인 한미경<sup>1</sup> 김성진<sup>2</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학나노과학부 <sup>2</sup>이화여대 화학과

$\text{Bi}_2\text{Te}_3$ -based compounds are considered the most suitable thermoelectric materials for use near room temperature but need more enhancement of efficiency. It has been known that the intercalation of small amounts of 3d transition metal between the van der Waals layers is a good way to increase the thermoelectric figure-of-merit (ZT) of  $\text{Bi}_2\text{Te}_3$ -based compounds. We prepare polycrystalline Cu intercalated  $\text{Bi}_2\text{Te}_3$ -based bulk samples using Bridgman method, and study thermoelectric properties as a function of Cu doping in  $\text{Bi}_2\text{Te}_3$ . In particular, the composition of  $\text{Cu}_{0.07}\text{Bi}_2\text{Te}_3$  achieves the highest ZT (ZT ~ 1.15 at 300K). To optimize the thermoelectric properties of  $\text{Cu}_{0.07}\text{Bi}_2\text{Te}_3$ , we have synthesized and characterized p-type  $\text{Cu}_{0.07}\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$  and n-type  $\text{Cu}_x\text{Bi}_2\text{Te}_{2.5}\text{Se}_{0.5}$  solid solution at various compositions. The structure and composition of the samples are characterized by using XRD and EDS. The temperature dependence of Seebeck coefficient and the conductivity of  $\text{Cu}_{0.07}\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$  and n-type  $\text{Cu}_x\text{Bi}_2\text{Te}_{2.5}\text{Se}_{0.5}$  samples are measured. The p-type  $\text{Cu}_{0.07}\text{Bi}_1\text{Sb}_1\text{Te}_3$  has the highest power factor of  $23\mu\text{W}/\text{cmK}^2$  at 300K,

and the power factor of n-type  $\text{Cu}_{0.03}\text{Bi}_2\text{Te}_{2.5}\text{Se}_{0.5}$  reaches to  $20\mu\text{W}/\text{cmK}^2$  at 350K. Thus, intercalating 3d transition metal is an effective method to improve thermoelectric property.



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발표코드: MAT.P-1108

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of $\text{Bi}_2\text{Te}_3$ Nanotubes as Thermoelectric Materials

김하영 김소영<sup>1</sup> 한미경<sup>2</sup> 김성진

이화여대 화학과 <sup>1</sup>이화여대 화학나노과학과 <sup>2</sup>이화여대 화학나노과학부

We have successfully developed an ethylene glycol mediated one-pot solution phase synthetic method for highly crystalline  $\text{Bi}_2\text{Te}_3$  nanotubes. Highly uniform  $\text{Bi}_2\text{Te}_3$  nanotubes with a length of 1  $\mu\text{m}$  and a diameter of 40 nm can be synthesized through a simple and fast solution process by using ultrathin Te nanowires as sacrificial templates. Different from previous template-directed hydrothermal synthesis, here we used heating mantle as the reactor for preparing  $\text{Bi}_2\text{Te}_3$  nanotubes, which makes the reaction perform more efficiently. As-synthesized  $\text{Bi}_2\text{Te}_3$  nanotubes have a rhombohedral-phase single crystalline structure. It was found that using ethylene glycol as solvent and precise controlling reaction temperature and time were crucial to obtain high-quality single crystal  $\text{Bi}_2\text{Te}_3$  nanotubes. The tube size and morphology can be controlled by adjusting the concentration of NaOH and PVP on the formation mechanism of  $\text{Bi}_2\text{Te}_3$  nanotubes. The crystal structure and morphologies of nanotubes were investigated by powder X-ray diffraction, FE-SEM, and HR-TEM. Thermoelectric properties of nanotubes are discussed.

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발표코드: MAT.P-1109

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## First principles study of electronic properties of graphene and SiO<sub>2</sub> interface

이진희

광주과학기술원 신소재공학과

Graphene is promising material due to its high mobility. Electronic properties of graphene can be affected by supporting substrates. SiO<sub>2</sub> is the most widely used material as a substrate. First principles calculation was performed to investigate electronic property changes between graphene and SiO<sub>2</sub>. Dispersion corrected Density Functional Theory (dispersion corrected DFT) was used, and it described well than DFT. Three different SiO<sub>2</sub> surface states were set on which graphene was adsorbed. Reconstructed surface is fully coordinated oxygen atoms at top. Hydroxylated surface is two OH-terminated, in which the oxygen bonded to silicon. Graphene was adsorbed on two different positions. Hydrogen added surface is that a hydrogen atom passivates three-oxygen-coordinated silicon. A carbon atom of graphene was adsorbed on top of an oxygen atom of SiO<sub>2</sub> (top), or a center of graphene hexagonal lattice was on top of an oxygen atom (hollow). Among them, hydrogen added surface was the most reactive, and hydroxylated surface was the least reactive. Binding energy, charge transfer, and size of band gap were larger when



graphene was adsorbed on much reactive surface. Band gap was in particular dependent to graphene adsorption site. When graphene adsorbed on surface as top position, relatively large band gap was opened. Stronger repulsive interaction at the position considers to splits energy degeneracy at Dirac point. Electrons were transferred from graphene to substrate after adsorption, and graphene was doped to p-type and charged positively. Inhomogeneous charge distribution makes graphene mobility decreased. Thus, reactive  $\text{SiO}_2$  surface state can lead to mobility decreasing although it can induce larger band gap.



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발표코드: MAT.P-1110

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of GaAs<sub>1-x</sub>P<sub>x</sub> nanowires using vapor-liquid-solid mechanism of CVD method

임형순 김한성<sup>1</sup> 박정희<sup>1</sup>

고려대 미세소자공학협동/마이크로소자공학<sup>1</sup> 고려대 소재화학과

GaAs<sub>1-x</sub>P<sub>x</sub> ( $0 < x < 1$ ) nanowires were synthesized by the CVD(chemical Vapor Deposition) method. Zinc blende and Wurtzite are different crystal in cubic structure. Our NWs(avg.diameter = 100nm) grown along the [111] direction and has stacking faults and segments. The percentage of P(phosphine) determine length of segments and their number of stacking faults. Percentage and morphology is shown the XRD, SEM, TEM, UV and RAMAN spectroscopy.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Thermal radiation coating composition research and development

장진호 김육중 조정연 반성태 김근수 이지은

(주)HYTC 연구소

There are various types of thermal radiation material that are in use today, but only little quantity of the material can be added and the effect of thermal radiation is quite low as the technology to disperse the material is still in its infancy. It is possible to adopt the materials for the thermal radiation, such as Metaloxid and Carbon nano Tube-Graphite, by dispersing a dispersant, for example a surfactant. However issues arose concerning the actual thermal property and stability of these materials. This research shows that there is improvement in the effectiveness of the thermal radiation by comparing the results from applying either the high-thermal radiation coating liquid or the existing coating liquid. As a results, it is found that the use of high-thermal coating liquid allow the surfaces to radiate the heat more effectively as well as to prevent them from contamination and corrosion.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development and Modification of OMC(Ordered Mesoporous Carbon) for Removing Heavy Metal Ions

김순근 김지만<sup>1</sup>

경기과학기술연구원 화학생명과학부 <sup>1</sup>성균관대 화학과

Resolution of water pollution is environmental issue. Especially due to water contamination by heavy metal, methods for resolution of these problems are studied in many research groups. Absorption is one of the most famous method for removing these heavy metal ions. We used OMC(Ordered Mesoporous Carbon) for solving this problem. OMC consists of carbon same as charcoal which has high efficiency in cohesion with the other elements, and the electrical adsorption by varying precursors can increase the removing effect. Uniformity of meso-sized pores of OMC were analyzed with X-ray diffraction analysis and nitrogen adsorption. While differentiating carbonization temperature, concentration of heavy metals, the precursor of the OMC, concentration after adsorption was measured, and we found the best condition for absorption of heavy metal using OMC. It showed over than 90% of efficiency when we used OMC made in 900℃ using Quinoxaline (have nitrogen for hetero elements) for precursor. We compared the absorption efficiency with common absorbents such as activated carbon and zeolite. Different absorbents

showed lower than 40% of absorption efficiency. Finally we used SEM-EDS for finding the way how the hetero elements differentiate the absorption efficiency.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Sn nanoparticles by laser ablation and their Electrochemical Application

조용재 김창현 김한성 임형순<sup>1</sup> 임영록 박정희

고려대 소재화학과 <sup>1</sup>고려대 미세소자공학협동/마이크로소자공학

Laser ablation of Sn nanoparticles (NPs) synthesis by gas-source has been performed using a Nd:YAG laser in a vacuum. The Sn NPs are coated with carbon sheath, forming a Sn/C core/shell structure. 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). The Sn NPs/Reduced Graphene Oxide Composites showed excellent lithium ion storage properties. The results showed that the electrochemical performance of composites was greatly enhanced, indicating that the composites might have a promising future as application in Li-ion battery.

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발표코드: MAT.P-1114

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **ZnO on Si nanowires core/shell Nanocable Arrays and their Application**

**임영록 조용재 명운 김한성 박정희**

고려대 소재화학과

The ZnO on Vertically-aligned Si nanowires core-shell nanocable arrays were synthesized by hydrothermal method at a large area of substrates. The length of the Si nanowires is controlled in the range 30 ~ 50 $\mu$ m. 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). Their electrical and physical properties of these nanowires were also investigated.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Assaying Gallium Sulfide (GaS) Nanosheets Character by Transmission Electron Microscopy

백승혁 김한성 정찬수 박정희 안재평<sup>1</sup>

고려대 소재화학과 <sup>1</sup>KIST 산업화지원센터

We aim to prepare graphene-like GaS, which are quasi-two-dimensional compounds in which the atoms within the layer are held together by strong covalent forces while Van der Waals interaction enables stacking of the layers. The products of these reactions were characterized by transmission electron microscopy (TEM), atomic force microscopy (AFM), scanning electron microscopy (SEM), X-ray diffraction (XRD). As a result of TEM analysis, SAED pattern is indexed to [001] zone axis of hexagonal GaS crystal. And line scan and mapping confirmed homogeneous distribution over the whole nanostructure. Last, we also prove Atomic and distance's relation through TEM image & ED pattern on GaS sheet.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Wide-field Raman spectroscopy for high throughput graphene imaging

구은혜 오현규<sup>1</sup> 주상용

연세대 화학과 <sup>1</sup>연세대 화학

Raman spectroscopy, inelastic scattering due to the molecular vibrations (*i.e.* phonon) is widely used to probe carbon materials because of their crystalline structures. Since graphene consists of one layer of 2 dimensional  $sp^2$  honeycomb lattice, Raman spectroscopy is useful to characterize graphene properties, such as the number of layers, doping type, electron-phonon interaction and defects. Although mapping carbon materials with confocal micro-Raman is largely used, it has many difficulties in detection. This technique has low throughput, limited image acquisition speed limited by raster-scanning pixel size and thus is hard to image large area. To overcome these limitations of confocal micro-Raman, wide-field Raman is newly operated as alternative. Wide-field Raman is accomplished by illuminating an area of interest by a defocused spot, collecting the Raman scattered light with an objective. Among various advantages in contrast with confocal Raman imaging, Wide-field Raman Imaging (WRI) is used to rapidly visualize carbon materials on a variety of substrates and characterize the quality, revealing spatial inhomogeneities in film quality that is undetected with point Raman spectroscopy. Moreover, wide-field

Raman is valuable to monitor dynamic processes in carbon material synthesis with high spatial and spectral resolution over a large area in real time.[1] ACS Nano 2012, 6 (1), 373[2] Nanotechnology 2007, 18, 165707



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**[발표취소] Sol-gel method preparation of TiO<sub>2</sub> that has a organic functional group in low temperature**

**김성필 최현철**

전남대 화학과

**발 표 취 소**

본 논문은 발표취소된 논문입니다.

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발표코드: MAT.P-1118

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and Synthesis of Inherently Conducting Polymer composites

YARU 조원제 유국현

동국대 화학과

In nowadays, the Conductive polymers have wide perspective and practicability in many fields, because they are easy to synthesize, in the meanwhile, they have series of excellent characteristics, such as high conductivity, high electrochemical properties and etc. Among them, polyaniline, polypyrrole have been widely applied as Conductive polymers. However, they have some drawbacks which can limit their application in some particular field. Conductive polymer composites was a new kind of functional polymer materials, the research and application of conducting polymer composites was widely paid attention in recent years. the major research challenges in the development of conducting polymer composite materials is reducing the filler content as much as possible while improving the electrical conductive and the stability of electrical properties. In my research I mixture these three Conductive polymers with Conductive polymers-DADMAC (Diallyldimethyl ammonium chloride) which is well studied recently and synthesize them together to form a new Conductive polymer composite which can be

used in many field for its outstanding property. the experimental results show that, Conductive polymer-DADMAC composites has high conductivity and thermal stability



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effective separation of metallic components using supercritical fluids treated SWCNT

김효선 서영수<sup>1</sup>

세종대<sup>1</sup> 세종대 나노공학과

For the electrical applications, it is essential for separating metallic and semiconducting components of single-walled carbon nanotubes (SWCNTs). We applied supercritical fluids (SCF) to SWCNT to separate the metallic component effectively using gel chromatography. It could be because SCF treated SWCNTs are more debundled than pristine one. Metallic component were quantitatively analyzed using Near-IR spectroscopy. Thin films of the separated SWCNT were made via vacuum filtration method using anodic aluminum oxide membrane with 0.1 $\mu$ m pore and in turn transferred on to PET film. Sheet resistance of the films will be compared with the chemical properties of it, which were measured using Raman spectroscopy and UV-Vis spectroscopy

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## One-Pot Synthesis of Pt-Graphene-Layered Titanate Nanocomposites with Improved Functionality as an Electrocatalyst for Oxygen Reduction

신수인 고아라<sup>1</sup> 이영미<sup>1</sup> 황성주<sup>2</sup>

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Three-component nanocomposites consisting of layered titanate nanosheets, graphene nanosheets, and Pt nanoparticles are synthesized to investigate the effect of the incorporation of layered titanate nanosheet on the electrocatalytic activity and physicochemical properties of Pt-graphene nanocomposite. The Pt-graphene-layered titanate nanocomposites are prepared by the crystal growth of Pt nanoparticles on the surface of the colloidal mixture of layered titanate nanosheets and graphene oxide nanosheets. According to powder X-ray diffraction and Fourier transformed-infrared spectroscopic analysis, the obtained nanocomposites are composed of face-centered cubic Pt metal and the mixed nanosheets of layered titanate and reduced graphene oxide (RGO). Field emission-scanning electron microscopy-energy dispersive spectrometry clearly demonstrates the homogeneous hybridization between the Pt nanoparticles and the layered titanate/RGO nanosheets with house-of-cards type porous stacking

morphology. The homogeneous distribution of Pt nanoparticles on the surface of graphene and titanate nanosheets is confirmed by high resolution-transmission electron microscopy. All of the present Pt-RGO-layered titanate nanocomposites display promising functionality as an electrocatalyst for oxygen reduction. The catalytic activity of the Pt-RGO nanocomposite is remarkably improved by the incorporation of layered titanate nanosheet, underscoring the beneficial role of layered titanate phase.





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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effects of supercritical fluid treatment on CNT films prepared by a filtration method

최진혁 서영수<sup>1</sup>

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Electrical conductivity of CNT films prepared using a filtration method was measured as a function of optical transmittance of the films. Supercritical fluid treated CNT which showed better dispersion in aqueous solution, however, exhibits lower conductivity and less-stiff percolation behavior in the optical transmittance-conductivity curve than non-treated one. This result may be due to tight binding of surfactant on the tubes during the SCF treatment. After acid treatment on the films, conductivity of the film prepared from SCF-treated CNT was more enhanced. Chemical composition of the film will be analyzed using Raman spectroscopy and others.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Size Effects of Au Nanoparticles on the Performance of Dye-Sensitized Solar Cells

장윤희 김동하

이화여대 화학나노과학과

Plasmonic metal nanoparticles (NPs) have widely applied in various research fields such as optoelectronics, optical sensing, and nanoplasmonics due to their unique optical and electrical properties from bulk materials. Especially, the metallic NPs can be effective in solar cell system since the performance of the cell can be enhanced due to not only near field enhancement through the localized surface plasmon resonance but also light scattering effect. Herein, we experimentally investigate the effect of the inclusion of Au NPs with various sizes into TiO<sub>2</sub> layers as tailor-designed plasmonic photoanodes in dye-sensitized solar cells. The composite photoanode layers show intense light absorption and enhanced photocurrent density due to increased local field intensity and light pathways, and thereby cell efficiency was improved.

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## **Metal Nanoparticles at the Periphery of Poly(4-vinylpyridine) shell in designed Core@Shell Nanostructures for LSPR-Based Sensing and Electrocatalysis**

이지은 김동하

이화여대 화학나노과학과

Bimetallic Core@shell nanoparticles have demonstrated distinctly different properties and potential uses in electronics, magnetism, catalysis, optics, and sensors. Their versatility in a wide range of applications stems from their unique physical and chemical properties directly related to particle size, shape, and interparticle distance and surface properties. The properties of the gold nanoparticles (AuNPs) are based on localized surface plasmon resonance (LSPR), the coupling of light into the resonant oscillation of charge density on the nanostructured noble metal surface. Core@shell type nanospheres have also been utilized as a platform for integration of functionalities into both the core and shell. The interaction between two types of metal NPs selectively located in the core and shell may alter the LSPR property, depending on the relative amount of the two metal components, the relative distance between them and the shell thickness. We suggest a unique strategy to generate core@shell nanoparticles based on pH-

sensitive AuNPs decorated with polymer shell. Concretely, pH-sensitive AuNPs having P4VP on the surface were first fabricated through SI-ATRP. Then, they were mixed with selected metal precursor solutions followed by reduction using reducing agent. The metal NPs thus incorporated were distributed uniformly in the P4VP polymer shells. We investigate the structural alteration during the sequential synthetic process. The bimetallic nanostructures of AuNP@PVP nanocomposites containing another type of metal NP at the PVP periphery exhibit a controlled optical sensing property based on LSPR coupling phenomenon and a typical electrocatalytic activity for methanol oxidation reaction.



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## **Incorporation of Carbon-Doped Mesoporous TiO<sub>2</sub> onto Graphene Sheets and Their Visible Light Active Photocatalysis**

**Saji Thomas 김동하**

이화여대 화학나노과학과

Titanium dioxide (TiO<sub>2</sub>) is one of the most promising functional inorganic materials for photocatalysis. However, the wide bandgap energy (3.2eV) of TiO<sub>2</sub>, restricts its photocatalytic activity under the entire range of solar spectrum. Many efforts such as dye sensitization, metal/non-metal doping, and introduction of plasmonic nanostructures have been made to synthesize TiO<sub>2</sub>-based nanocomposites for the inhibition of electron-hole recombination and extending its absorption to visible region. Among them, non-metal doping may lead to chemically stable photocatalysts compared to others, but quenching of electron-hole recombination is still a problem to be addressed. Graphene is considered as a good support for the loaded nanoparticles to achieve a uniform distribution without any aggregation. When graphene is combined with carbon-doped TiO<sub>2</sub>, at the interface the excitons of TiO<sub>2</sub> can be transferred from the conduction band of TiO<sub>2</sub> to graphene owing to the energy level structure, resulting in an effective separation of electrons and holes. Here, we use amphiphilic triblock copolymer (P-123) as scaffold and carbon source

to fabricate mesoporous carbon-doped TiO<sub>2</sub>. A desired amount of titanium isopropoxide was mixed with aqueous solution of P-123 and the solution was left for evaporation-induced self-assembly (EISA). The obtained membrane was calcined under inert atmosphere to obtain carbon doped mesoporous TiO<sub>2</sub>. This was then mixed with graphene oxide and reduced to form graphene. The visible light photocatalytic efficiency of thus obtained nanocomposites was exploited using p-nitrophenol as target dye.



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## Graphene-Based Hybrids for Supercapacitor Applications



**최문형 백승민**

경북대 화학과

Graphene Nanosheets are widely used in key technologies, such as catalysis, gas sensors, and energy storage materials. On the other hand, metal nanoparticles also have attracted much attention as promising materials because they could exert synergetic functionality by the hybridization with layered compounds. We describe the synthesis of graphene nanosheet/metal hybrids through a soft-chemical synthetic process. The nanohybrid material was characterized by X-ray diffraction technique, scanning electron microscopy (SEM). X-ray diffraction (XRD) studies show that the graphene nanosheets are homogeneously hybridized with nanoparticles. According to the SEM images of these hybrids, the nanosized metal particles are distributed inbetween the graphene nanosheets. These nanohybrids are also characterized using BET method, FT-IR and TG Analysis. The present hybrids result in an enhanced specific capacitance in comparison with the starting materials.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparison of lithium adsorption capacity between $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ and $\text{Li}_{1.6}\text{Mn}_{1.5}\text{M}_{0.2}\text{O}_4$ (M=Co, Fe) as lithium adsorbents

권지희

충남대 화학과

The spinel-type lithium manganese oxide  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  is the most suitable for recovery of lithium from seawater, because it has a high selectivity for lithium ions, large adsorptive capacity, and high chemical stability. It is also known that the chemical stability of transition metal substituted spinel materials is better than the spinel lithium manganese oxides. Therefore, it is interesting to see how the lithium adsorption capacity of the transition metal substituted spinel materials is varied based on the dopants such as Cr, Co and Fe etc. In this work  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  and metal-doped  $\text{Li}_{1.6}\text{Mn}_{1.5}\text{M}_{0.2}\text{O}_4$  (M=Co, Fe) materials are prepared using sol-gel method followed by calcination at  $450^\circ\text{C}$  for 24h. And then the  $\text{Li}^+$  extraction were performed in a 0.5M HCl solution. The  $\text{Li}^+$  uptake experiments are performed to find a close relationship between  $\text{Li}^+$  adsorption capacity and transition metal substituents. The physicochemical properties of the product were characterized by thermo gravimetric analysis (TGA)/differential thermal



analysis (DTA), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), and inductively coupled plasma atomic emission spectroscopy (ICP-AES).



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of spinel $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ from $\beta\text{-MnO}_2$ using flux method and its lithium uptake capacity for lithium adsorbent

채창완

충남대 화학과

$\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  phase is the most promising lithium adsorbent due to its high lithium-uptake capacity and chemical stability. In order to synthesize  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  phase with various morphologies, we have prepared  $\beta\text{-MnO}_2$  with various morphologies through hydrothermal method. For example, the  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  has been synthesized from needle-like and seed-like  $\beta\text{-MnO}_2$  through flux method using relatively low reaction temperature to prevent phase transition of  $\beta\text{-MnO}_2$  occurred at more than  $500^\circ\text{C}$  due to the loss of oxygen. In order to evaluate the lithium uptake capacity of the as-prepared  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  with various morphologies difference, the  $\text{Li}^+$  extraction was performed by acid treatment and  $\text{Li}^+$  uptake was carried out in lithium-enriched solution. SEM observation showed that the morphology of  $\beta\text{-MnO}_2$  was maintained through the whole processes, which means that the morphology control of the precursor compounds such as  $\beta\text{-MnO}_2$  can provide a route to control the morphology of the final products such as  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ . The physicochemical properties of the  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  and  $\text{H}_{1.6}\text{Mn}_{1.6}\text{O}_4$  were characterized by

X-ray powder diffraction (XRD), inductively couple plasma-atomic emission spectroscopy (ICP-AES) and thermogravimetric analysis (TGA)/differential thermal analysis (DTA).



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Copper(I) sulfide Counter Electrode for Photoelectrochemical Cell

최진웅 정찬수 김한성 박정희

고려대 소재화학과

Copper(I) sulfide, with an indirect band gap of approximately 1.2 eV, is an appealing photovoltaic material. The synthesis of vertically aligned Copper(I) sulfide nanowires has been described. Briefly, a Cu foil electrochemically polished then placed in a quartz tube, where a mixture of H<sub>2</sub>S, oxygen gas flowed over the surface of the Cu foil. The reaction took place at room temperature. Analyze the Cu<sub>2</sub>S NWs by Transmission electron microscope(TEM), Scanning electron microscope(SEM), X-ray diffraction(XRD), Raman spectrum.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Computational screening and organic syntheses of three monoethanolamine derivatives as potential CO<sub>2</sub> absorbents

조은희 전영호 심재웅 김자현

송실대 화학과

Aqueous monoethanolamine (MEA) captures quickly CO<sub>2</sub> in flue gas through forming water-soluble carbamate, and is regenerated when the carbamate solution is heated at 120 °C. To find amines which can compete with MEA in terms of reactivity and regeneration energy, eleven MEA derivatives have been considered for calculating their nucleophilic reactivity and accessibility to CO<sub>2</sub>. Based on the analysis of the electronic reactivity indices with those of MEA, three candidate compounds have been chosen and synthesized by alkylation reactions of amines, their corresponding alkylhalides or epoxides. After purification in a Kugelrohr apparatus, the products were characterized by FAB-MS, IR, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR spectroscopy.

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발표코드: MAT.P-1130

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Organic pcu net Framework Connected by Salicylbisimine Octahedral Cages

고낙은 최상범 심재웅 김태민<sup>1</sup> 김자현

송실대 화학과 <sup>1</sup>송실대

A new covalent-organic framework was synthesized by a one-step Schiff base condensation reaction between triamine unit and fused salicylbisaldehyde. Instead of salicylbisaldehyde, fused salicylbisaldehyde was used to connect the six vertices of the octahedral organic cage to make a three-dimensional pcu type framework. The salicylbisimine framework is amorphous and insoluble in common organic solvents. Its measured surface area is smaller than that of a proposed structure, implying framework interpenetration.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fabrication of magnetic core-shell particles and its photocatalytic activity

김도연 정진승<sup>1</sup>

강릉원주대 화학신소재학과 <sup>1</sup>강릉원주대 화학과

Multifunctional  $\text{Fe}_3\text{O}_4@\text{TiO}_2$  core-shell particles were fabricated by atomic layer deposition (ALD) process that induces the magnetic particles to be coated with a  $\text{TiO}_2$  shell. Multifunctional core/shell particles are characterized by field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), x-ray diffraction (XRD). Magnetic measurement indicates that the as-synthesized  $\text{Fe}_3\text{O}_4@\text{TiO}_2$  core-shell particles are superparamagnetic at room temperature. Photocatalytic experiment is demonstrated by utilizing the oxidation reaction of rhodamine B with the photofunctional magnetic core-shell particles.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -Lectin

강경태 채원식<sup>1</sup> 정진승

강릉원주대 화학과 <sup>1</sup>한국기초과학지원연구원 강릉센터

Superparamagnetic submicron materials have become particularly crucial in research area for biomedical applications such as drug delivery, biosensor, bioseparation, and photocatalyst. In order for magnetic submicron materials to be applied in this kind of applications, it needs to be soluble in water solution and have high saturated magnetization in mild magnetic field. To detect of glycoproteins in relation to adult cancer diseases, we made lectin-immobilized magnetic particles which can mix with blood sample separate particles by using magnetic field. These lectin-immobilized superparamagnetic particles have synthesized by following methods. Firstly, magnetic  $\text{Fe}_3\text{O}_4$  submicron particles were synthesized by solvothermal reduction method, and then, formed  $\text{Fe}_3\text{O}_4@\text{SiO}_2$  using sol-gel method. After modifying silica surface, we got the lectin-immobilized  $\text{Fe}_3\text{O}_4@\text{SiO}_2$  particles. Microstructure of the  $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -Lectin is characterized by FE-SEM, TEM, XRD, FLIM, FT-IR spectroscopy.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Titania Films and CdS Nanoparticles Sequentially Coated on Core/Shell Silica Microspheres for Hydrogen Evolution**

**이강혁 장혜령 강승희 허남희**

서강대 화학과

We have synthesized titania-coated core/shell silica microspheres, which contain CdS nanoparticles (NPs) within mesoporous silica shells. First CdS NPs are embedded within mesoporous silica shells in core/shell silicas and then titania films are coated on the microspheres. Depositions of CdS NPs and titania films were repeated a couple of times to encapsulate more CdS NPs into mesoporous shells. Finally the microspheres were annealed under the CS<sub>2</sub>/Ar atmosphere at 573 K. The resulting microspheres, meso-SiO<sub>2</sub>@CdS/TiO<sub>2</sub>, were characterized by various means such as transmission electron microscopy, scanning electron microscopy, photo luminescence (PL), UV-visible spectroscopy, and X-ray powder diffraction. The Pt-loaded meso-SiO<sub>2</sub>@CdS/TiO<sub>2</sub> microspheres show photocatalytic activity, which produce efficiently hydrogen under visible light. An important feature of the meso-SiO<sub>2</sub>@CdS/TiO<sub>2</sub> microsphere is that it can encapsulate CdS and Pt NPs within the titania shell, which prevents the loss of active NPs in the course of photolysis.

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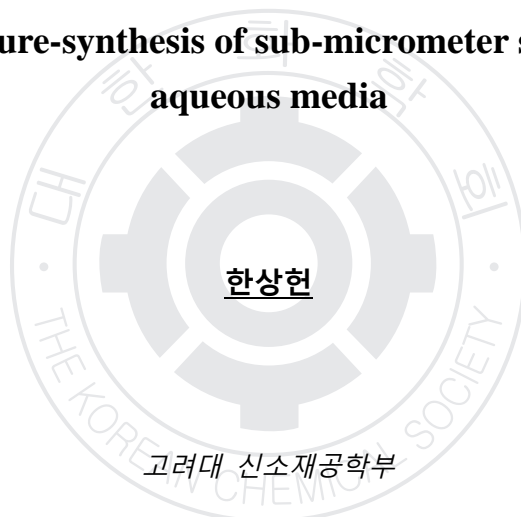
장소: 일산KINTEX

발표코드: MAT.P-1134

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Room temperature-synthesis of sub-micrometer silver particles in aqueous media



We have developed a facile method for synthesizing sub-micrometer silver particles using poly(4-vinylbenzenesulfonate sodium salt) as a structure directing reagent in aqueous media at room temperature. We have demonstrated that molecular weight and concentration of the polymer can effectively and systematically control the sub-micrometer silver particle structures. The chemical and physical properties of sub-micrometer silver particles have been investigated and taken advantage of for diagnostic applications.

일시: 2012년 4월 25~27일(수~금) 3일간

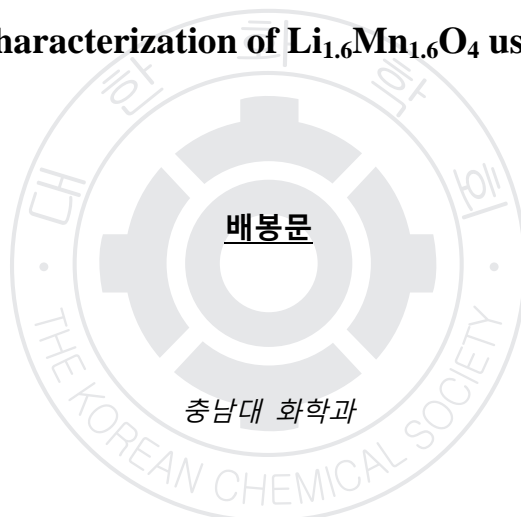
장소: 일산KINTEX

발표코드: MAT.P-1135

발표분야: 재료화학

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## Synthesis and characterization of $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ using flux methods



$\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  has received considerable attention as lithium selective adsorbent. Unlike other manganese oxide adsorbents that contain Mn(III), the absolute Mn(IV) is present in  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  and the redox reaction cannot occur during lithium extraction/insertion reaction. Therefore, the chemical stability is sufficiently high. In addition, the ion-exchange capacity may be markedly larger than that of the other manganese oxides because the theoretical exchange capacity reaches 69 mg/g on the basis of the chemical composition. However, the synthesis of  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  cannot be done easily due to other competing phases using conventional high temperature reactions. In this study, we are quite successful in preparing homogeneous  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  using lithium-containing fluxes at relatively low temperature. The characterization of  $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$  is performed X-ray powder diffraction (XRD), scanning electron microscope (SEM) and inductively coupled plasma-atomic emission spectroscopy (ICP-AES).

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Size-Controlled Electron Transfer and Photocatalytic Activity of ZnO-Au Nanoparticle Composites

김덕한 이재일<sup>1</sup> 이명순<sup>1</sup> 이동일

연세대 화학과 <sup>1</sup>Nanomaterials Lab, U.S.A

This Letter describes size-controlled photocatalytic activity of ZnO nanoparticles coated with glutathione-protected gold nanoparticles with diameters of 1.1, 1.6, and 2.8 nm. The photocatalytic activity of the ZnO-Au composites was found to increase with increasing gold size for both oxidative and reductive catalytic reactions. Photoluminescence decay dynamics of the composites showed that the electron-transfer rate from the photoexcited ZnO to gold nanoparticle also increased as the gold size increased. These results demonstrate that the photogenerated electron transfer and the resulting catalytic activity of the composites can be controlled by the size of the mediating gold capacitors.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) using hydrothermal reaction method

허지수

충남대 화학과

Hematite as one of the most stable iron oxide under ambient conditions, is widely used in commercial and industrial applications, such as catalysts, pigments, fine ceramics, sensors, environment protection, and hydrogen storage. The physical and chemical properties of materials largely depend on the size and morphology. Therefore much attention has been paid to the controlled synthesis of hematite particles. There are a lot of ways to synthesize hematite, for example gel?sol processing, forced hydrolysis processing, and hydrothermal methods. Among them hydrothermal method is one of the most promising methods because the powders prepared through hydrothermal route have high purity, narrow particle size distribution and precise composition. In the hydrothermal process, the pH value of the solution plays a great part in modifying the morphology, phase and size of the products. In our study to synthesize the iron oxide cubes, the aqueous solution containing formic acid and ferric chloride was maintained in a Teflon-lined autoclave at 180°C for 30h. The characterization of the samples by XRD confirmed the formation of

$\alpha$ -Fe<sub>2</sub>O<sub>3</sub> (hematite). SEM (scanning electron microscope) analysis was carried out to study the morphology and particle size of the hematite prepared.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nitrogen oxide removal of nanoporous carbons by template method

배경민 김병주<sup>1</sup> 박수진

인하대 화학과 <sup>1</sup>전주기계탄소기술원 탄소밸리사업단

In this work, nanoporous carbons (NCs) were prepared by self-assembly of polymeric carbon precursors and block copolymer template in the presence of tetraethyl orthosilicate (TEOS) and colloidal silica. The NCs' pore structures and total pore volumes were analyzed by reference to  $N_2/77$  K adsorption isotherms and their surface morphologies were characterized using a transmission electron microscope (TEM). The porosity and nitrogen oxide removal of NCs were increased by activation with carbon dioxide. It could be concluded that nitrogen oxide removal ability of NCs depends on the textural properties, and NCs were good materials for nitrogen oxide removal.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of anodic oxidation on the surface and mechanical properties of carbon fiber-reinforced epoxy resin composites

배경민 김병주<sup>1</sup> 박수진

인하대 화학과 <sup>1</sup>전주기계탄소기술원 탄소밸리사업단

The effect of anodic oxidation on the surface and mechanical properties of carbon fiber-reinforced epoxy resin composites was investigated. The surface properties of the anodized carbon fibers were studied through the measurement of contact angles and through SEM and XPS analyses. The mechanical interfacial properties of the composites were studied through measurements of interlaminar shear strength (ILSS), critical stress intensity factor ( $K_{IC}$ ). It was shown that the surface functional groups containing oxygen on the anodized carbon fibers exert great effects on the surface energetics of fibers and the mechanical interfacial properties.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Elemental mercury adsorption of porous carbons based on polymeric resin

배경민 김병주<sup>1</sup> 박수진

인하대 화학과 <sup>1</sup>전주기계탄소기술원 탄소밸리사업단

Porous carbons (PCs) were prepared from polystyrene-based cation-exchangeable resin (PSI). The influence of the method of activation was studied in the elemental mercury adsorption behaviors of the porous carbons. The textural properties were studied by BET and D-R methods with N<sub>2</sub>/77K adsorption isotherms. The PCs activated by chemical activation have much better textural parameters and elemental mercury adsorption behaviors than those activated by physical activation. This was probably due to the elemental mercury adsorption ability of PCs depends on the method and procedure of activation as well as on their textural parameters.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Au nanoflowers coated indium-doped tin oxide substrate fabricated by combining chemical assembly and electro-deposition methods**

**Bu yanru 이상화**

경원대 화학생명공학과

In this work, a new method combining chemical assembly and electro-deposition methods was used to prepare Surface Enhanced Raman Scattering (SERS) active substrate. Small Au nanoparticles (5nm) were arrayed as seeds on the indium-doped tin oxide (ITO) glass with the assistance of 3-aminopropyltrimethoxysilane (APTMS), followed by the constant potential deposition. We systematically investigated the effect of the concentration of  $\text{HAuCl}_4$ , depositing potential, depositing time on the substrate morphology (such as the density, size, and structure of the Au nanoflowers) and their coupling state. In Raman measurement, o-Chloro Thiophenol was chosen as a probe molecule to check the uniformity and activity of the as-prepared substrate. Moreover, the variation of Raman intensities as the function of the probe concentration was also investigated to realize the quantitative detection of o-Chloro Thiophenol using this SERS substrate. Key words: Au, concentration, depositing time, depositing potential, Raman intensity

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발표코드: MAT.P-1142

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Surface modification of Melanin-like Nanoparticles and Fabrication of Organic-Soluble Melanin-like Nanoparticle/Polymer Composite Film

황대웅 주국연 이진규

서울대 화학부

Melanins are naturally occurring dark-colored pigments ubiquitously found in most organisms and they exhibit various interesting properties such as broad semiconductor-like absorption spectra, radical scavenging, antioxidative behavior and metal-binding properties. Melanin-like nanoparticles (MLNPs) are an unprecedented synthetic melanin model providing nanoparticle character of natural melanin with similar physicochemical property to the natural melanin. Accordingly, they have great potential for a melanin-based functional material originated from the melanin's various biological functions. To devise a MLNP-based functional material, however, developing a suitable surface modification method for the MLNPs is essential. In this regard, we examined the surface modification of MLNPs with alkyl amines and could generate organic solvent-dispersible MLNPs. Furthermore, an organic composite film could be fabricated by solvent casting and spin-coating a mixture of the surface-modified MLNPs and a commercially available polymer.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Au@Pd core-shell nanocubes with Finely- and Well-Controlled Sizes: Synthesis and Their Optical Properties**

**김도열 최경우 임상혁<sup>1</sup> 박오욱**

KAIST 생명화학공학과 <sup>1</sup>한국화학연구원 소자재료센터

We report a facile method for the synthesis of uniform Au@Pd core-shell nanocubes with finely- and well-controlled sizes by seed-mediated growth. Using single-crystal seeds of Au spheres with a uniform size, we could reproducibly obtain Au@Pd core-shell nanocubes with a narrow size distributions (98%). Moreover, the size of Au@Pd core-shell nanocubes could be finely and readily tuned in a controllable fashion from 11.4 to 41.1 nm in an edge length by varying the concentration of Na<sub>2</sub>PdCl<sub>4</sub>, the amount of seeds, or both. We have also investigated the localized surface plasmon resonance (LSPR) properties of Au@Pd core-shell nanocubes as a function of Pd shell thickness.

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발표코드: MAT.P-1144

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication of multifunctional phosphor films, layered rare-earth hydroxide nanosheets and SiO<sub>2</sub> nanoparticles**

**이병일 변송호**

경희대 화학과

Multifunctional luminescent films, which have antireflection, antifogging, and luminescence properties, were fabricated by a layer-by-layer assembly of layered gadolinium hydroxide(LGdH) nanosheets and SiO<sub>2</sub> nanoparticles on the quartz glass plates. Eu, Tb, and Dy were selected as activator cations for red, green, and blue displays in LGdH host matrix. These thin-film coatings of layered rare-earth hydroxide nanosheets and SiO<sub>2</sub> nanoparticles of ~20 nm in diameter led to a significantly reduced reflective losses in the visible region, exhibiting an attractive and potentially useful antireflection property, nanoporosity-derived superhydrophilicity, and antifogging property. Highly improved transmittance enabled us to display combinatorial color luminescence, which can be achieved by multiply overlapping individual films with different combinations, without significant loss of transparency. Triple overlap of red/green/blue films generated an excellent white-light under 254 nm UV irradiation.

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장소: 일산KINTEX

발표코드: MAT.P-1145

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Water soluble upconverting nanoparticles with photoswitchable fluorescence

배정수 장다은 안광현<sup>1</sup> 변송호

경희대 화학과 <sup>1</sup>경희대 응용화학과

Well crystallized hexagonal-phase  $\beta$ -NaYF<sub>4</sub>:Yb,Tm nanoparticles, known as highly efficient IR-to-visible upconverting nanoparticles(UCNPs), were synthesized via user-friendly route. The surfaces of UCNPs were modified with block copolymer, such as pluronic F-127 composed of a long hydrophobic chain and two hydrophilic head groups. Photoswitchable fluorescence organic dyes (a series of diarylethene) were then intercalated into the inner shell by hydrophobic interaction. Photoswitching and upconversion photoluminescence properties of the resulting aqueous suspension were measured with UV (~312 nm) and Near-IR laser (~980 nm), respectively. Bio-compatibility of organic dye-implanted UCNPs with high water solubility showed a potential application for NIR fluorescent bioimaging.

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발표코드: MAT.P-1146

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Simple and easy synthesis of magnetic nano-capsules

최제남 차진명<sup>1</sup> 이진규<sup>1</sup>

서울대 화학과 <sup>1</sup>서울대 화학부

나노 물질은 크기, 모양, 형태에 따라 물질의 물리적? 광학적? 화학적 특성이 변하므로 이를 조절 하기 위한 많은 노력들이 있어왔다. 특히, hollow structure 는 구조 내 빈 공간과 넓은 표면적, 작은 밀도 등의 장점을 가지고 있어 다양한 분야에 응용될 수 있을 것으로 기대되고 있다. 본 연구에서는 akaganeite( $\beta$ -FeOOH)를 출발 물질로 기존의 polyol 방법을 변형하여 template 없이 매우 간단한 방법으로 자성 나노 캡슐을 합성하였다. 합성 방법은 미리 합성한 스핀들 모양의  $\beta$ -FeOOH 를 sodium acetate (NaOAc) 존재 하에, ethylene glycol 을 용매로 reflux 하였다. 정확한 합성 메커니즘은 아직 명확하게 이해 되지 않았지만, ethylene glycol 에 의한 부분적인 환원( $\text{Fe}^{3+} \rightarrow \text{Fe}^{2+}$ )에 의해  $\beta$ -FeOOH 에서  $\text{Fe}_3\text{O}_4$  로 상 변화가 일어나며, hollow structure 를 만드는데 NaAc 가 결정적 역할을 하는 것으로 생각된다. 이러한 hollow structure 합성법은 기존의 방법과 달리 매우 간단하며 경제적이다. 합성 메커니즘과 합성된 물질은 X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron

microscopy (TEM), Brunauer-Emmet-Teller (BET) 측정을 통해 분석하였고, vibration sample magnetometer (VSM)으로 자성 특성을 보았다.





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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ultrasmall PbS quantum dots for energy applications

최혜경 정소희<sup>1</sup> 김영조

충북대 화학과 <sup>1</sup>한국기계연구원 나노기계연구본부

We investigated a synthetic route and characterization for ultrasmall PbS quantum dots having extreme quantum confinement with 1.5 to 2.9 nm in diameter. To get a series of PbS quantum dots with first absorption wavelength ranging from 580 to 820 nm (2.1-1.5 eV), they were controlled by adjusting growth temperature in the range of 70 - 95 °C, growth time. In photoluminescence (PL) spectra we found that red shift with respect to the first absorption peak increases with decreasing PbS quantum dots size. Ultrasmall PbS quantum dots solids were further assembled to demonstrate the transport properties for energy applications. This work was supported by the Global Frontier R&D Program by the Center for Multiscale Energy Systems funded by the National Research Foundation under the Ministry of Education, Science, and Technology, the Industrial Core Technology Development Program funded by the Ministry of Knowledge Economy (No. 10035274).

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발표코드: MAT.P-1148

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Oxidation Behaviors of Carbon/Carbon Composites with TEOS

정건 박수진<sup>1</sup> 서민강<sup>2</sup>

전북대 고분자나노공학과 <sup>1</sup>인하대 화학과 <sup>2</sup>전주기계탄소기술원 전략기획실

In this work, the tetraethylorthosilicate(TEOS) used as an oxidation inhibitor was impregnated with phenolic resins to improve the anti-oxidation properties of Carbon/Carbon composites in different concentrations of 0, 1, 2, and 3 wt.%. Thermogravimetric analysis(TGA) was executed to evaluate the thermal decomposition mechanism and thermal stability of the composites in the temperature range of 30-850°C. All the mechanical interfacial properties of the composites were also studied with interlaminar shear stress (ILSS) measurement.

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발표코드: MAT.P-1149

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Ge nanoparticles by laser ablation and their applications

김창현 장동명 명윤 김한성 조용재 임형순<sup>1</sup> 박정희

고려대 소재화학과 <sup>1</sup>고려대 미세소자공학협동/마이크로소자공학

Laser ablation of Ge nanoparticles (NPs) synthesis by gas-source has been performed using a Nd:YAG laser in a vacuum. The formation of the Ge NPs morphology, strain and composition with the number of laser pulses incident on the same part of the surface, have been studied using X-ray diffraction, transmission electron microscopy and Raman spectroscopy.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Influence of KOH Activation on Porosity of Styrene-acrylonitrile (SAN)-based Carbons**

이지한 박수진

인하대 화학과

In this work, we prepared styrene-acrylonitrile (SAN)-based porous carbons by chemical activation using potassium hydroxide (KOH). Activations were performed at different temperatures with 1:4 SAN-based carbon/KOH ratio to investigate the influence of thermal treatment on porosity of SAN-based carbons during activation. The textural characteristics of activated SAN-based carbons were determined by  $N_2/77$  K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and BJH method. The morphologies of the activated carbons were investigated by scanning electron microscope (SEM) and transmission electron microscopy (TEM). Also, the structural properties of the activated carbons were characterized by X-ray diffraction spectroscopy (XRD).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Influence of KOH activation on electrochemical performance of coaltar pitch-based activated carbon for supercapacitor**

**허지훈 서민강<sup>1</sup> 박수진<sup>2</sup>**

전북대 유기소재파이버 공학과 <sup>1</sup>전주기계탄소기술원 전략기획실 <sup>2</sup>인하대 화학과

In this work, coaltar pitch-based activated carbons (ACs) were prepared as supercapacitor electrode materials. The effect of KOH activation temperature on electrochemical performance of the ACs was investigated. The textural properties and morphologies of the ACs were analyzed by reference to  $N_2/77\text{ K}$  adsorption isotherms and field emission scanning electron microscope (FE-SEM), respectively. The electrochemical performance of the ACs was confirmed by cyclic voltammograms (CV). The experimental results indicated that the specific capacitance of the ACs increased with developing the pore structures by activation temperature increase.

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발표코드: MAT.P-1152

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Au triangular-shaped nanostructure For Sensitivity Enhancement of Surface Plasmon Resonance Sensor

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. SPR has been widely employed for biosensor applications because of the capability for label-free detection of biomolecular interactions. Nanosphere lithography (NSL) is an inexpensive, simple to implement, inherently parallel, high throughput, materials general nanofabrication technique capable of producing an unexpectedly large variety of nanoparticle structures and well-ordered 2D nanoparticle arrays. In this study, we used Au triangular-shaped nanostructure for SPR sensitivity enhancement. The Au based thin film was evaporated by sputter on the flat  $18 \times 18 \text{ mm}^2$  cover glass substrates. Periodic particle array surfaces have been prepared using identical single-layer Nanosphere lithography (NSL) masks made by Langmuir-Blodgett (LB) method of silica nanospheres with a variety of diameter ( $D = 150, 300, \text{ and } 500$ ). The Au nanostructured SPR chip was fabricated by e-beam evaporation on the Au based thin film substrates. The Au nanostructured SPR chips showed a remarkable

shift of resonance angle for analytes such as water and ethanol aqueous solution compared with that of conventional Au chip. The peaks of near resonance angle were widened especially when 150 nm sized silica particle template based chip was used. In comparison to conventional flat Au chips, sensitivity enhancement was up to 120% on the 150 nm sized silica particle template based chip. The tendency for the sensitivity enhancement change in bulky refractive index remains the same as previous Au nanostructured SPR researches.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of MoO<sub>3</sub> on Friction and Wear Properties of Carbon/Carbon Composites

정건 박수진<sup>1</sup> 서민강<sup>2</sup>

전북대 고분자나노공학과 <sup>1</sup>인하대 화학과 <sup>2</sup>전주기계탄소기술원 전략기획실

In this work, the molybdenum oxide (MoO<sub>3</sub>) used as an oxidation inhibitor was impregnated with phenolic resins to improve the friction and wear properties of Carbon/Carbon composites in different concentrations of 0, 5, 10, and 15 wt.%. The friction and wear properties of the composites were investigated using a constant speed wear test apparatus in an oxidation environment. To investigate the surface microstructure of the composites, the friction surfaces after wear tests were examined using the scanning electron microscope (SEM) and atomic force microscope (AFM).



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Zeolite MFI Nanosheet with a Single-Pore Thickness Synthesized by a Zeolite-Structure-Directing Surfactant**

정진환 조창범 조강희 유룡

KAIST 화학과

Zeolite MFI nanosheets have been hydrothermally synthesized using a surfactant with the formula of  $[\text{C}_{18}\text{H}_{37}\text{-N}^+(\text{CH}_3)_2\text{-C}_6\text{H}_{12}\text{-N}^+(\text{CH}_3)_2\text{-C}_6\text{H}_{12}\text{-N}^+(\text{CH}_3)_2\text{-C}_{18}\text{H}_{37}][\text{Br}^-]_3$  as the zeolite structure-directing agent. These nanosheets correspond to an extremely thin slice of MFI zeolite crystal of 1.5-nm thickness, which is smaller than a b-lattice parameter (1.97 nm) of single unit-cell dimension. Despite the small thickness, the nanosheet still exhibits high steam-thermal stability as well as acid strength comparable to bulk MFI zeolite. The zeolite nanosheet could be used as a heterogeneous catalyst for acid-catalytic reaction involving bulky molecules that could not enter the micropore of conventional zeolite.

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발표코드: MAT.P-1155

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and properties of Nobel D- $\pi$ -A Sensitizers for Dye Sensitized Solar Cells

김종형 계광열<sup>1</sup> 정영삼<sup>2</sup>

(주)솔라시스 <sup>1</sup>아주대 화학과 <sup>2</sup>고려대 화학과

Phenothiazine containing dyes for the DSSCs(Dye Sensitized Solar Cells) have been synthesized. Photocurrent and voltage were measured from a solar simulator (class AAA). The J-V curve and overall efficiency for the DSSCs based on the dyes were presented and compared with N719 dye.

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발표코드: MAT.P-1156

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Generation of Three-Level Pore Hierarchy in Nanoscale by Zeolite-Structure-Directing Surfactant

조강희 나경수 김재현 유통

KAIST 화학과

Zeolite was hydrothermally synthesized using a surfactant equipped with a micropore-generating functional group. Two-level pore hierarchy of mesopore and micropore was generated in the zeolite structure, whereas the surfactant molecules were assembled into micelles in the mesoscale while each functional group acted as a template for a micropore. An additional macroporosity could occasionally appear to exhibit a totally three-level pore hierarchy. The hierarchically porous morphogenesis has been investigated with X-ray diffraction and electron microscopy, using diatomaceous earth as a silica source. This investigation has unveiled that the two-level pore hierarchy can be developed in case where the crystalline zeolite phase is generated after full migration of the silica source through the solution phase as dissolved. The three-level pore hierarchy is developed in the case of pseudomorphic transformation, in which the solid-state silica source is transformed into a crystalline zeolite before sufficient migration into

the solution phase. Furthermore, it has been demonstrated that the hierarchical morphogenesis can be controlled by synthesis conditions and surfactant structures.



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발표코드: MAT.P-1157

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Properties of Coumarin Containing Dyes for Dye Sensitized Solar Cells

유용재 계광열<sup>1</sup> 정영삼<sup>2</sup>

솔라시스 연구소 <sup>1</sup>아주대 화학과 <sup>2</sup>고려대 화학과

Coumarin containing dyes for the DSSCs(Dye Sensitized Solar Cells) have been synthesized. Photocurrent and voltage were measured from a solar simulator (class AAA). The J-V curve and overall efficiency for the DSSCs based on the dyes were presented and compared with N719 dye.

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발표코드: MAT.P-1158

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Properties of Phenothiazine containing Dyes for Dye Sensitized Solar Cells

정영삼 계광열<sup>1</sup> 유용재<sup>2</sup>

(주)솔라시스 <sup>1</sup>아주대 화학과 <sup>2</sup>솔라시스 연구소

Phenothiazine containing dyes for the DSSCs(Dye Sensitized Solar Cells) have been synthesized. Photocurrent and voltage were measured from a solar simulator (class AAA). The J-V curve and overall efficiency for the DSSCs based on the dyes were presented and compared with N719 dye.

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발표코드: MAT.P-1159

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Coralyme-Induced Rapid Hybridization of DNA-Functionalized Gold Nanoparticle Probes for Colorimetric Detection**

오주환

고려대 신소재공학부

We have developed a new colorimetric assay to detect coralyme based upon the hybridization kinetics of DNA-functionalized gold nanoparticles (DNA-AuNPs). In presence of coralyme, the DNA-AuNP hybridization kinetics was dramatically enhanced by non Watson-Crick base pair interactions of adenine-adenine (A-A), where coralyme strongly intercalates the poly-A/poly-A duplex via A-coralyme-A chemistry. By controlling the DNA loading on the nanoparticle probes, the sensitivity and selectivity of assay have been significantly improved.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Three-Dimensional Structure of Helical $\text{Ge}_3\text{Sb}_2\text{Te}_6$ and $\text{Ge}_3\text{Bi}_2\text{Te}_6$ Nanowires Using Electron Tomography

김한성 백승혁 정찬수 박정희 안재평<sup>1</sup>

고려대 소재화학과 <sup>1</sup>KIST 산업화지원센터

Recently, interest in 3-dimensional (3D) nanostructures has been steadily increasing, owing to their attractive morphology and mechanical/electrical/optical properties. All of the helical and zigzagged structures in these previous studies were analyzed by examining their 2-dimensional (2D) projections using TEM, which provides a first insight into their size and morphology. There are, however, potentially some cases where important 3D structural information is missed or erroneous information may be obtained when using simply this technique. Electron tomography, which is a method of reconstructing the 3D morphologies from a series of 2D transmission electron microscopy (TEM) images or projections, has been successfully applied to analyze the morphology of various 1D nanostructures. We were synthesized by the thermal evaporation for the  $\text{R}_2\text{Te}_3(\text{GeTe})_n$  ( $\text{R} = \text{Sb, Bi}$ ) alloy nanowires. Among the nanowires, the  $\text{Ge}_3\text{Sb}_2\text{Te}_6$  and  $\text{Ge}_3\text{Bi}_2\text{Te}_6$  nanowires consist of a unique helical morphology and superlattice structures. We employed both electron tomography and high-resolution TEM images to study the 3D structure of



helical  $\text{Ge}_3\text{Sb}_2\text{Te}_6$  and  $\text{Ge}_3\text{Bi}_2\text{Te}_6$  nanowires. Their 3D reconstruction images, acquired from a series of 2D projections, were obtained by high-angle annular dark field (HAADF) scanning TEM (STEM).



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발표코드: MAT.P-1161

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Microporous Zeolite Materials from Recycling of Mesoporous Silicate Waste

김윤경 김정호<sup>1</sup> 유종성<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

The amount of chemical waste have been increasing, especially chemical wastes. The waste products are often hazardous and need to be treated before disposal. To reduce the waste treatment expenses, certain waste products can be recycled or reused. Recently, we have reported the fabrication of mesoporous materials by recycling of mesoporous silicate waste. It was confirmed by analysis of <sup>29</sup>Si-NMR and ICP-MS that sodium silicate and silicate waste that used to recycling works were absolutely similar. In this study, we have synthesized LTA and MFI type of zeolite using the method which was reported previously by our group using the silicate wastes. The present study aims to achieve the goals as: (i) selective etching of silica template from mesoporous carbon/silica composite by NaOH solution, (ii) recycling silicate wastes to obtain zeolites (LTA, MFI), and (iii) characterization of synthetically recycled zeolites though methods such as X-Ray Diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy, <sup>27</sup>Al and <sup>29</sup>Si Nuclear Magnetic Resonance (NMR) spectroscopy, Scanning Electron Microscopy (SEM), BET

surface area determination and Transmission Electron Microscopy (TEM). This straight forward green chemistry route is not only recycling the chemicals, but also decreasing the waste for better improvement in the environment.



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발표코드: MAT.P-1162

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhanced Photovoltaic Properties of a Cobalt Bipyridyl Redox Electrolyte in Dye-sensitized Solar Cells

이충혁 강바울 이완인

인하대 화학과

Dye-sensitized solar cells (DSCs) with cobalt-based mediators with efficiencies surpassing the record for DSCs with iodide-free electrolytes were developed by selection a suitable combination of a cobalt bipyridine complex and an organic sensitizer. Mass transport of  $[\text{Co}(\text{bpy})_3]^{2/3}$  redox electrolyte is found to strongly depend on porosity and pore size of mesoporous  $\text{TiO}_2$  film. So, we have synthesized the different size of  $\text{TiO}_2$  nanoparticle to control the porosity. Photovoltaic performance is improved by increasing the  $\text{TiO}_2$  nanoparticle size from 20nm to 70nm.

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장소: 일산KINTEX

발표코드: MAT.P-1163

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Mesoporous Iron Oxide Heterjunction Film Based on a Solution-Based Nanoparticle Approach for Enhanced Photoelectrochemical Water

Splitting

Jingling Liu 권영욱<sup>1</sup>

성균관대 나노과학기술학부 <sup>1</sup>성균관대 화학과

Mesoporous iron oxide( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) thin film has been produced using a commercial triblock copolymer F127 as the structure-directing agent and iron(III) nitrate as the molecular precursor based on a simple solution-based nanoparticle approach. Mesoporous  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> thin film was derived by the nanoparticles after removing the organic template. Scanning electron micrographs (SEM) and transmission electron microscope (TEM) observation revealed that the as-prepared mesoporous  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> thin film has mesopores in a uniform size range of 10 nm. The characterization of this film was also examined by Small and Wide angle XRD, UV-vis and Raman spectroscopy. To the best of our knowledge, for overcoming the limitation of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> by poor light absorption, a small hole diffusion length and poor conductivity for solar hydrogen production, the ultrathin heterjunction layer of SnO<sub>2</sub>/WO<sub>3</sub> was

induced, and the photoelectrochemical property of the mesoporous  $\alpha$  -  $\text{Fe}_2\text{O}_3$  film was dramatically enhanced because of the specific band structure of  $\text{SnO}_2/\text{WO}_3/\text{Fe}_2\text{O}_3$ .



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Comparative Study on Photocatalytic Activity of Sol-gel Derived $W_{18}O_{49}/TiO_2$ and $WO_3/TiO_2$ Heterocomposite Under Visible Light Irradiation

Rawal Sher Bahadur SANDIPAN BERA 김학진 이완인

인하대 화학과

Blue colored transition metal oxide  $W_{18}O_{49}$  nanorod structure was synthesized by one-pot thermally induced crystal growth process. The size of the nanorods was found to be ~100 nm.  $WO_3$  with similar morphology was obtained by heating  $W_{18}O_{49}$  at 400°C identified from x-ray diffraction pattern. Then heterojunction structure,  $W_{18}O_{49}/TiO_2$  and  $WO_3/TiO_2$  were formed by covering the surface of  $W_{18}O_{49}$  and  $WO_3$  with polycrystalline  $TiO_2$  by sol-gel process. It was found that  $W_{18}O_{49}$  shows a profound absorption over the visible range, and its valence band (VB) is located lower than that of  $TiO_2$ . Under visible light irradiation ( $\lambda \geq 420$  nm),  $W_{18}O_{49}/TiO_2$  showed a notable photocatalytic activity in removal of gaseous 2-propanol (2P) and evolution of  $CO_2$ . Therefore the higher photocatalytic efficiency of the  $W_{18}O_{49}/TiO_2$  photocatalyst compared to  $WO_3/TiO_2$  under visible light irradiation was deduced to be caused by the inter-semiconductor electron-hole transfer between the VB of  $W_{18}O_{49}$  and  $TiO_2$ .

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발표코드: MAT.P-1165

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Influence of fluorine treatment on electrochemical performance of PAN-based carbon nanofibers for supercapacitor**

**허지훈 서민강<sup>1</sup> 박수진<sup>2</sup>**

전북대 유기소재파이버 공학과 <sup>1</sup>전주기계탄소기술원 전략기획실 <sup>2</sup>인하대 화학과

In this work, we investigated the electrochemical performance of porous PAN-based carbon nanofibers (P-CNFs) by fluorine treatment. The effect of fluorine treatment time on electrochemical performance of the P-CNFs was investigated. The textural properties and morphologies of P-CNFs were analyzed by reference to N<sub>2</sub>/77 K adsorption isotherms, and field emission scanning electron microscope (FE-SEM), respectively. The electrochemical performance of P-CNFs was confirmed by cyclic voltammograms (CV). As results, the electrochemical performance of fluorine treated P-CNFs was higher than that of untreated P-CNFs. This was suggested that the fluorine functional groups on the P-CNFs led to the combination effect of both electric double-layer capacitor and pseudocapacitance in the present system. Key word: PAN nanofibers, fluorine treatment, supercapacitor, pseudocapacitor, electrochemical performance



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발표코드: MAT.P-1166

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of superhydrophobic surface on nanoporous polycarbonate

고승철 안용현

단국대 화학과

Industrial or academic research on superhydrophobic in the lot is being progressed. Superhydrophobic property is controlled by both the geometrical structure of a surface and low surface energy material coating. Using both, the first polycarbonate plate dipping in the Methylene chloride. The water contact angle increase from 80 on the normal surface to 93 on the nanoporous structure. Next, The coating of surfaces with silanes is well known. So evaporated trichloromethylsilane (TCMS) using etched PC-plate on the coating. The water contact angle increase from 93 on the normal surface to 140 on the deposited surface. Surface morphology changes could be confirmed by FE-SEM.

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발표코드: MAT.P-1167

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Multi functional thin layer coating for flexible display prepared by sol-gel method

서용성 홍유진 김대진 유국현

동국대 화학과

High transparency multi functional coating-Anti reflection and anti pollution organic-inorganic hybrid thin layer was prepared by sol-gel method. The organic-inorganic hybrid layer was synthesized with TEOS (Tetraethoxysilane), Organosilane, Titanium isopropoxide and Fluoroalkylsilane. It was prepared to have high adhesion ability to various substrates. It was coated on the surface of glass and polymer plate and measured anti reflection and anti pollution ability. Anti reflection property was measured through the light transmittance and refraction index. Anti pollution properties-anti finger printing and easy clean abilities were measured contact angle and slide angle. Contact angle and slide angle was measured for water and n-hexadecane that was shown prohibits repellent ability to the moisture and oil. As a result, this hybrid layer has an ability to prohibit reflection on surface that means it has possibility to improve visibility of display

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Superhydrophobic surface coatings using silica  
particles/poly(trimethoxysilyl)propyl methacrylate nanocomposites:  
Enhancing mechanical durability**

**윤종해 황은지 신재호**

광운대 화학과

Superhydrophobic surface coatings with high static water contact angle ( $>150^\circ$ ) have been receiving tremendous attention in recent years. The applications of superhydrophobic coatings are diverse due to their unique water-repellency, self-cleaning ability, and anti-biofouling property. Various methods have been proposed to fabricate superhydrophobic surfaces mimicking the lotus surface structure, including lithographic patterning, plasma etching, electrochemical deposition, and chemical vapor deposition. However, these methods often require harsh synthetic conditions and complex fabrication techniques. Furthermore, the poor mechanical stability of superhydrophobic coatings formulated on the surface is generally another limitation in their widespread applications. Herein we demonstrate on a one-step facile spray-coating technique to fabricate a superhydrophobic surface modified with silica particle/poly(trimethoxysilyl)propyl methacrylate nanocomposites. The superhydrophobic surface

coatings prepared are characterized in term of the water contact angles and the surface roughness/morphology by using a scanning electron microscopy (SEM). Futhermore, abrasion resistance of the fabricated superhydrophobic coatings was evaluated by a home-made scratch tester, which was composed of a piece of sandpaper and weights of different masses.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Au Nanoparticles Decorated Polymer Nanocapsule

윤경원 백강균 이지영 김지홍 김기문

포항공과대 지능초분자연구단, WCU 첨단재료과학부, 화학과

Metal nanoparticles are important for a wide range of applications including catalysis, photonics, electronics, and biomedical sensing. Protecting agents such as surfactants, dendrimers and polymers are needed to stabilize the nanoparticles (NPs) from self aggregation. However, these protecting agents have strong affinity towards the surface of NPs and restrict the chemical activities of NPs. We utilized a novel polymer nanocapsule, which not only stabilized the NPs (Au-NPs), but also provided a uniform distribution of NPs over the surface of the nanocapsule. Polymer nanocapsules are synthesized via polymerization of (allyloxy)<sub>12</sub>cucurbit[6]uril which has a rigid core and multiple polymerizable allyl groups at the periphery. The structure of Au-NPs on polymer nanocapsule has been characterized by transmission electron microscopy. Combination of nanocapsule with NPs may find useful applications in the area of catalysis and hyperthermia therapy. Details of the synthesis and characterization of the NPs on nanocapsule will be presented.

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발표분야: 재료화학

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## Highly Efficient Flexible Dye-Sensitized Solar Cell Using Compression Method

유소라 유선미 김은이 이완인

인하대 화학과

Recently, dye-sensitized solar cell (DSC) has attracted extensive attention due to low production cost of electricity and relatively high energy conversion efficiency. Development of flexible device is crucial to diversify its commercial applications, in accordance with rapidly growing technologies in plastic electronics. Herein, we introduced a compression method in fabricating highly efficient DSC at low temperature. Flexible DSCs prepared with ITO substrate and Degussa P-25  $\text{TiO}_2$  powder, N719 dye or TA-St-CA organic dye and an electrolyte containing LiI and  $\text{I}_2$ . Electrochemical impedance spectroscopy (EIS) analysis indicated conversion efficiency enhancement and reduction of resistance at  $\text{TiO}_2$  films after compression method. As a result, it can provide photoelectric energy conversion efficiency up to 6.67% with N719 dye and 4.12% with TA-St-CA dye.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrospun TiO<sub>2</sub> Nanofibers for Efficient Electron Transport Layers of Inverted Polymer Solar Cells

서요한 김원배

광주과학기술원 신소재공학부

Polymer solar cells have some prominent properties because of this device system have some advantages such as simple and cheap processes to make photovoltaic devices from spin-casting and ink-jet method, but polymer-based photovoltaic devices still have lower power conversion efficiency than another photovoltaic devices in spite of these advantages of polymer-based photovoltaic device. One of the major factors of increasing the performance of polymer solar cells is the development of efficient electron transport layer to efficiently deliver electrons separated from excitons toward cathode. In this work, we applied electrospun TiO<sub>2</sub> nanofibers on TiO<sub>2</sub> buffer layers as an electron transport layer of inverted polymer solar cells. Although TiO<sub>2</sub> has good electron acceptability and large band gap, the electron transport layer with thin film structure has confined contact area with polymer layer and limited electron pathways. However, one-dimensional TiO<sub>2</sub> nanofibers can provide continuous electron pathways and large interfacial area with P3HT:PCBM blend layer. After characterizing the structural and electronic

properties of electrospun TiO<sub>2</sub> nanofibers, we fabricated the inverted polymer solar cells using TiO<sub>2</sub> nanofibers. Our devices using TiO<sub>2</sub> nanofibers have remarkably increased short circuit current, fill factor and power conversion efficiency, comparing to the device without TiO<sub>2</sub> nanofibers. These results could explain that electrospun TiO<sub>2</sub> nanofibers have suitable morphological and electronic properties for electron transport layer of inverted polymer solar cells.

**Acknowledgment** This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 20110016600 (Mid-career Researcher Program)), the Global Frontier R&D Program on Center for Multiscale Energy System, and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. R15-2008-006-03002-0).





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발표코드: MAT.P-1172

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of Two-Dimensional GaS Nanobelts for rechargeable lithium ion batteries

정찬수 조용재 임형순<sup>1</sup> 박정희

고려대 소재화학과 <sup>1</sup>고려대 미세소자공학협동/마이크로소자공학

Gallium sulfide is one of the most important materials, among the III-VI group of semiconductor materials, with two different stoichiometries, i.e., GaS and Ga<sub>2</sub>S<sub>3</sub>. Hexagonal GaS crystallizes in layered structure with double layer of nonmetal atoms, consisting of S-Ga-Ga-S sheets, stacking along c axis, having intralayer Van der Waals bonding and interlayer covalent bonding and is structurally similar to graphite. Recently, 2D nanomaterials, including nanoflakes, nanoplates and nanosheets, used as anode materials have attracted considerable attention owing to their rapid ionic and electronic diffusion during the cyclic reaction, which lead to higher discharge/charge capacities and cyclic stability. Interestingly, the pores, either existing in the attached structure or as intrinsic defects of nanomaterials can minimize the volume change during the cyclings and thus enhance the cyclic performances. Herein, the first report concerning the cyclic performance of GaS nanosheets electrodes is presented.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Neutron diffraction analysis and ionic conductivity of $\text{Na}_3\text{Ga}(\text{PO}_3)_3\text{N}$

김민웅 김재겸<sup>1</sup> 정재훈 김승주

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Sodium-gallium-nitridophosphate,  $\text{Na}_3\text{Ga}(\text{PO}_3)_3\text{N}$  was prepared by solid state reaction of  $\text{NaPO}_3$  and  $\text{Ga}_2\text{O}_3$  under ammonia gas flow. The crystal structure of  $\text{Na}_3\text{Ga}(\text{PO}_3)_3\text{N}$  has been determined from neutron diffraction data(HRPD). The unit cell is cubic system with space group  $P2_13$  ( $Z = 4$ ) and cell parameters, 9.3643(7) Å. In the structure of  $\text{Na}_3\text{Ga}(\text{PO}_3)_3\text{N}$ , phosphorous atom is coordinated to three oxygen atoms and one nitrogen atom to form a  $\text{PO}_3\text{N}$  tetrahedron. The  $(\text{PO}_3)_3\text{N}$  entity is formed by three  $\text{PO}_3\text{N}$  tetrahedra sharing the corner occupied by the nitrogen atom. A gallium atom is coordinated to six oxygen atoms to form a octahedron and the six oxygen atoms are connected to the three  $(\text{PO}_3)_3\text{N}$ . The thermal behavior and the ionic conductivity of  $\text{Na}_3\text{Ga}(\text{PO}_3)_3\text{N}$  can be compared to that of  $\text{Na}_3\text{Al}(\text{PO}_3)_3\text{N}$ .

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발표코드: MAT.P-1174

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Structure of a New Mixed-metallic Phosphate, $\text{Na}_x(\text{V}_{2-y}/\text{Nb}_y)(\text{PO}_4)_3$ ( $x = 0.78$ , $y = 0.95$ )

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The structures and properties of Na phosphates have been intensively investigated with a view to understanding their structural variations that seem to be contingent upon the type of the transition metals. As a result of our efforts to design new phosphates from the known phase, a new mixed-metallic phosphate,  $\text{Na}_{0.78}(\text{V}_{1.05}/\text{Nb}_{0.95})(\text{PO}_4)_3$ , has been prepared as single crystals and its crystal structure has been characterized through X-ray diffraction. In this compound the metal sites of trans-corner-sharing  $(\text{V}/\text{Nb})\text{O}_6$  octahedra are occupied by statistically disordered V and Nb atoms which are linked together by tetrahedral  $\text{PO}_4$  groups and the polyhedra share O atoms to form a three-dimensional framework with large empty channels. The Na ions stay in this space and its stoichiometry seems to be adjusted by the sum of the oxidation states of each metal. Therefore, the classical charge balance of the title compound can be represented as  $[\text{Na}^+]_x[\text{V}^{3+}]_{2-y}[\text{Nb}^{5+}]_y[\text{P}^{5+}]_3[\text{O}^{2-}]_{12}$ .

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## Single-cation type ionic liquids and double-cation type ionic liquids of electrical characterization

이원길 조원제 유국현

동국대 화학과

Ionic liquids (ILs) were well known for green solvent and efficient electrolyte for lithium ion battery. The non volatile and high electro conductivity properties were made high value for replacement materials of re-chargeable battery's electrolyte. But, the high viscosity at room temperature and low electro conductivity were high barrier of need to improve. On this study, we will show the single-cation ILs and the double-cation ILs system in one molecule for improving viscosity and electro conductivity. Double-cation ILs were synthesized from di-terminals aliphatic halide and several quaternary amines. Two sort of different type of double-cation ILs were synthesized which substituted the same quaternary amines (symmetric type ILs) or different quaternary amines (asymmetric type ILs) in one molecule terminals. We used microreactor for synthesis of double-cation ILs. Microreactor is brand-new glassware for micro fluidics chemistry. Microreactor has several of advantages accuracy temperature control, high safety, high

yield, continuous process and easy to scale up. In the conclusion, the synthesized ILs of different functional group terminals has higher electro conductivity compare to same functional group terminal ILs.



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## Synthesis and Characterizations of a New Mixed-Metallic Phosphate, $\text{Na}_{3.7}\text{V}_{1.8}\text{Ta}_{6.2}\text{P}_6\text{O}_{35}$

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The new single-crystalline mixed metallic phosphate,  $\text{Na}_{16x}\text{V}_{8x}\text{Ta}_{8-8x}\text{P}_6\text{O}_{35}$  ( $x=0.23$ ), has been prepared with the use of the metal halide, NaCl as a reactive flux. This compound has been structurally characterized by single-crystal X-ray diffraction techniques. The title compound crystallize in the space group *Pbam* of the orthorhombic system with unit cell parameters  $a = 8.4686(2) \text{ \AA}$ ,  $b = 15.3354(5) \text{ \AA}$ ,  $c = 10.3962(3) \text{ \AA}$ ,  $V = 1350.15(7) \text{ \AA}^3$  and  $Z = 2$ . The framework consists of  $[\text{Ta}_3\text{P}_2\text{O}_{17}]$  layers and they are linked via corner-sharing  $\text{TaO}_6$  octahedra to form the  $[\text{Ta}_6\text{P}_4\text{O}_{31}]$  bilayer. These bilayers are linked along the crystallographic *c* axis through  $[\text{Ta}_2\text{P}_2\text{O}_4]$  units, which is built up from the two edge-sharing  $\text{TaO}_6$  octahedra connected to the two  $\text{PO}_4$  tetrahedra. There are three and two crystallographically independent metal and Li sites, respectively exist in the title compound. Metal 1 and 3 sites are fully occupied by  $\text{Ta}^{5+}$  ions, whereas the metal 2 site is occupied by statistically disordered  $\text{V}^{3+}/\text{Ta}^{5+}$  ions. The Li1 site is fully

occupied but the Li2 site is partially occupied for charge neutrality. The classical charge valence of the title compound can be represented by  $[\text{Na}^+]_{3.7}[\text{V}^{3+}]_{1.8}[\text{Ta}^{5+}]_{6.2}[\text{P}^{5+}]_6[\text{O}^{2-}]_{35}$ .



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## Molecular Layer Deposition of Titanium Aryloxide

한규석 성명모

한양대 화학과

We fabricated organic-inorganic hybrid thin films using layer-by-layer vapor phase reaction which are called molecular layer deposition (MLD). Titanium chloride and hydroquinone were used as precursors to deposit hybrid 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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## Oxidation Resistance of Fe and Cu Foils Coated with Reduced Graphene Oxide Sheets

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The protection of metals such as Fe and Cu, which are widely used in industry, is of great importance because of necessity to preserve their surface properties. Traditional protection methods may lead to negative influences on physical property and surface deformation. In this study, we demonstrate oxidation resistance of Fe and Cu foils by coating them with reduced graphene oxide (rGO) sheets. The rGO-coated Fe and Cu foils were prepared by transferring rGO multilayers on SiO<sub>2</sub> substrate to Fe and Cu foils. The oxidation resistance of the rGO-coated metal substrates was investigated by Raman spectroscopy and scanning electron microscopy after heat treatment at 200 °C in air for 2 h. The bare metal surfaces were severely oxidized, whereas the rGO-coated metal surfaces were protected from oxidation. The results indicate that the rGO thin film plays a role as an oxidation-resistive barrier. The simple solution process using rGO is the advantage of the present study

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## Solid-State Synthesis of Silver Nanoparticles in the Presence of Poly(3-hexylthiophene)

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Metal nanoparticles have been recently used as additives in polymer solar cells due to their plasmonic effect for improving the efficiency. Poly(3-hexylthiophene) is one of the conjugated polymers used as an electron donor material in the active layers of polymer solar cells. Therefore, silver nanoparticles were synthesized in the presence of poly(3-hexylthiophene) using a solid-state synthesis method for direct application in polymer solar cells. The size of the nanoparticles thus produced was found to be in the range of 3 - 8 nm. The silver nanoparticles were characterized by UV-Vis spectroscopy, X-ray diffraction, and transmission electron microscopy. In addition, the morphology of the films was analyzed by atomic force microscopy and scanning electron microscopy.

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## Synthesis and Characterization of Novel p-type Oligomer TFT Containing Anthracene

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Solution processed Organic thin film transistors (OTFTs) based on polymeric semiconductors as an active layer have attracted wide attention due to their potential use in low-cost, lightweight and flexible electronic devices. Due to the high stability of conducting polythiophenes, extensive efforts have targeted new thiophene architectures that allow for enhanced materials properties, easier processing, and higher stability. The anthracene derivatives for organic thin film transistors were synthesized by Sonogashira coupling reaction. The oligomers were characterized by <sup>1</sup>H NMR and thermal properties were investigated by differential scanning calorimetry, thermogravimetric analysis. These oligomers showed high thermal stability. And their spectroscopic and electrochemical properties investigated by cyclic voltammetry, UV-vis. These oligomers were fabricated into the device by solution process. The OTFT devices of the oligomers measured charge carrier mobilities.. These oligomers showed high thermal

stability with 5% weight loss at 327 °C and 426 °C. The anthracene derivatives for OTFT will be fabricated and further discussed.



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## **A novel p-Type anthradithiophenes based semiconducting oligomers for Organic Thin-Film Transistors**

**홍정아 고혜진<sup>1</sup> 한희원 하종진 김윤희<sup>2</sup> 권순기<sup>3</sup>**

경상대 고분자공학과 <sup>1</sup>경상대 고분자공학전공 <sup>2</sup>경상대 화학과 <sup>3</sup>경상대 나노신소재공학부

Organic thin film transistors (OTFTs) have been the focus of much research activity as a promising alternatives to conventional Si-based FETs for low-cost, large-area, and simple device structure. Therefore, the devices need to follow a solution-processing technologies, such as spin-coating and inkjet printing. So, we designed and synthesized a novel p-type naphthalene(TESADT-Na) and benzothiophene(TESADT-BT) substituted anthradithiophenes based oligomers by Suzuki coupling reaction. The newly designed oligomers are expected to have good morphology and charge carrier mobility due to the anthradithiophene derivatives with a planar  $\pi$ - $\pi$  system. Side group naphthalene increases the  $\pi$ - $\pi$  stacking characteristics and can increase the solubility in the common organic solvents such as chloroform, toluene and chlorobenzene. TESADT-Na oligomer's mobility is  $0.0004\text{cm}^2/\text{Vs}$  and TESADT-BT oligomer's mobility is  $0.0002\text{cm}^2/\text{Vs}$ .

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## **Fabrication and Photocatalytic Activities of TiO<sub>2</sub> Nanostructures Prepared from Metal-Organic Framework Precursors, TiBDC and TiBDC-NH<sub>2</sub>**

임지혁 강은영<sup>1</sup> 김자현<sup>1</sup> 박종래

서울대 재료공학부 <sup>1</sup>충실대 화학과

Nanostructured TiO<sub>2</sub> materials were fabricated from thermolysis of metal-organic framework (MOF) precursors, TiBDC and TiBDC-NH<sub>2</sub> which were composed of Ti ions and benzene-1,4-dicarboxylate (BDC) or 2-amino-benzene-1,4-dicarboxylate (BDC-NH<sub>2</sub>) linkers, respectively. Using several characterization tools, we confirmed that the aggregates of anatase TiO<sub>2</sub> nanoparticles were formed during thermal decomposition of two Ti-containing MOFs. To investigate photocatalytic properties TiO<sub>2</sub> nanostructures, photodecomposition behavior of organic pollutants under UV or VIS irradiation was monitored.

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## Effects of Strain-induced Crystallization of Electrospun Conjugated Polymer Nanoweb in Organic Photovoltaic Cells

김성균 김태훈 박종래

서울대 재료공학부

Crystallinity of conjugated polymer is closely correlated with performance of organic photovoltaic (OPV) cells. Improved crystallinity leads to an increase in hole mobility and optical absorption of the low-photon-energy region due to the increased conjugation length and  $\pi$ - $\pi$  stacking of conjugated polymer. The higher hole mobility induces successful charge transportation and the higher optical absorption generates more charge carriers. As a result, these cause better photovoltaic performance. Until now, thermal annealing or solvent annealing was used for increasing the crystallinity of conjugated polymer in bulk-heterojunction (BHJ) structured OPV cells. However, these methods are limited to a few crystalline conjugated polymers such as poly(3-hexylthiophene) (P3HT). Also, there is room for improving the crystallinity of P3HT in BHJ structured OPV cells. Thus increasing the crystallinity of both amorphous conjugated polymers and P3HT is an important issue for achieving higher power conversion efficiency. Electrospinning is a facile method to fabricate most of polymers to nanofibers and nanowebs.

Crystallinity of polymers is increased during the electrospinning process due to the elongation by electric field, and it can be enhanced by subsequent strain-induced crystallization. Thus the combination of electrospinning and strain-induced crystallization can be an easy and effective method to improve the crystallinity of amorphous conjugated polymers for better photovoltaic performance. In this work, crystallinity of electrospun conjugated polymer nanowebs was controlled by strain-induced crystallization. OPV devices composed of the electrospun fibers were prepared to study correlation between the crystallinity and power conversion efficiency of the OPV device.





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## Various Edge-functionalized graphite via simple and eco-friendly methods

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Graphene, a single layer of carbon atom bonded together in a hexagonal lattice, has attracted tremendous attention because of its remarkable electronic, optical and physical properties. Thus, graphene is considered having potential applications such as display, transparent electrode, transistor, etc. Various methods such as drawing method, epitaxial growth method, reduced graphite oxide (rGO), chemical vapor deposition (CVD) are reported to prepare graphene. We reported a new approach that graphite was exfoliated by grafting various organic molecular wedges to the defect sites located mainly on the edges of graphite via Friedel-Crafts acylation reaction in poly(phosphoric acid) /phosphorous pentoxide medium. This is the first attempt to large-scale “direct” chemical exfoliation of graphite without harsh conditions that are known to damage carbon framework. We also developed a simple and eco-friendly (CO<sub>2</sub>-capturing) ball milling process to efficiently produce edge-carboxylated graphite (ECG) in solid state without involving hazardous chemicals. The resultant ECG was demonstrated to be highly dispersible in

various polar solvents suitable for solution casting. The resultant exhibited many superior structure-property characteristics with respect to its GO and H-GO counterparts. In result, the organic molecular wedges and ball milling technique developed in this study could be regarded as a general approach toward low-cost, high-yield production of edge-functionalized graphene (EFG) with various functional groups of practical significance for mass production of multifunctional materials and devices based on graphene.



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## Easy and smart functionalization of lithium niobate crystal toward the application of SAW device

김효설 이승윤 성소희 김재호

아주대 분자과학기술학과

Although, lithium niobate ( $\text{LiNbO}_3$ ) is one of good candidate for the substrate of SAW device along with Lithium tantalite ( $\text{LiTaO}_3$ ), it is very difficult to modify its surface for the functionalization since the stable binding energy of crystal surface. In this study, the functionalization of lithium niobate surface has been successfully obtained by the grafting of 3-aminopropyltriethoxysilane (APTES) after 5 min UV/O<sub>3</sub> treatment. This functionalization has been proved by X-ray photoelectron spectroscopy and contact angle measurement. In addition, through the immobilization of FITC onto the lithium niobate surface, we could confirm the successful induction of surface amine group. The data show that the stability of the self-assembled monolayer (SAM) film on the APTES-modified lithium niobate surface is largely due to the formation of a siloxy-niobate ( $?\text{Si?O?Nb?}$ ) bond via a condensation reaction between ethoxysilane ( $-\text{Si-O-C-}$ ) and niobate hydroxide ( $?\text{NbOH}$ ). The extremely hydrophobic and stable SAM on lithium niobate could have useful applications in surface acoustic waves (SAW) device.

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## Formation of graphitic carbon nitride in layered aluminosilicates

김가인 양재훈 최진호

이화여대 화학·나노과학과

Graphitic carbon nitride was synthesized in layered aluminosilicates via solid state reaction. At first, metal-urea complexes such as magnesium chloride-urea and iron(III) nitrate-urea, eutatic solution, were intercalated into layered aluminosilicates via solid state reaction at 105 °C for 3 hours. According to X-ray diffraction analysis, the basal spacing of metal-urea / layered aluminosilicates was expanded to 1.76 nm compared to one of Na<sup>+</sup> intercalated layered aluminosilicates, 0.96 nm, indicating that metal urea complex was successfully intercalated into layered aluminosilicates. By calcining the prepared metal-urea/layered aluminosilicates nanohybrid at 500 °C for 3 hours, urea in the interlayer of layered aluminosilicates was polymerized to form graphitic carbon nitride. UV-visible spectrum shows that the calcined sample has an absorption edge at around 450 nm, thus making the nanohybrid pale-yellow, which is similar to one of bulk graphitic carbon nitride.

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## Aminoacid intercalated layered double hydroxides for removing CO<sub>2</sub>

LI QIULI 양재훈 최진호

이화여대 화학·나노과학과

Layered double hydroxide (LDH) has attracted great attention due to the ability of incorporating negatively charged (bio-)organic molecules and inorganic clusters into the interlayer spaces. In this study, we have directly incorporated aminoacid molecules into layered double hydroxides such as Zn-Al LDH, Mg-Al LDH, and Ca-Al LDH via traditional co-precipitation method. Since the amine group of intercalated aminoacid can capture CO<sub>2</sub> by forming carbamic acid, aminoacids with different number of amino-group such as valine, phenylalanine, lysine, and arginine, were incorporated into the layered double hydroxides in order to compare the CO<sub>2</sub> removal activity depending on the number of amine group in aminoacid. The interlayer structures of aminoacid intercalated LDH are characterized with X-ray diffraction analysis. The activity of removing CO<sub>2</sub> was evaluated with volumetric CO<sub>2</sub> gas adsorption-desorption isotherm analysis at different temperatures. The CO<sub>2</sub>-removal property of aminoacid intercalated LDH nanohybrids will be discussed in terms of the number of amine group in the aminoacid and the kind of layered double hydroxides.

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## **In vivo chemotherapeutic application of anticancer drug encapsulated layered double hydroxides**

최고은 최진호

이화여대 화학.나노과학과

Drug delivery systems have been intensively studied in the last few decades because they enable drugs to be effectively delivered to target sites, and increase the therapeutic efficacy with minimum side effects through controlled release manner. In this study, an anticancer drug, methotrexate (MTX), has been successfully encapsulated into layered double hydroxides (LDHs) through co-precipitation route to produce MTX-LDH nanohybrids. According to the Powder X-ray diffraction (PXRD), spectroscopy analysis and thermogravimetric analysis, MTX molecules are stabilized in the interlayer space of LDHs by electrostatic interaction, maintain their functional groups and structural integrity. We also investigated the anti-tumor effect of MTX-LDH nanohybrid in orthotopic breast cancer model, and found that the drug efficacy of MTX-LDH was more significantly increased than that of MTX only.

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## A Computational Study on the Aluminum Oxide Formation at Al/La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> Interface for Resistance Random Access Memory Applications

이노도

광주과학기술원 신소재공학부

Resistance random access memory (ReRAM) has been intensively studied as a promising candidate for post-NAND flash memory device. In particular, a simple capacitorlike structure with a metal such as aluminum (Al) or titanium (Ti) and a mixed-valence manganite such as La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> ( $x \sim 0.3$ ; LSMO) widely investigated because of their relatively stable operation as well as better device performance. Previous studies on a metal/LSMO device showed that oxygen ions in LSMO move to interface and oxidize a reactive metal under an electric field, resulting in resistive switching. Although, the microscopic mechanisms of switching are not yet clear, defects and their migrations have been considered as a key factor for origin of the switching behavior. First-principles calculations have been performed to study the formation of interfacial aluminum oxides of Al/LSMO and to analyze the switching properties. We investigated the change in structure, energy, and diffusion properties of oxygen ions during the oxygen

ions migration at Al/LSMO interface. Especially, we focused on the stability of various types of interfacial aluminum oxides during the oxidation process. Based on our results, we suggest a model for resistive switching and their microscopic origin of resistive switching phenomena.





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## Bio-compatible Ca/Fe Layered Double Hydroxides

Ahmad Imran 양재훈 최진호

이화여대 화학·나노과학과

Inherent chemical inertness along with the safety and stability of hydrotalcite-type layered double hydroxides (LDHs) in the bio-system make them promising candidates for pharmaceutical applications such as the development of drug delivery system (DDS) with controlled release and sustained drug activity. The potential cellular toxicity of various LDHs has been reported in recent decades. However, cytotoxicity study of hydrocalumite-type calcium-based layered anionic clays has not been reported. In this study, we have synthesized nitrate and chloride forms of hydrocalumite-type Ca/Fe LDH by conventional co-precipitation route and evaluated the cytotoxicity of them. Thus prepared hydrocalumite-type Ca/Fe LDHs were physico-chemically characterized with X-ray diffraction (XRD) analysis, fourier transform infrared (FT-IR) spectroscopic analysis and thermo-gravimetric (TG/DT) analysis. XRD patterns of the prepared Ca/Fe LDHs showed the basal spacings of 0.87 and 0.78 nm for chloride and nitrate forms respectively. Morphological examinations by scanning electron microscopy (SEM) and tunneling electron microscopy (TEM) revealed typically plate-like particles with numerous small and

regularly well-defined hexagon shaped crystals. To evaluate the toxicological effect of these synthesized Ca/Fe LDHs in vitro, two different cell lines: human normal lung cells (L-132) and HeLa cells are used. Both the forms of Ca/Fe LDHs have no substantial cytotoxicity in terms of inflammation response, oxidative stress, and membrane damage.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## A Novel Thermo-Responsive Microspheres Design for Controlled Drug Release

박소현 장정호<sup>1</sup>

한양대 신소재공학과 <sup>1</sup>한국세라믹기술원 바이오IT융합센터

We report a new drug delivery system by bioabsorbable calcium phosphate (CaP) microspheres and thermo-responsive Poly(*N*-isopropylacrylamide). The drug delivery system was core-shell type PNIPAm coated CaP microspheres. CaP microspheres were prepared enzymatic decomposition of urea and accomplished by emulsification process (water-in-oil). The prepared CaP microspheres were coated with SiO<sub>2</sub> in order to stabilize weak structures and easy functionalization. PNIPAm grafted silica coated CaP microspheres (PNIPAm/SiCaP microspheres) were synthesized by using 3-MOP as a silane coupling agent to introduce double bond onto silica coated CaP microspheres and the radical copolymerization of MOP-SiCaP microspheres and NIPAm monomers. Indomethacin and Alendronate(ALD) were added to the PNIPAm gels and CaP microspheres for release, respectively. When the temperature rises (above the lower critical solution temperature-LCST), the polymer gel shrinks, squeezing the drug into the porous. ALD into the CaP microspheres was slowly diffuses than Indomethacin into the PNIPAm because coated

SiO<sub>2</sub> and PNIPAm. PNIPAm/SiCaP microspheres were characterized by Fourier transform infrared (FT-IR), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and thermal gravimetric analysis (TGA). Drug release of thermo-responsive microspheres was investigated by ultraviolet-visible (UV) spectrophotometry.



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발표코드: MAT.P-1192

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of novel acceptor-donor-acceptor type conjugated molecules for organic solar cells

전수지 박상혁

공주대 화학과

Organic photovoltaics possess many benefits such as light-weight, low cost, facile fabrication for large area, and mechanical flexibility. However, there are still problems 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 planned to improve PCE of organic solar cells. Commonly, 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.

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발표코드: MAT.P-1193

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development of donor-acceptor type small molecules for photovoltaic solar cells

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 thermogravimetric 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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발표코드: MAT.P-1194

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## ITO전극을 실버나노와이어 투명 전극으로 대체한 유연 유기태양

전지 개발

황인영 박상혁

공주대 화학과

미래 대체 에너지원 중 하나인 유기태양전지는 환경적인 면에서는 좋은 평가를 받고 있지만 전극으로 사용되는 indium의 높은 가격으로 인해 기업 혹은 개인이 활용하기 위한 비용적인 면에서 외면을 받고 있다. 따라서 본 연구는 ITO 전극 대신에 실버나노와이어를 전극으로 활용한 유연 유기태양전지 연구에 초점을 두고 있다. 유기태양전지가 상용화에 성공하기 위해서는, 현재 가장 많이 사용되고 있지만 상대적으로 고가인데다 유연하지 못한 ITO 전극을 대체하는 것이 중요하다. 본 연구에서는 실버나노와이어를 활용한 투명 전극을 개발하고 유연기판 위에서 bulk-heterojunction 유기태양전지의 부착력과 bending 각을 테스트한 결과 ITO 전극의 대체 가능성을 확인하였다.

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발표코드: MAT.P-1195

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Successive Seed-Mediated Growth of Ag Nanoplates on a Solid Substrate for Development of Surface-Enhanced Raman Scattering Platform

김영관 민달희<sup>1</sup>

KAIST 화학과 <sup>1</sup>서울대 화학과

The metal nanostructures have attracted much research attention because of their unique opto-electrical properties such as surface Plasmon resonance (SPR) and surface enhanced Raman scattering (SERS). Their unique properties were successfully controlled by tailoring their structures and harnessed to devise highly sensitive biosensor and imaging tool. Therefore, it is one of the important issues that the development of an appropriate synthetic strategy of metal nanostructures with structural diversity. In this study, we have developed a strategy for the direct growth of Ag nanoplates on a solid substrate by using seed-mediated growth approach. The synthesized Ag nanoplates were further grown by simply repeating seed-mediated growth under the same synthetic condition. Based on the present strategy, the size and surface density of grown Ag nanoplates were increased with repeated growth, thus, the SPR band of synthesized Ag nanoplate grown substrates was changed according to their structural development during



repeated successive growth cycles. The resulting Ag nanoplate grown substrates showed excellent performance as a SERS platform. We believe that the present strategy will be an important addition to the fabrication of SERS-based sensing platform with high sensitivity and reproducibility because of cost-effectiveness and simple fabrication processes with excellent performance.



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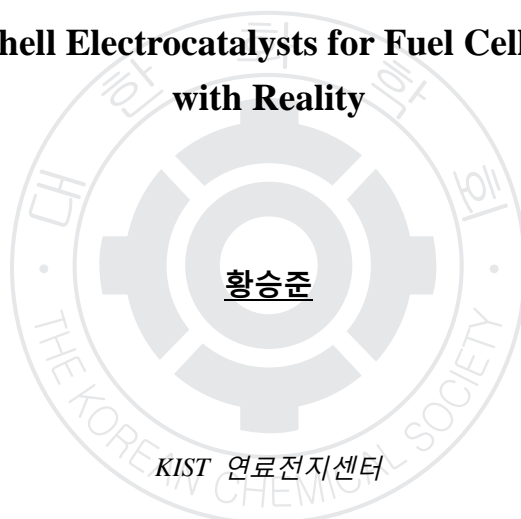
장소: 일산KINTEX

발표코드: MAT.P-1196

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Supported Core-Shell Electrocatalysts for Fuel Cells; Close Encounter with Reality



In this study, we screened the most probable core-shell combination by using computational method and then devised a facile synthetic route for synthesizing the proposed core-shell structure. Finally, we characterized the fuel cell performance and durability in a single cell level. Firstly, in order to find the most probable core-shell combinations for ORR reaction, we performed density functional theory (DFT) calculations. Two simple descriptors were used for screening. One is oxygen adsorption energy on Pt-shell as a measure of reactivity. The other is vacancy formation energy of Pt in Pt-shell as a criterion for stability. Especially, the searching process has been focused on finding a stable core-shell combinations since durability of nano-catalysts is crucial to commercialize for fuel cell applications. According to the simulation, PdCu@Pt core-shell was predicted to show superior reactivity and stability. This combination was expected to reduce the adsorption energy of oxygen on Pt shell, which is believed to show better reactivity. The charge accumulation between Pt and PdCu interface enhanced the bonding strength of

PdCu and Pt interface, which stabilizes Pt shell. Two simple descriptors used in this study can be extended to find another core-shell combination for ORR reaction before synthesizing core-shell nanocatalysts.



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발표코드: MAT.P-1197

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Patterned Growth of ZnO Nanowire by Tetramethylammonium Hydroxide in Aqueous Solution

김용희 백남섭 정명애<sup>1</sup> 정상돈

한국전자통신연구원 신경계인터페이스연구팀 <sup>1</sup>한국전자통신연구원 융합기술미래기술부

We present herein a simple protocol of growing a patterned ZnO nanowire by etching of ZnO seed layer in the tetramethylammonium hydroxide (TMAH) solution. The ZnO seed layer was fabricated by sol-gel method using zinc acetate solution and ZnO seed layer was patterned by using photolithographic method. Patterned ZnO seed layer was etched in the TMAH solution and subsequently grown by hydrothermal method. Remarkable point of this patterned ZnO nanowire that the development of photoresist and etching of ZnO seed layer was continued concurrently in aqueous TMAH solution. The properties of ZnO nanowire was investigated by XRD data which show the high purity and good crystallinity.

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장소: 일산KINTEX

발표코드: MAT.P-1198

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Single-Cell-based Neuronal Patterning using Site-Specific Photocrosslinking of Cell-Repellent Polymer

백남설 김용희 정상돈 정명애<sup>1</sup>

한국전자통신연구원 신경계인터페이스연구팀 <sup>1</sup>한국전자통신연구원 융합기술미래기술부

Single-cell-based neuronal networks on the micropatterned substrate fabricated by photocrosslinking of poly(styrene-*co*-methacryloxybenzophenone) were demonstrated. For this study, we synthesized the polystyrene derivative as a cell-repellent layer using radical polymerization method and fabricated micro-sized photopatterns on transparent indium tin oxide and SiO<sub>2</sub> substrate for neuronal patterning. This photocrosslinking method provides well-organized micropatterns with 3  $\mu$ m line resolution and excellent pattern fidelity, resulting in the formation of single-cell-based neuronal networks.

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발표코드: MAT.P-1199

발표분야: 재료화학

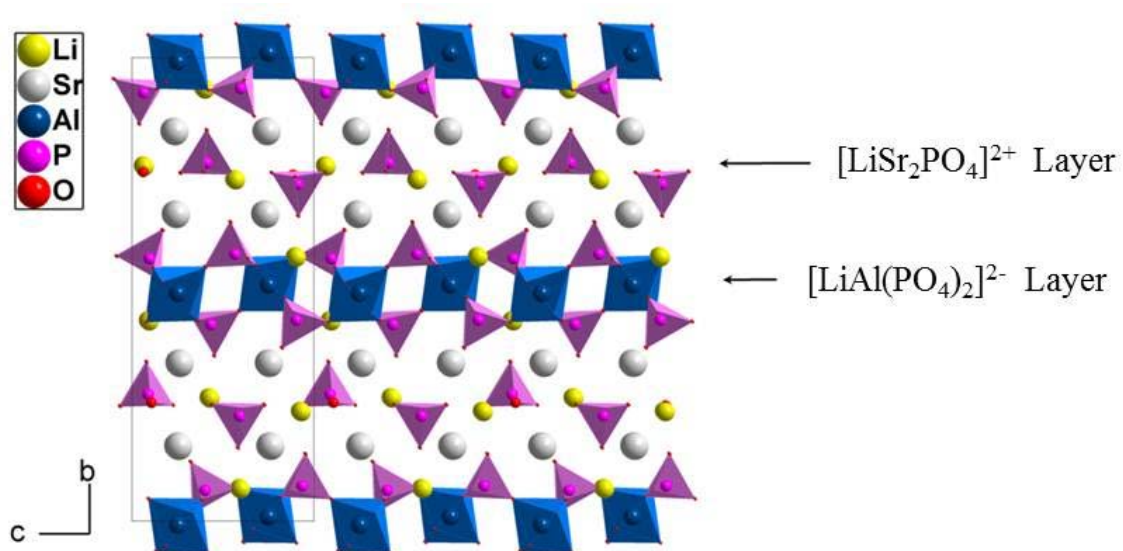
발표종류: 포스터, 발표일시: 수 18:00~21:00

## The structure analysis and ion conductivity measurement of new Li-containing phosphate, $\text{Li}_2\text{AlSr}_2(\text{PO}_4)_3$

정재훈 손혜진<sup>1</sup>

아주대 에너지시스템학부 <sup>1</sup>아주대 화학과

A new Li-containing phosphate,  $\text{Li}_2\text{AlSr}_2(\text{PO}_4)_3$  was synthesized by molten salt method (crystal) and solid state reaction (powder). The structure of  $\text{Li}_2\text{AlSr}_2(\text{PO}_4)_3$  was determined by single crystal X-ray diffraction. It crystallizes in the monoclinic space group  $\text{P}1\ 2_1/\text{n}$  (No. 14) with lattice parameters  $a = 4.945\ \text{\AA}$ ,  $b = 22.088\ \text{\AA}$ ,  $c = 8.632\ \text{\AA}$  and  $\beta = 91.47^\circ$ . This compound composed of alternating layers of  $[\text{LiAl}(\text{PO}_4)_2]^{2-}$  layer and  $[\text{LiSr}_2\text{PO}_2]^{+2}$  layer. Ionic conductivity was measured by impedance spectroscopy. Temperature dependences of the bulk ionic conductivity show Arrhenius behavior. Conductivity was found to be  $\sigma = 2.65 \times 10^{-4}\ \text{S/cm}$  at 667 K with activation energy  $E_a = 0.53\ \text{eV}$ .



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발표코드: MAT.P-1200

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Physicochemical Properties of Individually Suspended SWNT in Non-Ionic Surfactant

Nur Elida M.Z 이승윤 김효섭 김재호

아주대 분자과학기술학과

Triblock copolymer, Poloxamer 407 or commercially known as Pluronic F127, was used for dispersing Single-walled Carbon Nanotubes (SWNTs) in aqueous solution. Due to strong van der Waals interaction between tubes, SWNTs experienced hydrophobicity properties and required surface modification. Non-covalent method of dispersing SWNTs using Pluronic polymer has the advantages of maintaining the intrinsic properties of SWNTs structure. In this study, the physicochemical properties of carbon nanotubes were analyzed in terms of size, surface modification, stability and concentration. The SWNT dispersion prepared by using probe sonication method exhibited good stability with average CNT diameter and length of  $4\pm 2$  nm and 100-600 nm, respectively. The dispersion stability and hydrodynamic size were also discussed. Raman analysis was carried out in order to analyze diameter, chirality, and purity. High frequency tangential T modes or known as G band can be observed at  $1591\text{ cm}^{-1}$  which



represent semiconducting SWNT. Exfoliation of SWNT bundle into individual tubes was observed using SEM dan TEM.



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발표코드: MAT.P-1201

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Superhydrophobicity of ITO nanorods fabricated by sputtering deposition

박후근 윤성웅<sup>1</sup> 도영락

국민대 생명나노화학과 <sup>1</sup>국민대 화학과

A droplet on superhydrophobic surfaces forms a nearly perfect spherical pearl with contact angle higher than  $150^\circ$ . Tin-doped indium oxide (ITO) nanorods were fabricated on ITO substrate via radio frequency (rf)-magnetron sputtering deposition, and their height was approximately 700nm. For hydrophobization of ITO nanorods surface, the prepared ITO nanorods were treated under a liquid phase with perfluorodecyltrichlorosilane (PFS) self-assembled monolayers (SAMs). Although the ITO nanorods are very hydrophilic, they could become superhydrophobic by modifying them with a coating of PFS. Static, advancing and receding contact angles of ITO nanorods were measured by a contact angle analyzer in order to demonstrate superhydrophobicity of ITO nanorods. The structural and morphological properties of ITO nanorods were investigated by performing scanning electron microscopy (SEM) and atomic force microscopy (AFM).

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발표코드: MAT.P-1202

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation and characterization of CdSe/ZnS Quantum-Dots coated glass beads

윤지수 오지혜<sup>1</sup> 조영식<sup>2</sup> 도영락<sup>1</sup>

국민대 나노화학과 <sup>1</sup>국민대 생명나노화학과 <sup>2</sup>단국대 화학과

CdSe/ZnS quantum dots (QDs) were synthesized by a hot-injection single step method using reactivity difference between Cd and Zn precursors and that between Se and S precursors. The QDs have a core-shell structure with chemical composition gradients and a high photoluminescent property. We used glass beads as binder in order to prevent aggregation of QDs in different solutions. For fabricating a glass beads?QDs composite, (3-mercaptopropyl)trimethoxysilane (MPTS) are used as linker between glass beads and QDs. Dithiol was coated on the glass beads with QDs layer to raise the number of QDs layer. The structural, morphological and optical properties of the glass bead-QDs composites were investigated by performing scanning electron microscopy (SEM), and photoluminescence (PL) measurements.

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발표코드: MAT.P-1203

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile Synthesis and Characterization of I-III-VI-ZnS Nanocrystals

홍성표 김민채<sup>1</sup> 도영락<sup>2</sup>

국민대 생명나노화학 <sup>1</sup>국민대 화학과 <sup>2</sup>국민대 생명나노화학과

For synthesis of high luminescent  $\text{AgIn}_x\text{S}_{(3x-1)/2}$ -ZnS-alloyed nanocrystals,  $\text{AgIn}_x\text{S}_{(3x-1)/2}$  cores were prepared by injecting sulfur source into a mixture of silver and indium precursors in the presence of 1-dodecanethiol.  $\text{AgIn}_x\text{S}_{(3x-1)/2}$ -ZnS-alloyed nanocrystals were synthesized by diffusing Zn into  $\text{AgIn}_x\text{S}_{(3x-1)/2}$  cores without further heating. The obtained  $\text{AgIn}_x\text{S}_{(3x-1)/2}$ -ZnS-alloyed nanocrystals were characterized by UV-vis spectroscopy, PL spectroscopy, X-ray diffraction and Transmission electron microscopy. Absorbance, PL emission wavelength and quantum yield of the obtained  $\text{AgIn}_x\text{S}_{(3x-1)/2}$ -ZnS-alloyed nanocrystals can be tuned easily via variation of the mole ratio of their components. Also these photoluminescent properties were influenced by experimental variables including reaction temperature, time and concentration.

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장소: 일산KINTEX

발표코드: MAT.P-1204

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Facile Method for rGO FET: Selective Adsorption of rGO on SAM-Treated Gold Electrode by Electrostatic Attraction

양지은 신현석

울산과학기술대 에너지공학부

A facile method for fabrication of negatively and positively charged reduced graphene oxide (rGO) field effect transistor (FETs) is proposed, which utilizes electrostatic attraction between electrodes and rGO sheets. The pre-patterned gold electrode on SiO<sub>2</sub>(300 nm)/Si wafer is prepared, followed by forming self-assembled monolayers (SAMs) with negative or positive charges on the electrode. Negatively and positively charged rGO sheets are functionalized with carboxylic acid and amine groups, respectively. The electrode with SAMs is immersed in a solution with negatively or positively charged graphene oxide (GO) sheets. Then, the GO sheets are selectively adsorbed on the gold electrode via electrostatic attraction. The FET of amine-functionalized rGO exhibits n-doping effect. Furthermore, FET devices fabricated by this method exhibited high mobility of carriers: maximum 82.5 and 27.5 cm<sup>2</sup>/Vs for hole and electron, respectively, in -rGO devices and maximum 6.7 and 1.8 cm<sup>2</sup>/Vs for hole and electron, respectively, in +rGO devices.

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장소: 일산KINTEX

발표코드: MAT.P-1205

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Efficient siRNA delivery in vitro and in vivo using mesoporous silica nanoparticles with large pores

나희경 민달희<sup>1</sup>

KAIST 화학과 <sup>1</sup>서울대 화학과

RNA interference (RNAi) is an evolutionarily conserved biological process in which a double stranded RNA inhibits gene expression by degrading target mRNA or by blocking the translation pathway of a specific gene. The application of RNAi using siRNA (small interfering RNA) in biomedical area might have great potential to treat diseases that cannot be treated by conventional small molecule drug. Mesoporous silica materials appear to possess immense potentials in catalysis, biosensors and drug delivery systems due to their tunable pore and particle size, high surface area, large pore volume, and biocompatibility. In particular, monodispersed silica spheres with large pores are very important for the incorporation of large molecules such as metal complexes and proteins into mesopores, and for the retention of pore space after grafting of organic functional groups. Here, we report an efficient siRNA delivery system based on pore expanded silica nanoparticle. It is shown that newly developed siRNA delivery system is novel and powerful gene delivery vehicle in vitro and in vivo. Our study demonstrates

that siRNA-pore expanded silica nanoparticle complex can serve as potential gene silencing therapeutics for treating various diseases.



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발표코드: MAT.P-1206

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## High-performance n-type organic field-effect transistors based on single-crystal fullerene nanowires

박경선 조보람 백장미 이기석 성명모

한양대 화학과

We generated single-crystal fullerene nanowire array using a direct printing method, liquid-bridge-mediated nanotransfer molding (LB-nTM). LB-nTM is able to simultaneously synthesize, align, and pattern of nanowires using molecular ink solution. Using this method, fullerene nanowires were synthesized by self-assembly and crystallization of fullerene molecules within the nanoscale channels of molds, and these nanowires were directly transferred to the substrates by a direct printing process. This method was utilized to fabricate high-performance n-type organic field-effect transistors that can be integrated into device arrays on flexible plastic substrates.



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발표코드: MAT.P-1207

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Phase-selective and Rapid Crystallization of Metal-organic Frameworks with Non-conventional Heating Methods

전재우 박은영 Nazmul Abedin Khan 정성화

경북대 화학과

Metal-organic frameworks (MOFs) attract much attention because of possibility of designing a structure with a particular pore size/shape, huge porosity and many potential applications [1]. So far, the MOFs, especially, structures that are stable to air or water have been crystallized by hydrothermal or solvothermal syntheses with conventional electrical heating [1]. In this presentation, the crystallizations of MOFs with nonconventional heating methods like ultrasound (US) and microwave (MW) will be discussed. The rapid and facile syntheses of MOFs with US and MW will be presented [2]. Moreover, a phase-selective crystallization of a MOF, especially less stable phase, with MW heating will also be illustrated [3]. The phase-selective crystallization will be explained with phase-conversion to a more stable structure with prolonged crystallization time [3]. Acknowledgement This work 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. G. Férey, "Hybrid porous solids:

past, present, future”, Chem. Soc. Rev., 37, 191 (2008). 2. E. Haque, N. A. Khan, J. H. Park, S. H. Jhung, "Syntheses of a metal-organic framework material, iron-terephthalate under ultrasound, microwave and conventional electrical heating: A kinetic study", Chem. Eur. J., 16, 1046 (2010). 3. N. A. Khan, S. H. Jhung, "Phase-transition and phase-selective synthesis of porous chromium-benzenedicarboxylates", Crystal Growth Des., 10, 1860 (2010).



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

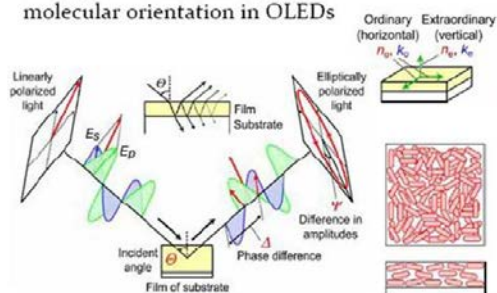
## **Dual efficiency enhancement by delayed fluorescence and dipole orientation in high-efficiency fluorescent organic light-emitting diodes**

**김범진 박종욱**

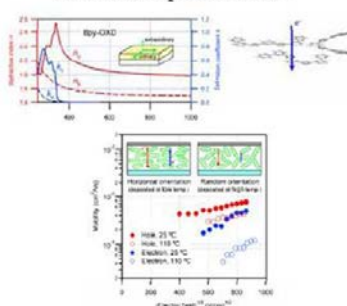
가톨릭대 화학과

To explain the origin of extremely high efficiencies of deep-blue fluorescent OLEDs with anisotropic-shaped anthracene derivatives, the enhancements of singlet-exciton generation efficiency and outcoupling efficiency were investigated by transient electroluminescence measurement and spectroscopic ellipsometry, respectively. This dual efficiency enhancement is important for understanding and further improving high-performance fluorescent OLEDs.

## Analysis of the anisotropy and molecular orientation in OLEDs



## Relationship between orientation and device performance

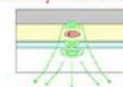


### Vertically oriented molecules



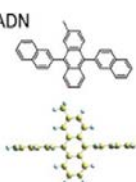
Low out-coupling efficiency

### Horizontally oriented molecules

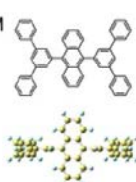


High out-coupling efficiency

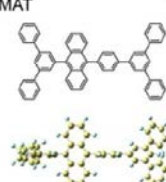
MADN



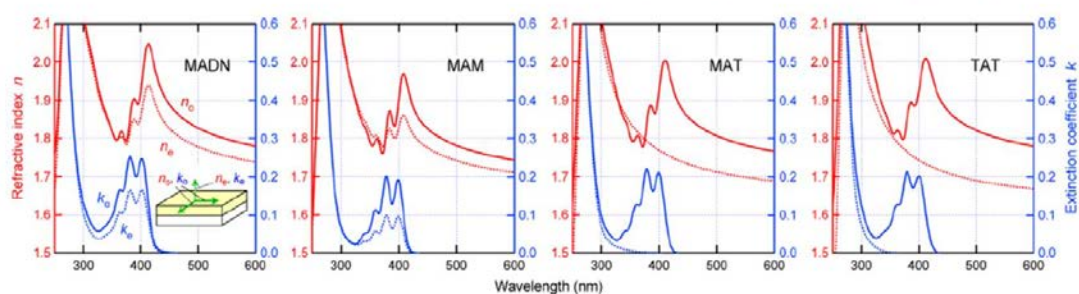
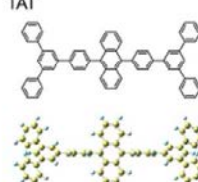
MAM



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TAT



일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: MAT.P-1209

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Optoelectronic property of graphene functionalized with spiropyran

장아람 강동우 신현석<sup>1</sup>

울산과학기술대 친환경에너지공학부 <sup>1</sup>울산과학기술대 에너지공학부

Graphene is functionalized with spiropyran, a well-known photochromic molecule, via non-covalent bonding. The field-effect transistor (FET) with spiropyran-functionalized graphene exhibits 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 of neutral form (colorless spiropyran) and charge separated form (purple colored merocyanine) on UV-Vis light irradiation. The merocyanine form is produced during UV light irradiation, inducing the shift of the Dirac point of graphene toward negative gate voltage. This result indicates that carrier density was changed by dipole moment of separated charges. Also, the reverse process to neutral spiropyran form occurred during visible light irradiation, inducing the shift of the Dirac point toward positive gate voltage. The change of Dirac point by UV and visible light was reproducibly repeated. Furthermore, spiropyran molecules improve photocurrent response of graphene. Details on experimental process and optoelectronic property of graphene functionalized with spiropyran will be presented.

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발표코드: MAT.P-1210

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Luminescent Eu(TTA)<sub>3</sub>Phen in PEO matrix for Detecting Traces of Water

최푸른 구은희<sup>1</sup>

연세대 신소재공학과 <sup>1</sup>한국세라믹기술원 바이오IT융합

Promising next generation of Flexible electronics which are flexible e-book, thin film solar cell, flexible lighting, and flexible OLED provide the availability of robust, light weight, portable and rollable function. However, one of the major obstacles of the technology is the extraordinary sensitivity of organic based active materials to water trace and oxygen molecules. The requirement of WVTR (Water Vapor Transmission Rate) is 10<sup>-6</sup>g/m<sup>2</sup>/day for flexible OLED. However, it is difficult to measure the permeability of 10<sup>-6</sup>g/m<sup>2</sup>/day by current technologies like MORCON, calcium to jump over the hurdle; opto-chemical method is promising using luminescent nana-materials, which are sensitive to oxygen or water. It can be used for not only estimating the permeability of a trace of target molecules, but also measuring defect of barrier film which affects its WVTR. In this study, Eu-complex is synthesized and characterized as a fluorescent material for detecting a trace of water molecule. Eu-complex is incorporated in poly (ethylene oxide). Eu-complex in polymer matrix is not tricky to manage. It has

strong red-fluorescence, but is easily quenched by a trace of water. The optical property and water sensitivity of the film which is incorporated with Eu-complex has been investigated and characterized using SEM, Ellipsometry, Uv-vis, and PL spectrometer.



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발표코드: MAT.P-1211

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## a fluorescent nitric oxide(NO) sensor with Rh-complex in silica beads

양난희 구은희<sup>1</sup>

고려대 바이오마이크로시스템 <sup>1</sup>한국세라믹기술원 바이오IT융합

Nitric oxide (NO) has been interested in chemistry and biology since it was identified as the endothelium-derived relaxation factor. In addition, NO was established a ubiquitous messenger molecule in the cardiovascular, nervous and immune systems and tumor progression. However NO is highly reactive and it can be converted to other species quickly, thus it is very difficult to detect and monitor the concentration of NO in vivo. SO many methodologies of detecting NO have been developed include electrochemical, EPR, chemiluminescent, and fluorescence signaling. Our method in developing sensors that utilize the formation of transition-metal complex to trigger a change in fluorescence is based on a strategy that takes advantage of the well-known fluorescence-quenching properties of transition metal complexes with partially filled d-shells. Furthermore our nanohybrids incorporated system can sense NO reversibly by turn-on emission and display more effectively than solution environment.



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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of Silica microbeads incorporated with water-soluble Quantum dots for ultrasensitive DNA sensor applications

이지혜 구은희<sup>1</sup>

고려대 <sup>1</sup>한국세라믹기술원 바이오IT융합

Ultrasensitive DNA detection is necessary in clinical diagnostics, gene analysis, and a variety field of biomedical studies. In microarray gene analysis, signal amplification is the most critical issue and is typically achieved by fluorophores, such as organic dyes to the DNA probes. Semiconductor Quantum dots (QDs) have novel optical properties such as simultaneous excitation, size-tunable emission, high stability against photobleaching and narrow, symmetrical emission peak. Silica microbeads incorporated with QDs have several advantages compared with organic dyes in bioanalysis array system. First, large number of QDs are encoded a single micro beads, which produces a strong fluorescence signal when it is excited properly. Second, the microbead is highly photostable, when they are inside the silica network. Third, the silica surface is easily modified as a biocompatible and versatile substrate for the immobilization of biomolecules. In this study, we have investigated the silica microbeads incorporated with water-soluble QDs and modified silica microbeads surface for applied more usefully to biological

systems. Furthermore, the microstructure, optical properties and the sensitivity of the microbeads incorporating with water-soluble QDs were characterized by transmission electron microscopy, scanning electron microscopy, Fluorescence microscopy, UV-Vis spectroscopy, respectively.



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발표코드: MAT.P-1213

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 4,4'-sulfonylbis(4,1-phenylene) bis(4-(3-(acryloyloxy)propoxy)benzoate)

### 합성과 액정성 평가

김도연 전윤태 도윤선

애경화학 기술연구소

반응형 액정은 액정 분자 말단에 중합가능한 관능기들을 가지면서도 액정으로써의 결정성 성질과 유동성을 가지는 물질이다. 중합가능한 반응형 액정을 이용 광학필름(TAC, PET 등)에 코팅을 통하여 LCD 디스플레이에 사용되는 각종 보상필름, 위상차필름, FPR 필름으로 상업적 활용이 이루어지고 있다. 본 연구에서는 고 굴절률을 가지는 반응형 액정 물질 4,4'-sulfonylbis(4,1-phenylene) bis(4-(3-(acryloyloxy)propoxy)benzoate) 를 합성하여 NMR, GC-Mass, IR 등을 통하여 확인하였고, 편광현미경, DSC, TGA 를 통하여 열적성질을 확인하였다. 위 합성된 반응형 액정 물질을 이용하여 상업적으로 널리 활용되는 RM-257(Merck 社)제품에 혼합사용을 통하여 부족하였던 액정상 온도범위, 굴절을 부분을 보완하여 사용될 수 있음을 연구하였다.

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장소: 일산KINTEX

발표코드: MAT.P-1214

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Study on surface morphology for Nylon 4,6 thin film deposited by Molecular Layer Deposition

양다슬 성명모

한양대 화학과

Molecular Layer Deposition(MLD) is based on sequential and self-terminating surface reactions analogous to ALD and results in the formation of self-assembled organic monolayer in each sequence. We fabricated Polyamide 4,6(Nylon) thin film by MLD using Adipoyl chloride and 1,4-butadiamine. Polyamide 4,6 film was grown at 70°C and the growth rate is 3.5 Å/cycle. The thickness was measured by Ellipsometer. The surface morphology was investigated by Atomic Force Microscopy(AFM) and roughness is proportional to number of growing cycles. It can be used as encapsulation layer by fabricating superlattice with Aluminum oxide.

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발표코드: MAT.P-1215

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **C<sub>60</sub>-Organosilicon Nanocomposites**

**Dao Duy Tung 최진규 정현담**

전남대 화학과

Fullerene (C<sub>60</sub>) and its derivatives have attracted much attention due to their promising applications in a variety of fields. However, its poor solubility and processability pose difficulties in utilizing C<sub>60</sub> for practical applications. Incorporation of C<sub>60</sub> with siloxane moieties is a useful alternative way to improve the solubility and processability. The new material C<sub>60</sub>-organosilicon composites was synthesized from C<sub>60</sub> and 1,1,3,3,5,5-hexamethyltrisiloxane in the presence of Karstedt catalyst via hydrosilylation. The electrical and optical properties of the C<sub>60</sub>-organosilicon composites thin films were investigated.

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장소: 일산KINTEX

발표코드: MAT.P-1216

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Condensable InP Quantum Dot Solids

Dao Duy Tung Mai Xuan Dung 정현담

전남대 화학과

InP quantum dots capped by myristic acid (InP-MA QDs) were synthesized by a typical hot injection method using MA as stabilizing agent. The current density across the InP-MA QDs thin film which was fabricated by spin-coating method is about  $10^{-4} \text{ A/cm}^2$  at the electric field of 0.1 MV/cm from I-V measurement on a metal-insulator-metal (MIM) device. The low conductivity of the InP-MA QDs thin film is interpreted as due to the long interdistances among the dots governed by the MA molecules. Therefore, replacing the MA with thioacetic acid (TAA) by biphasic ligand exchange was conducted in order to obtain TAA capped InP QDs (InP-TAA). InP-TAA QDs were designed due to: 1) the TAA is very short molecule; 2) the thiolate groups on the surface of the InP-TAA QDs are expected to undergo condensation reaction upon thermal annealing which connects the QDs within the QD thin film through a very short linker -S-; and 3) TAA provides better passivation to the QDs both in the solution and thin film states which minimizing the effect of surface trapping states.

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장소: 일산KINTEX

발표코드: MAT.P-1217

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

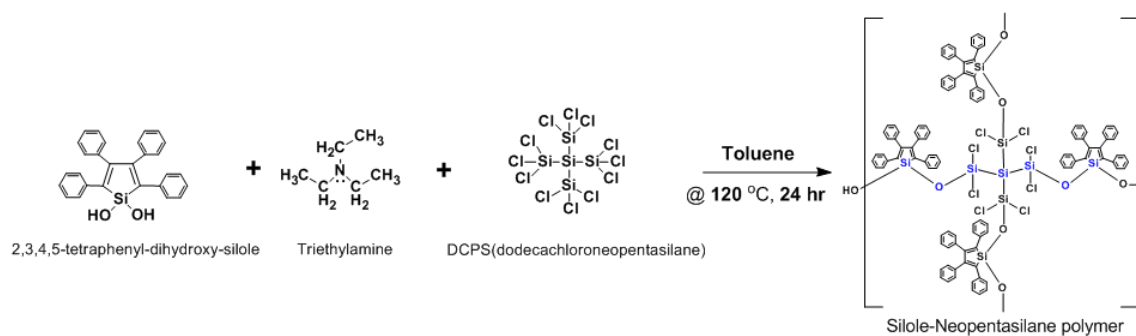
## Synthesis and Electron Trap Properties of Silole-Neopentasilane Hybrid Thin Films

이돈성 최진규 손홍래<sup>1</sup> 정현담

전남대 화학과 <sup>1</sup>조선대 화학과

Charge trapping is a key factor determining the performance of charge trap flash memory devices. Nowadays, organic-inorganic hybrid materials have drawn much attention for the charge trap materials due to merging their advantages; functionality and electrical/thermal stabilities from organic and inorganic parts, respectively. A new kind of organic-inorganic hybrid polymer, silole-neopentasilane (SNPS), was invented and synthesized for realization of its charge trap properties. Organic portions consisting of (tetraphenyl)silole rings were responsible for negative charge (electron) trapping, while the Si-O-Si inorganic linkages provided the intrachain energy barrier for controlling electron transport. The SNPS was synthesized by solution process from dihydroxy (tetraphenyl)silole (DS) and dodecachloroneopentasilane (DCPS) with a catalyst of triethylamine. The molecular structure and weight of the SNPS were analyzed by <sup>1</sup>H-nuclear magnetic resonance (NMR) spectroscopy, Fourier transform infrared spectroscopy (FT-IR), and gel permeation chromatography (GPC). Then, the SNPS thin films

were fabricated by spin-coating onto Si-wafers. The electron trapping of the SNPS thin films was confirmed from the positive flat band shift ( $\Delta V_{FB}$ ) in the capacitance-voltage (C-V) measurements performed within the metal-insulator-semiconductor (MIS) device structure.





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발표코드: MAT.P-1218

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Sergeant and soldiers effects: Helix-inducing placement of chiral residues in peptoid sequences

신혜민 서지원<sup>1</sup> 윤명한

광주과학기술원 신소재공학부 <sup>1</sup>광주과학기술원 기초교육학부

Natural molecules such as proteins, nucleic acids and carbohydrates have specific functions, which are mainly originated from their 3D structures. Hence, many biomimetic molecules such as artificial peptides and peptoids are being investigated to fold into specific secondary structures. Peptoids, oligo-N-substitute glycines, have achirality of backbone and lack of hydrogen bond donors, so difficult to form  $\alpha$ -helical structure. Yet, peptoids with  $\alpha$ -chiral, aromatic side-chains form stable polyproline-like helices in both organic and aqueous solutions. Even though peptoid structures such as  $\alpha$ -helix, threaded-loop, and cyclic peptoid have been discovered, there is still lack of understanding on the precise control of peptoid structures that lie in between fully helical and unstructured. In this study, we report the synthesis and characterization of a family of structured peptoids with varying an  $\alpha$ -chiral residue location to investigate how effectively peptoid helicity is controlled via regiochemistry of  $\alpha$ -chiral residue. Circular dichroism studies of the sequenced peptoid heptamers reveal that stronger helicities are induced by  $\alpha$ -chiral residue

on the first position from the C-terminus than the other positions and those peptoids' helicities are maintained stably in acetonitrile solution at temperatures up to 75 °C. These results will be the foundation of peptoids' sequence-structure relationships.



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발표코드: MAT.P-1219

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Solution-processed zinc tin oxide thin film semiconductors with semiconductor-insulator interlayer modifications**

**손기철 윤명한**

광주과학기술원 신소재공학부

Conductive metal oxides have attracted much attention as active materials in transparent thin film transistors (TFTs) and transparent electrodes in LCD, LED and touch panel display. Unlike conventional thin-film fabricating methods such as chemical vapor deposition (CVD), pulse laser deposition (PLD) and sputtering, solution-based deposition method utilizing metal precursors has several advantages including film uniformity over large area, relatively low fabrication cost, low processing-temperature, and etc. Despite these advantages, there remain unsolved issues on poor adhesion and minority carrier formation at the interface between metal oxide and dielectric layers. In this study, we fabricated and characterized solution-processed zinc tin oxide (ZTO) TFTs by sol-gel process and embedded carbon nanostructures at the interface between semiconductor and gate insulator layers. We believe that this study will contribute to our understanding of the interfacial modification effect on metal-oxide TFT performance and development of high-performance metal-oxide TFTs via low-temperature solution-process.

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발표코드: MAT.P-1220

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## InP Quantum Dot-Organosilicon Nanocomposites

Mai Xuan Dung 최진규 정소희<sup>1</sup> 정현담

전남대 화학과 <sup>1</sup>한국기계연구원 나노기계연구본부

InP quantum dot (QD)-organosilicon nanocomposites were synthesized and their photoluminescence was mainly investigated because of their applicability to white LEDs (light emitting diodes). The InP and InP/ZnS QDs, which are synthesized by conventional method using fatty ligand such as myristic acid, hexadecylamine, octylamine, etc, as stabilizing agent, are incompatible with typical silicone encapsulants due to the large differences in their solubility parameters. Therefore, direct chemical bonding is needed to overcome this incompatible problem. In the first approach, post ligand exchange from myristic acid (MA) to 3-aminopropyltrimethylsilane (APTMS) are able to generate soluble InP QDs bearing silylable Si-H groups, which allow embedding the QDs into vinyl-functionalized silicones through direct chemical bonding. However, the photoluminescent efficiency is greatly reduced upon ligand exchanging from MA to APTMS, which is interpreted by surface corrosion of the QD induced by the stronger electron donating ligand based on theoretical studies. Vinyl functionalized InP QDs were then designed in the second approach, in which vinyl terminated amine (10-undecene-1-amine) is used as co-stabilizing agent. The

new synthesizing effort is expected to produce highly luminescent QDs being able to chemical bonding to various silane compounds.



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발표코드: ELEC.P-1221

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Battery Performance of Morphology-Controlled $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Cathodes

홍순기 여인형<sup>1</sup> 모선일

아주대 에너지시스템학부 화학 <sup>1</sup>동국대 화학과

Nickel substituted  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  spinel is one of the most promising candidates with a high operating voltage at 4.7 V versus  $\text{Li}^+/\text{Li}$ . In the case of  $\text{LiMn}_2\text{O}_4$  spinel, the cathodes suffer from poor cycling efficiency for long life operating, especially at high temperature, which was caused by the structural instability and the dissolution of manganese ions. The  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  spinel has a good cycling performances and good thermal stability by doping nickel into the lattices. In addition to the intrinsic properties of the material, the morphology plays a key role in its electrochemical performance. The morphology controlled  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  has different characteristics, due to their structural variety, surface composition and diffusion lengths for Li ion. In this work, octahedral- and rod-shaped  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  was prepared by hydrothermal and by using proper precursors and by following heat treatment. Each morphology cathodes has different space group as Fd-3m and P4<sub>3</sub>32. Crystalline phases, structure, and the morphology were characterized by using an X-ray diffraction (RigakuD/max 2700V/VP), Neutron

diffraction and a scanning electron microscope (JEOL JSM-6380). 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. The comparing of those materials will be discussed in detail.



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발표코드: ELEC.P-1222

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical Preparation of $\text{Li}_2\text{MnSiO}_4$ Nanocrystalline And Polypyrrole Composite film

유다연 Hung-Cuong Dinh 여인형<sup>1</sup> 모선일

아주대 에너지시스템학부 화학 <sup>1</sup>동국대 화학과

$\text{Li}_2\text{MnSiO}_4$  has been an attractive cathode material for rechargeable lithium ion batteries. The main advantages of  $\text{Li}_2\text{MnSiO}_4$  are relatively lower cost, less toxicity, environmental friendliness, and high theoretical capacity  $333 \text{ mAhg}^{-1}$ . However, this material has a disadvantage of low conductivity. Conducting polymer, polypyrrole, has characteristics of high electrical conductivity and stability with flexibility. Nanosized  $\text{Li}_2\text{MnSiO}_4$  was prepared by simple hydrothermal method using  $\text{LiOH}$ ,  $\text{SiO}_2$ ,  $\text{MnCl}_2$ . And then  $\text{Li}_2\text{MnSiO}_4$ /polypyrrole composite film was made by an electrochemical method. Composite film containing the  $\text{Li}_2\text{MnSiO}_4$  in the conductive polymer network (polypyrrole) was galvanostatically grown on a working electrode in three electrode system. The characteristics of  $\text{Li}_2\text{MnSiO}_4$ /polypyrrole composite film, morphology and electrochemical properties were examined by X-ray powder diffraction (XRD) and scanning electron microcopy (SEM). Electrochemical properties change was also systematically examined and will be discussed.



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발표코드: ELEC.P-1223

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Battery Performance of C-coated Nanocrystalline LiMnPO<sub>4</sub> Cathode

Hung-Cuong Dinh 여인형<sup>1</sup> 모선일

아주대 에너지시스템학부 화학 <sup>1</sup>동국대 화학과

As new class of intercalation compounds, phosphates with olivine structure rather than oxides, has emerged that overcome many of the weaknesses inherent to earlier cathode candidates. LiMnPO<sub>4</sub> olivine structure is attracted much attention as the most promising material for rechargeable Li-ion batteries, due to high energy density (ca. 701 Whkg<sup>-1</sup>), the redox potential of 4.1 V vs. Li/Li<sup>+</sup>, and high theoretical capacity of 171 mAhg<sup>-1</sup>. However, the very low electronic conductivity is preventing high rate performance of the LiMnPO<sub>4</sub> cathode. To improve electrochemical characteristic of LiMnPO<sub>4</sub>, optimizing particle size to nano-scale is necessary owing to its high specific surface area, short diffusion lengths for Li-ion. In this work, well-crystallized LiMnPO<sub>4</sub> nanoparticles were prepared by a simple hydrothermal method using LiOH, H<sub>3</sub>PO<sub>4</sub>, Mn(CH<sub>3</sub>COO)<sub>2</sub>·4H<sub>2</sub>O, glucose. After that, the LiMnPO<sub>4</sub> nanoparticles were coated with carbon on surface by pyrolysing sucrose in an inert atmosphere. The structure, morphology and electrochemical properties, carbon content were analyzed by the X-ray powder diffraction (RXD) patterns, scanning electron microscopic (SEM) images, Raman spectrometer, and thermal gravimetric

analyzer (TGA). The lithium batteries with the C-coated LiMnPO<sub>4</sub> nanoparticles cathode were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled galvanostatically a potential range of 2.0-4.4 V using a multichannel battery test mode (Maccor 4000).



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발표코드: ELEC.P-1224

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Heterostructured Cobalt Iron Prussian blue analogues embedded in porous silica matrix by wet-coating : Electrochemistry and Spectroelectrochemistry

정영희 곽준영 김영일

부경대 화학과

Prussian blue and its analogues have been attracting for their physical and chemical properties such as magnetism, ion selectivity and electrochromicity. We synthesized the hybrid metal hexacyanoferrate particles by co-precipitation of  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Fe}(\text{CN})_6^{3-}$  and  $\text{Fe}(\text{CN})_6^{4-}$  for modification of color tone and redox potential range. Various PBA films embedded in silica matrix were prepared by wet-coating on PET/ITO. Co-Fe-PBA films kept the unique voltammetric redox peaks of single component PB and Co-PBAs; on the other hand it showed new absorption band at 730nm in visible spectrum due to increasing of the oxidation potential ( $\text{Fe}^{II}\text{Co}^{II} \rightarrow \text{Fe}^{III}\text{Co}^{III}$ ). Hybrid Co-Fe-PBA films showed reversible color changes (blue- transparent olive brown) depending on the electrochemical reactions in the potential range -0.4V to 1.5V vs SCE (0.1M KPF<sub>6</sub>/PC). The stability of single component PB, Co-PBA, mixed Co-Fe-PBA and hybrid Co-Fe-PBA films in non-aqueous solution were almost same.

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발표코드: ELEC.P-1225

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical Detection of Heavy Metal Ions using the Different Doping Leveled BDD Electrodes

윤장희 원미숙 한송이

한국기초과학지원연구원 부산센터

The boron doped diamond (BDD) electrodes having different boron doping levels (800 ppm, 8000 ppm) were tested for the simultaneous detection of heavy metal ions (Cd, Pb, Cu, Zn and Hg) using the electrochemical method (anodic stripping voltammetry, ASV and differential pulse anodic stripping voltammetry, DPASV). Various experimental parameters that affect on response, such as pH, deposition time, deposition potential, and pulse amplitude were carefully optimized with the BDD electrodes. Using ASV and DPASV, the logarithmic linear response range for the heavy metal ions (Cd, Pb, Cu, Zn and Hg) were in the range of 5 ppb to 50 ppb. The detection limits for heavy metal ions (Cd, Pb, Cu, Zn and Hg) were in the range 1.0 ppb to 5.0 ppb. The results were compared to the ICP-Mass spectrometry. Key words: boron doped diamond (BDD) electrode, anodic stripping voltammetry (ASV), differential pulse anodic stripping voltammetry (DPASV), heavy metal ions

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발표코드: ELEC.P-1226

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical sensors utilizing a micro-liquid/gel interface for Cr(VI) ions

이상혁 이해진

경북대 화학과

본 포스터는 환경유해물질인 Cr(VI)이온 검출을 선택적으로 검출하기 위한 전기화학적 기반의 센서 개발에 관한 내용이다. 서로 혼합될 수 없는 액체/액체 계면에서의 크롬 이온의 전이반응 시 일어나는 전류의 변화를 활용하고자 하였으며 이를 위해 66 마이크로홀어레이를 고분자 지지체에 제작하고 이에 3% PVC-NPOE(polyvinylchloride - 2nitrophenyloctylether)와 TOATB (tetraoctylammoniumtetrakis(pentafluorophenyl)borateetherate)로 구성된 유기성 젤을 도포시켜 수용액/젤 마이크로홀 계면을 형성하였다. 개발한 마이크로홀 어레이 수용액/젤 계면에서 다양한 산화물을 형성하는 Cr(VI) 이온들의 이동반응을 이용하여 크롬 이온을 정량적으로 분석하였다. 또한 크롬 이온과 선택적으로 결합하여 Cr(VI) 이온들이 선택적으로 수용액/유기상 젤 계면을 전이하도록 도와주는 리간드로 Aliquat 336 를 유기성 젤에 도입하여 크롬 이온을 선택적으로 검출할 수 있는 새로운 전기화학적 센서를 개발한 연구 내용을 발표하려 한다.

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장소: 일산KINTEX

발표코드: ELEC.P-1227

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Characterization of covantly bonded Pt with thiolated carbon nanostructures and their electrocatlytic performance to $H_2O_2$

유정민 김대근 전승원

전남대 화학과

Modified electrodes prepared from thiolated carbon nanostructures multi-walled carbon nanotubes (t-MWCNT) and graphene oxide (t-GO) with covalent bonded platinum (Pt) nanoparticles were used in the electrocatalytic reduction of hydrogen peroxide ( $H_2O_2$ ).  $H_2O_2$  biosensors were developed from poly(diallyldimethylammonium chloride) coated t-MWCNT-Pt and t-GO-Pt on glassy carbon electrodes. They were easily and quickly prepared and showed improved sensitivity to the electrocatalytic reduction of  $H_2O_2$ . The Pt nanoparticles covalently bonded to the thiolated carbon nanostructures were characterized by transmission electron microscopy, X-ray photoelectron spectroscopy, and energy dispersive X-ray spectroscopy. Cyclic voltammetry and amperometry were used to characterize the biosensors' performances. The proposed  $H_2O_2$  biosensors exhibited wide linear ranges and low detection limits, giving fast responses within 10s, thus demonstrating their potential for use in  $H_2O_2$  analysis.

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발표코드: ELEC.P-1228

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Catalytic oxygen reduction by different linked Graphene-Metal nanoparticles modified GCE in acidic solution

김대근 Mohammad Shamsuddin 전승원

전남대 화학과

We have reported four different linkers containing Graphene Oxide (GO) supported platinum (Pt) nanoparticles (NPs) catalysts that synthesized using a chemical method and employed an experimental characterization towards oxygen reduction reaction (ORR) in 0.5 M H<sub>2</sub>SO<sub>4</sub> solution acidic media. GO-Pt was characterized by X-ray photoelectron spectroscopy (XPS) transmission electron microscopy (TEM) and Energy-dispersive X-ray spectroscopy (EDX). The results showed that the attachment of Pt onto GO surface was successful. To investigate the relationships between the linker length and the catalytic activities of metal-decorated GO. Three samples were prepared with different linker molecules. Viz. HS(CH<sub>2</sub>)<sub>2</sub>SH, HS(CH<sub>2</sub>)<sub>3</sub>SH and HS(CH<sub>2</sub>)<sub>4</sub>SH. three different types of GO-Pt catalysts were characterized using electrochemical techniques such as cyclic voltammetry (CV), as well as rotating ring disk electrode (RRDE) to analyze the quantitatively obtain the ORR kinetic and the reaction mechanisms on glassy carbon electrode (GCE). All GO-Pt/GCE electrodes showed significantly improved ORR activity and

different ORR mechanisms. GO-Pt catalyst assigned to sites catalytically active towards the ORR, resulting in activity enhancement and a mechanism of a four-electron dominant reduction process.





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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemically characterization of various graphene nanosheets for the determination of serotonin

김슬기 김대근 전승원

전남대 화학과

Graphene nanosheets are delivered from easily available starting materials. We were synthesized chemically different types of graphene nanosheets, and used as electrocatalysts and their electrochemical properties were systematically characterized. We evaluated surface morphologies of graphene nanosheets via X-ray photoelectron spectra (XPS) and scanning electron microscopy (SEM). Also, we examine electrocatalytic activities using electrochemical impedance spectroscopy. Cyclic voltammetry, differential pulse voltammetry, and chronoamperometry were used for the electrochemical detection of serotonin which is an important neurotransmitter. A huge different results were observed with difference of graphene sheets due to reducing agent. Furthermore, the results obtained were compared with other graphene nanosheets. In all these experiments, graphene electrodes exhibited a better sensitivity, high signal-to-noise ratio, response time and possess higher stability than bare glassy carbon electrode.

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발표코드: ELEC.P-1230

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

**Four electron involved O<sub>2</sub> reduction reaction catalyzed by highly active multi walled carbon nanotubes-platinum nanocomposite in acidic media**

Mohammad Shamsuddin 김대근 전승원

전남대 화학과

The electrocatalyst for reduction of dioxygen (O<sub>2</sub>) has been synthesized and employed as doping agent. The surface of multi walled carbon nanotubes (MWCNT) was modified by platinum (Pt) in the chemical process. The O<sub>2</sub> reduction had done by several MWCNT-Pt modified glassy carbon electrode (GCE), denoted as MWCNT-Pt/GCE. The synthesis of MWCNT-Pt nanoparticles matrix was investigated by XPS, TEM and EDX. The electrocatalytic reduction of O<sub>2</sub> was investigated via cyclic voltammetry (CV), and rotating ring disk electrode (RRDE) techniques in 0.1 mol L<sup>-1</sup> HClO<sub>4</sub> aqueous solutions. The electrocatalytic reduction of O<sub>2</sub> at the MWCNT-Pt/GCE established a pathway of two and/or four-electron transfer reduction to hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) and H<sub>2</sub>O respectively. Especially, hydrodynamic voltammetry revealed the modified electrode was catalyzed effectively by the 4 electron reduction of dioxygen to H<sub>2</sub>O and the minimal generation of H<sub>2</sub>O<sub>2</sub> in the process of O<sub>2</sub> reduction. The

MWCNT-Pt showed the significant efficient electrocatalytic performance. It was found that MWCNT-Pt was an effective mediator for the reduction of dioxygen and responsible for the enhanced catalytic activity.



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발표종류: 포스터, 발표일시: 수 18:00~21:00

## On the Studies of Poly(L-lactic acid) Grafted Graphene Oxide Modified Glassy Carbon Electrode

한형순 정해상 김대근 전승원

전남대 화학과

In this study, chemically synthesized poly(L-lactic acid) grafted graphene oxide (GO-g-PLLA) was used as electrocatalysts and their electrochemical properties were systematically characterized. Methylene diphenyl diisocyanate (MDI) was used to create the anchor sites on GO. The synthesized GO-g-PLLA was characterized by the FT-IR and  $^1\text{H}$ -NMR spectroscopy methods. Again the composition and melt crystallization behavior was investigated by the TGA and DSC. In the DSC results, melting point of PLLA was appeared two peaks, such as melting point peak form is a typical characterization of the PLLA isomer. The surface morphologies of GO-g-PLLA were evaluated using scanning electron microscopy (SEM). The possibilities of employing graphenes for the electrochemical detection of important neurotransmitter, serotonin, were studied. Electrocatalytic activities were verified from cyclic voltammetry (CV) and differential pulse voltammetry (DPV).

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발표코드: ELEC.P-1232

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of graphene based on Pt nanoparticles for electrocatalytic oxidation of formic acid

김민수 김대근 전승원

전남대 화학과

The direct ethanol fuel cell (DEFCs) has received much attention due to their inherent high specific energy. We have studied Pt nanoparticles monodispersed on graphene oxide (GO) surface and were successfully prepared by the chemical reaction between  $K_2PtCl_6$  and GO. As-prepared catalysts were characterized by SEM, XPS and TEM. Highly dispersed Pt nanoparticles were observed on the graphene oxide composites that reduced by  $NaBH_4$ . The GO-Pt nanoparticles in  $H_2O$  were ultrasonically dispersed and loading onto glassy carbon electrode for formic acid oxidation, have been investigated using cyclic voltammetry and chronoamperometry methods. For the comparison the catalyst was employed to electrochemical formic acid oxidation in 0.5 M  $H_2SO_4$  and 0.5 M  $NaOH$ . The results show a significant electrolyte effect on formic acid oxidation in  $H_2SO_4$  solution. 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 DFAFCs successfully

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발표코드: ELEC.P-1233

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New anode redox polymer in the enzymatic biofuel cells

**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 lifetimes. This poster introduces a new anode redox polymer based on mediated glucose oxidation by glucose oxidase (GOx) which catalyzes the oxidation of glucose to glucose lactone. We report the electrooxidation of glucose to glucose lactone under physiological conditions (pH 7.4, 0.1 M NaCl, 37.5 °C). The immobilized electrocatalyst enabling the oxidation is the electrostatic adduct of glucose oxidase (GOx), and the redox polymer of poly (acrylicacid-4-vinylimidazole-acrylamide) complexed with  $[\text{Os}(\text{N},\text{N}'\text{-dimethyl-2,2'-biimidazole})_2]\text{Cl}_2$  cross-linked on the screen printed carbon electrodes (SPCEs). We have investigated enzymatic anode electrode formulations that have the potential to achieve higher current densities and longer stability on the electrodes.

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발표코드: ELEC.P-1234

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Electrochemical Immunoassay for detecting hippuric acid at ITO electrodes modified by electrodeposition of nickel pentacyanoferrates-antigen conjugates**

**전원용 최영봉<sup>1</sup> 김혁한<sup>1</sup>**

단국대 나노바이오효의과학과 <sup>1</sup>단국대 화학과

Electrochemical immunoassay for rapid and quantitative detection of hippuric acid (HA) in human urine was proposed in this work. The electrochemical immunoassay system for clinical diagnosis(or selectivity detection) has several advantages such as, simple instrumentation, relatively low cost, miniaturization, portability, disposability, and fully automation. The series of novel, formation of antigen-conjugated ferrate-nickel nanocomposite (Ni-Fe-HA) was electrodeposited onto indium tin oxide (ITO) electrode and then characterized using the electrochemical techniques. Also, the surface of the Ni-Fe-HA-electrodeposited on ITO electrode were identified by SEM image. The interaction between Os-HA-Bpy conjugate antigens and antibody-HA (anti-HA) was performed by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The redox currents of osmium complexes were linearly proportional to urinary HA in the range of 0.01 ~ 5.0 mg/mL, which is sufficient for use as an

immunosensor using a cutoff concentration of 2.0 mg/mL in urine samples. The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.





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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## New cathode redox polymer in the biofuel cells

이정민 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 lifetimes. This paper introduce a new cathode redox polymer based on mediated oxygen reduction to water by bilirubin oxidase (BOD). We report the electroreduction of  $O_2$  to water under physiological conditions (pH 7.4, 0.1 M NaCl, 37.5 °C). The immobilized electrocatalyst enabling the reduction is the electrostatic adduct of bilirubin oxidase from *Myrothecium verrucaria*, and the redox polymer of poly ( acrylicacid-4-vinylpyridine-acrylamide) (PAA-PVP-PAA) complexed with  $[Os(dicarboxylic\ acid-bipyridine)_2]^{2+/3+}$ , cross-linked on the screen printed carbon electrodes(SPCEs). We have investigated the enzymatic electrode formulations that have the high potential to achieve higher current densities and longer stability on the electrodes.

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발표코드: ELEC.P-1236

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical Properties of Dopamine and Ascorbic acid at Dendritic Au Rod Surfaces: Selective Detection of Dopamine

안미리 김종원

충북대 화학과

전기화학적 석출을 통해 형성한 dendritic Au rod (DAR) 의 나노구조 표면을 이용하여 아스코브산과 도파민의 전기화학적 거동과 도파민의 선택적인 검출에 대해 연구하였다. Au(I) 을 포함한 아황산염을 기본으로하는 전해질의 간단한 전해석출로 100 nm 정도의 막대상에 뾰족한 돌기를 지닌 금 막대 모양의 DAR 구조의 전극을 만들수 있다. DAR 표면에서는 혼합 용액에서 측정시 아스코브산과 도파민의 두 물질의 봉우리가 분리되어 나타났고, 변형되지 않은 평평한 금 전극의 표면에서는 분리되지 않은 하나의 봉우리로 관찰되었다. 도파민의 농도가 낮은 범위에서는 DAR/Bare 전류의 비율이 크게 나타나 DAR 전극이 평평한 금 전극보다 도파민 검출에 효과적인 것을 관찰하였는데, 이것은 DAR 상에 존재하는 뾰족한 금 구조에서 기인하는 것으로 추측된다. 혼합용액에서 아스코브산의 농도를 변화시켜도 도파민의 산화 피크는 영향을 받지 않아 DAR 전극 상에서 도파민의 선택적인 전기화학적

검출이 가능하였다. 0.1 mM 아스코브산 존재하에서 도파민의 검정곡선을 0.5-15  $\mu\text{M}$  범위에서 직선적으로 얻을 수 있었다.



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장소: 일산KINTEX

발표코드: ELEC.P-1237

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical detection of glucose at Nanoporous Black Gold surface in the presence of high concentration of chloride Ions

정화경 김종원

충북대 화학과

큰 표면적을 지니는 nanoporous gold 구조상에서 글루코오스의 전기촉매적 산화거동 및 염소 이온의 방해효과에 대한 연구를 수행하였다. 본 연구에서는 oxalate 용액을 전해질로 하여 금 표면상에서 양극 산화반응을 통해 형성시킨 nanoporous black gold(NPBG)를 활용하여, 다양한 Step time 을 적용시켜 구조와 표면적을 조절하고 이에 따른 글루코오스 산화거동의 변화를 관찰하였다. Step time 이 길어짐에 따라 pore 크기가 다소 증가했지만 큰 차이를 보이지 않았으나, 다공성 구조의 두께는 깊어졌으며 이에 따라 표면적이 증가되는 것을 확인했다. 염소 이온이 존재하지 않을 때에는 -0.15 V 와 0.2 V 에서 두 개의 산화 봉우리가 관찰되는데, 표면적의 증가에 따라 -0.15 V 의 산화 봉우리 전류는 지속적으로 증가했지만, 0.2 V 에서는 포화되는 경향을 보였다. 염소 이온이 존재하는 경우에는 -0.15 V 의 봉우리는 감소하고, 0.2 V 의 산화 봉우리만 상대적으로 크게 측정되었다. 염소이온 농도가 증가함에 따라 표면적의 변화에 따른 글루코오스 산화에 대한 표면활성의 변화 양상이 달라지는 것을

관찰하였다. 100 mM 의 높은 농도의 염소 이온이 존재하는 경우에는 표면적의 증가가 온전하게 글루코오스의 전기촉매적 산화효율의 증가에 반영이 되었다. 표면적이 매우 큰 NPBG 전극을 활용하여 정량적인 글루코오스의 전류법 검출이 높은 감도로 가능하였다.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Structure dependent surfaced-enhanced Raman scattering (SERS) activity at electrochemically fabricated nanostructured Au surfaces

최수희 김종원

충북대 화학과

다양한 형태의 나노 구조를 지니는 금 표면에서 표면 증강 라만 산란(surface-enhanced Raman scattering, SERS) 의 활성화에 대한 연구를 수행하였다. 네 가지 다른 형태의 금 나노 표면 구조: 1) 덴드라이트 금 막대 (dendritic Au rod, DAR) 구조, 2) 나노스파이크 금 (nanospike Au) 구조, 3) 나노다공성 금 (nanoporous gold, NPG) 구조 및 4) 나노플레이트 금 (nanoplate Au) 구조 에 대하여 주사 전자 현미경 (Scanning Electron Microscopy, SEM) 을 통해 표면 구조를 관찰하고, 각 표면 상에서 표면구조에 따라 달라지는 SERS 활성을 Rhodamine 6G 를 활용하여 관찰, 비교 분석하였다. SERS 활성은 표면에 형성된 나노구조의 모양과 크기에 따라서 크게 차이를 보였다. 100 nm 정도의 막대상에 뾰족한 돌기를 지닌 DAR 에서 가장 큰 SERS 활성을 나타 냈으며, nanospike Au 는 상대적으로 크기가 크고 매끈한 구조로 인해 DAR 구조에 비해 낮은 SERS 활성을 나타냈다. NPG 구조에서는 20 nm 크기의 인대/동공 구조를 지니고 있음에도 DAR 또는 nanospike Au 에 비해 확연히 낮은 SERS 활성이

관찰되었으며, nanoplate Au 구조는 SERS 활성을 거의 나타내지 않았다. 이러한 결과들을 바탕으로 금 구조의 모양과 크기가 SERS 활성에 미치는 영향에 대하여 고찰하였으며, 높은 SERS 활성을 나타내는 DAR 구조의 응용 가능성을 제시하였다.



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발표코드: ELEC.P-1239

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Platinum-Coated Porous Carbon Electrode for Hydrogen Evolving Catalyst in Carbonization of Carbon Dioxide

오세영 신운섭

서강대 화학과

Carbonization of CO<sub>2</sub> through electrolysis of saline water includes the production of hydroxide ions by hydrogen evolving reaction at cathode, followed by the addition of Ca<sup>2+</sup> or Mg<sup>2+</sup>. In this system, it is important that hydrogen gas evolves efficiently at low overvoltage. The development of highly porous electrode having a good H<sub>2</sub> evolving catalyst is a key factor. On a carbon paper polyaniline thin-layer was coated as an adlayer first and platinum was electrodeposited by voltage sweeping. The amount of deposited Pt could be controlled by changing the number of sweeping times. The SEM images of the electrode show that Pt particles are deposited homogeneously and the roughness factor was measured to be 231. The electrode evolved H<sub>2</sub> at 0.8 V vs. Ag/AgCl at 20 mA/cm<sup>2</sup> in 0.5 M NaHCO<sub>3</sub> (pH 8.3) when it was rotated at 2000 rpm speed. Note, the theoretical potential for H<sub>2</sub> evolution at pH 8.3 is -0.7 V vs. Ag/AgCl.



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발표코드: ELEC.P-1240

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ag/Ag<sub>2</sub>O Electroosmotic Pump Made of Polydisperse Silica Particles

엄태민 신운섭

서강대 화학과

The Ag/Ag<sub>2</sub>O/SiO<sub>2</sub>/Ag/Ag<sub>2</sub>O electroosmotic pump is non-gassing and energy efficient. The water is driven by protons produced in the anode reaction,  $2\text{Ag(s)} + \text{H}_2\text{O} \rightarrow \text{Ag}_2\text{O(s)} + 2\text{H}^+ + 2\text{e}^-$ , traveling through the porous membrane, consumed by hydroxide ions generated in the cathode reaction,  $\text{Ag}_2\text{O(s)} + 2\text{H}_2\text{O} + 2\text{e}^- \rightarrow 2\text{Ag(s)} + 2\text{OH}^-$ . In the pump 1  $\mu\text{m}$  monodisperse silica microspheres were used to make membrane, sandwiched between a pair of Ag/Ag<sub>2</sub>O plated carbon paper electrodes. We replaced the microspheres with cheap polydisperse (1~5 $\mu\text{m}$ , 80%) silica particles and tested the performances. The 13  $\mu\text{L}\cdot\text{min}^{-1}$  flow rate was obtained at 1 V and the flow was stable for 3 hours at continuous operation, consuming 80% of its coulometric capacity. When the voltage increased, the current increased proportionally. The flow rate was proportional to the applied voltage in the range of 0 ~ 20 V. The flow rate decreased proportional to the opposing pressure and the flow rate dropped to nil at 11 kpa at 1 V and 24 kpa at 2 V.

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2. Shin, W.; Zhu, E.; Nagarale, R. K.; Kim, C. H.; Lee, J. M.; Shin, S. J.; Heller, A. Anal. Chem. 2011, 83(12), 5023
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발표코드: ELEC.P-1241

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Improvement of the Flow-Stability of the Ag/SiO<sub>2</sub>/Ag<sub>2</sub>O Electroosmotic Pump

Enhua Zhu 신운섭<sup>1</sup>

서강대 바이오융합기술 <sup>1</sup>서강대 화학과

When a current or a voltage is applied across the ceramic membrane of the nongassing Ag/Ag<sub>2</sub>O-SiO<sub>2</sub>-Ag/Ag<sub>2</sub>O pump, protons produced in the anodic reaction  $2\text{Ag(s)} + \text{H}_2\text{O} \rightarrow \text{Ag}_2\text{O(s)} + 2\text{H}^+ + 2\text{e}^-$  are driven to the cathode, where they are consumed by the reaction  $\text{Ag}_2\text{O(s)} + \text{H}_2\text{O} + 2\text{e}^- \rightarrow 2\text{Ag(s)} + 2\text{OH}^-$ . The flow of water is induced by momentum transfer from the electric field-driven proton-sheet at the surface of the ceramic membrane. About  $10^4$  water molecules flowed per reacted electron. Because dissolved ions decrease the field at the membrane surface, the flow decreases upon increasing the ionic strength. For this reason Ag<sup>+</sup> ions introduced through the anodic reaction and by dissolution of Ag<sub>2</sub>O decrease the flow. Their accumulation is reduced by applying Nafion-films to the electrodes. The 20  $\mu\text{L min}^{-1}$  flow rate of 6 mm i.d. pumps with Nafion coated electrodes operate daily for 5 min at 1 V for 1 month, for 70 h when the pump is pulsed for 30 s every 30 min, and for 2 h when operating continuously.

## References

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일시: 2012년 4월 25~27일(수~금) 3일간

장소: 일산KINTEX

발표코드: ELEC.P-1242

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Fabrication and surface characterization of TiO<sub>2</sub> nano tube arrays by electrochemical oxidation in an H<sub>3</sub>PO<sub>4</sub>/NaOH/NH<sub>4</sub>F electrolyte**

**정의덕 백성림<sup>1</sup> 진종성**

한국기초과학지원연구원 부산센터<sup>1</sup> 부산대 화학과

TiO<sub>2</sub> nanotube array thin films (TiO<sub>2</sub> Nanotubes) were fabricated by anodic oxidation method using H<sub>3</sub>PO<sub>4</sub>/NaOH/NH<sub>4</sub>F electrolyte. The Average pore diameter and wall thickness of nanotubes was confirmed by Scanning electron microscopy(SEM). The X-ray diffraction (XRD) show a TiO<sub>2</sub> crystal phase. The Secondary ion spectroscopy (SIMS) and X-ray photoelectron spectroscopy (XPS) analysis investigate the surface analysis of TiO<sub>2</sub> NTs were utilized. It is expected that this technique will be applied in the preparation of lubricating, polymer bonded and hydrophobic surface on Ti substrate.

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발표코드: ELEC.P-1243

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrocatalytic Test of Nano-structured Pd in Alkaline Media

강민경 심준호<sup>1</sup> 이영미<sup>2</sup> 이종목<sup>3</sup>

이화여대 전기분석화학 <sup>1</sup>대구대 화학·응용화학과 <sup>2</sup>이화여대 화학나노과학과 <sup>3</sup>이화여대 화학  
과

Fine nano-structured Pd was potentiostatically electrodeposited on gold substrat. The concentration of palladium precursor was varied to control the morphology of structure of Pd. The surface morphology was characterized by SEM and HR-TEM. SAED pattern and XRD data indicate that the obtained Pd at some concentration has structure. Real surface area (RSA) and geometric surface area (GSA) of the electrodes were estimated by cyclic voltammetry and chronocoulometry, respectively. Voltammetry with rotating disk electrode (RDE) were used to test for oxygen reduction reaction (ORR) catalytic activity of as-prepared Pd in alkaline media. The number of electron (n) calculated from Koutecky-Levich plot was closer to 4. The results were compared with those of commercial platinum.

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장소: 일산KINTEX

발표코드: ELEC.P-1244

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Cu/Pd Nano-composites Including Electrocatalytic Activity Test

조아라 강민경<sup>1</sup> 심준호<sup>2</sup> 이영미 이종목<sup>3</sup>

이화여대 화학나노과학과 <sup>1</sup>이화여대 전기분석화학 <sup>2</sup>대구대 화학·응용화학과의 <sup>3</sup>이화여대 화학과

To control the morphology and composition, Cu/Pd nano-structured materials were synthesized in various concentration ratio of Cu and Pd mixture solutions, i.e., (Cu : Pd) of (100 : 0), (75 : 25), (50 : 50), (25 : 75), and (0 : 100). The solutions containing metal precursors were synthesized at the elevated temperature in alkaline media. The obtained nano-structured materials were characterized by SEM, TEM, and EDS. Three-dimensional porous structures were obtained in all mixture solutions except for the Cu only solution. Oxygen reduction catalytic activities were tested using rotating disk electrode voltammetry, where the better results revealed at the Cu/Pd composite materials than the pure Cu or Pd one.

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장소: 일산KINTEX

발표코드: ELEC.P-1245

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Au-Pd Hollow Nanoparticle Electrocatalyst for Direct Amperometric Glucose Sensing

차아름 심준호<sup>1</sup> 이영미<sup>2</sup> 이종목<sup>3</sup>

이화여대 나노화학과 <sup>1</sup>대구대 화학·응용화학과 <sup>2</sup>이화여대 화학나노과학과 <sup>3</sup>이화여대 화학과

Recent advances in nanotechnology have been applied to numerous nonenzymatic glucose electrochemical sensors based on nanostructured materials. We synthesized the Au-Pd bimetallic hollow nanoparticles, which exhibited reasonable nonenzymatic glucose sensing characteristics with good sensitivity and selectivity. The structure and composition of the Au, Pd and Au-Pd hollow catalysts were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy dispersive spectroscopy (EDS) to examine the morphology and to analyze the composition of respective metals. To investigate the glucose detection, the Au, Pd and Au-Pd hollow nanoparticles were loaded on a glassy carbon electrode with nafion as the capping agent for the nanocomposites. The GC/Au-Pd/Nafion electrode showed higher sensitivity for amperometric glucose detection than either GC/Au/Nafion or GC/Pd/Nafion electrode.



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장소: 일산KINTEX

발표코드: ELEC.P-1246

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Preparation and characterization of nano porous TiO<sub>2</sub> films fabricated by electrochemical oxidation**

**백성립 정의덕<sup>1</sup> 정옥상**

부산대 화학과 <sup>1</sup>한국기초과학지원연구원 부산센터

TiO<sub>2</sub> nanotube array thin films (TiO<sub>2</sub> NTs) were fabricated by anodic oxidation method using H<sub>3</sub> PO<sub>4</sub> /NaOH/HF electrolyte. X-ray powder diffractometry (XRD) and Scanning electron microscopy(SEM/EDX) were used to investigate the structure, morphology, length and pore diameter of the obtained TiO<sub>2</sub> NTs. Secondary ion spectroscopy (SIMS) analysis was used to investigate the surface atom image and depth profile analysis of TiO<sub>2</sub> NTs. By optimizing the electrochemical anodization conditions, TiO<sub>2</sub> nanotubes with tunable structures can be reproducibly prepared. It is expected that this technique will be applied in the preparation of lubricating, polymer bonded and Li ion battery material on Ti substrate.

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장소: 일산KINTEX

발표코드: ELEC.P-1247

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Development and Application of an Electrochemical Dual Microsensor for Simultaneous O<sub>2</sub>/pH Measurements

하예진 박선아<sup>1</sup> 심준호<sup>2</sup> 이영미

이화여대 화학나노과학과 <sup>1</sup>이화여대 화학 나노과학과 <sup>2</sup>대구대 화학·응용화학과

Simultaneous measurements of more than two biological analytes could be a key method for confirming their functional roles and relationship. For example, an O<sub>2</sub>/pH dual sensor is of interest since it can provide experimental data helpful to understand some biological mechanisms where O<sub>2</sub> as well as pH change are involved. In this presentation, we demonstrate the development and characterization of O<sub>2</sub>/pH dual sensors. The developed sensor is composed of a working electrode possessing two Pt microdisks and a Ag/AgCl reference/counter electrode. Two Pt disks of the working electrode are modified independently with gas permeable membrane and electrodeposited metal for analyzing O<sub>2</sub> concentration and pH, respectively. For an application, the O<sub>2</sub>/pH dual sensor is employed to measure O<sub>2</sub> and proton concentrations at different parts of the surface of a rat kidney. The current and potential in response to O<sub>2</sub> concentration and pH respectively, are measured simultaneously while the sensor is scanned over the rat kidney surface using scanning electrochemical microscope (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 (2011-0005623).



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발표코드: ELEC.P-1248

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Electrocatalytic Activity of Pd Nanoparticles Self-assembled on Graphene

김지연 심준호<sup>1</sup> 이종목<sup>2</sup> 이영미

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One of the most important challenges for the ultimate commercialization of fuel cells is the preparation of active, robust, and low-cost electrocatalysts. In particular, better electrocatalysts for the fuel cell cathode, where oxygen reduction reaction (ORR) requiring a high overpotential occurs, are needed to improve the efficiency and to lower the cost of fuel cells. In this respect, various nanostructured materials are of interest and have been studied for their catalytic activities. Since graphene was first discovered, it has been studied extensively and received great attention by scientists because of its low cost and advantageous characteristics over graphite, such as high electron mobility and intensity. Furthermore, it has large specific surface area. In this presentation, graphene coated with Pd nanoparticles is synthesized via self-assembly and characterized as fuel cell cathode catalyst. The structure, morphology and electrocatalytic activity of this product is characterized by scanning electron microscopy (SEM) and rotating disk

electrode (RDE). This research was supported by Mid-career Researcher Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology



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## Synthesis and Electrochemical Characterization of Bimetallic Au-Pd Nanocomposite

고아라 심준호<sup>1</sup> 이영미 이종목<sup>2</sup>

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Fuel cell research has been expanding in recent years as the demand for alternative fuels increases. Better catalysts for oxygen reduction reaction (ORR) are needed to improve the efficiency and to lower the cost of fuel cells. Pt and its alloys are still the best electrocatalysts for ORR, but the high cost and limited supply of Pt are the problem. As a catalyst based on non-Pt to reduce Pt usage, in this presentation, we demonstrate the synthesis and characterization of bimetallic Au-Pd nanocomposite. Bimetallic Au-Pd catalysts are prepared with the use of ascorbic acid as reductant at the various ratios of Au and Pd precursors. The structures and electrocatalytic activities of the bimetallic Au-Pd catalysts are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), cyclic voltammetry (CV), and rotating disk electrode (RDE) voltammetry. This research was supported by Mid-career Researcher Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2011-0015619).

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발표분야: 전기화학

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## Synthesis and Electrochemical Characterization of Silver-Gold Nanocomposites

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이화여대 화학나노과학과<sup>1</sup> 대구대 화학·응용화학과<sup>2</sup> 이화여대 화학과

Fuel cell has attracted much attention in recent years as a new energy system. Better electrocatalysts for oxygen reduction reaction (ORR) are needed to improve the efficiency and to lower the cost of fuel cells. 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 electronic, photonic, and sensing devices. This presentation reports the synthesis and characterization of one dimensional nanocomposites composed of Ag and Au (denoted Ag/Au). Ag/Au nanocomposites are prepared by galvanic replacement reaction between Ag nanowires and Au precursor at various concentrations (1, 10, and 100 mM HAuCl<sub>4</sub>). The structures, morphologies and electrocatalytic activities of these nanomaterials are characterized by scanning electron microscopy (SEM), rotating disk electrode (RDE) and cyclic voltammetry (CV). This research was supported by Basic Science Research

Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education,  
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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A construction of a new redox polymer wiring laccase cathode for the electrocatalytic reduction of O<sub>2</sub>**

강찬 김수정 신호설

전북대 화학과

An O<sub>2</sub> reduction cathode on which laccase enzyme was wired by PAA-PVI-[Os(tpy)(dme-bpy)]<sup>2+/3+</sup> (tpy = 2,2';6,2''-terpyridine ; dme-bpy = 4,4'-dimethyl-2,2'-bipyridyl ) redox polymer was constructed. The redox polymer was newly synthesized for the efficient electron transfer between the laccase redox center and the electrode surface. 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. Electro-reduction of O<sub>2</sub> catalyzed by laccase was measured by rotating disk voltammetry under the condition of pH 5.0 0.2 M citrate buffer and 37 °C. An optimal composition of redox polymer and laccase with the PEGDGE cross-linker content fixed was determined and an optimal loading was also determined. Stability was tested. Another bioelectrocatalyst film containing carbon nanotubes was prepared and a catalytic effect for the O<sub>2</sub> reduction was compared.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Electrochemical reactions of some electroactive biological compounds at carbon nanotube electrodes**

강찬 정혜란 신호설

전북대 화학과

Some biological compounds such as ascorbic acid, catechol, dopamine, and urate playing important roles in biological systems are electrochemically active. Electrochemical analyses of these compounds have difficulties because of the overlapped oxidation potentials, and enhancements of sensitivities are required. Carbon nanotube modified electrodes were prepared by coating oxidatively treated carbon nanotubes and employed for electrochemical reactions of those compounds. In cyclic voltammetric experiments at carbon nanotube modified electrodes, catechol, dopamine, urate showed positive shifts in the oxidation potentials with increases of the currents and, ascorbic acid showed a negative shift of the oxidation potential with a decrease of the current. The results were compared with those at conventional carbon electrodes.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Graphene-Vulcan Carbon Supported Electrocatalysts for Methanol Oxidation

우승희 김하석<sup>1</sup> 정택동 박원철<sup>2</sup>

서울대 화학부 <sup>1</sup>대구경북과학기술원 에너지시스템학과 <sup>2</sup>서울대 융합과학기술대학원 나노융합학과

In this study, we prepared a graphene through a simple chemical oxidation and loaded 40 wt% PtRu onto a graphene-Vulcan carbon composite using an improved impregnation method. Vulcan carbon was added as a nano spacer to enhance the utilization and electrochemical activities of the graphene-based materials. The results show that a PtRu catalyst loaded onto the graphene-Vulcan carbon composite exhibits high electrocatalytic activity and high stability toward methanol electrochemical oxidation owing to the special structure of the graphene-Vulcan carbon composite. In this poster, we will discuss the effect of spacing material between two-dimensional graphene sheets by electrochemical characteristics of methanol oxidation.

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## In situ Electrochemical Quartz Crystal Microbalance Studies on Reaction of Copper, Indium, and Selenium on Molybdenum Quartz

이상민 연유범 최익호 이치우<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

몰리브덴은 전이금속으로 태양전지, 배터리, 반도체, 전기로, 전극 등으로 많은 곳에 응용이 되고 있다. 몰리브덴은 10.22 g/cm<sup>3</sup> 의 밀도와 2610℃의 높은 융점을 가지며 상대적으로 높은 열전도도 (1.38W/CmK) 및 낮은 열팽창계수 (5.43 ppm/K)를 가질 뿐만 아니라 우수한 고온 기계적 특성 등으로 다양한 응용성을 가진 재료이다. 높은 융점과 낮은 음 접촉(ohmic contact) 및 셀레늄(Se) 분위기에서의 고온에 대한 안정성이 요구되는 CuInGaSe(CIGS) 박막의 전극으로 사용하기 위한 재료로도 각광 받고 있다. 본 실험에서는 CIGS 박막 전극을 사용되고 있는 Mo 전극을 이용하여 Electrochemical Quartz Crystal Microbalance(EQCM) 을 통한 Copper, Indium, and Selenium 의 반응을 관찰하였다.

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발표분야: 전기화학

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## 개미산 촉매독 측정을 위한 Iodine 흡착과 RDE system에서 발생

### 하는 촉매독양의 이해

신동완 이충균<sup>1</sup>

충남대 화학과 <sup>1</sup>충남대 화학과, 분석과학기술과

본 실험은 Pt 전극에서 발생하는 촉매독이 각각의 실험 상황에서 어떻게 다른지 이해하고, CA 전류 값이 작은 것이 RDE system 에서 발생하는 촉매독 양과 어떻게 상관 관계가 있는지 이해하는 실험이다. 실험은 Pt 전극에 흡착되어 있는 촉매독이 산화되는 것을 막기 위해 Iodine 을 추가로 흡착하여 진행하였다. 이러한 방법으로 각각 rpm 0 과 1000 일 때의 상황에서 발생하는 촉매독 양을 반복적으로 측정하여 회전하는 전극에 더 많은 electrolyte 가 공급되고 또한 더 많은 촉매독이 발생하여 전극의 활성을 떨어뜨린 다는 것을 확인하였다

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Electrochemical Characterization of $\text{LiMn}_2\text{O}_4$ and $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$ as Cathode for Lithium Ion Battery

한수철 배은경<sup>1</sup> 표명호<sup>1</sup>

순천대 인쇄전자공학과 <sup>1</sup>순천대 화학과

Spinel 구조인  $\text{LiMn}_2\text{O}_4$  양극물질에  $\text{Gd}^{3+}$ 을 doping 하여 Spinel 구조를 갖는  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$ 를 Sol-gel 방법으로 합성하였다. 본 연구에서는  $\text{LiMn}_2\text{O}_4$ 의 단점인 구조적 불안정성을 보완하기 위해서  $\text{Mn}^{3+}$  대신에  $\text{Gd}^{3+}$ 를 도핑하는 연구를 하였다. Cyclic voltammetry(CV)와 galvanostatic charge-discharge cycles test를 통하여 높은 C-rate 및 고온에서  $\text{Gd}^{3+}$ 을 도핑한  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$ 와 도핑하지 않은  $\text{LiMn}_2\text{O}_4$ 의 특성을 비교하였다.  $\text{LiMn}_2\text{O}_4$ 보다  $\text{Gd}^{3+}$ 이 도핑된  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$  ( $x = 0, 0.02, 0.04, 0.08$ ) 양극물질이 더 높은 가역 용량과 뛰어난 구조적 안정성을 갖는다는 사실을 확인할 수 있었다.  $\text{LiMn}_2\text{O}_4$ 의  $\text{Mn}^{3+}$ 를 대신해  $\text{Gd}^{3+}$ 를 도핑 함으로써, 1C와 5C의 초기 용량은 낮아진다. 하지만, 5C에서는 약 10cycle 이후부터  $\text{Gd}^{3+}$ 이 도핑된  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$  ( $x = 0.02$ ) 양극물질의 용량이  $\text{LiMn}_2\text{O}_4$ 보다 높아지는 것을 확인할 수 있었다. 그리고 10C에서는  $\text{LiMn}_2\text{O}_4$ 보다  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$  ( $x=0.02, 0.04$ )의 초기 용량이 더 높게 나왔고 cycling을 반복함에 따라  $\text{Gd}^{3+}$ 이 도핑된  $\text{LiGd}_x\text{Mn}_{2-x}\text{O}_4$ 의 가역용량이 상대적으로 (즉,

$\text{LiMn}_2\text{O}_4$  의 빠른 fading) 더 높아짐을 확인 하였다. 이러한 이유는,  $\text{Gd}^{3+}$ 이 도핑되지 않은  $\text{LiMn}_2\text{O}_4$  의 경우 cycling 중에  $\text{Mn}^{2+}$  이온이 용출 되는데 반해,  $\text{Gd}^{3+}$ 이 도핑된 경우  $\text{Mn}^{2+}$  이온의 용출이 줄어들기 때문이며, 이러한 현상은  $\text{Gd}^{3+}$  양이 높아질수록 뚜렷해 진다. 이상의 결과로부터  $\text{Gd}^{3+}$ 도핑은  $\text{LiMn}_2\text{O}_4$  에 구조 안정성을 부여하며, 이로 인해 높은 C-rate 및 고온에서 향상된 전기화학적 특성을 보이게 됨을 확인하였다.



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## Sol-gel 방법으로 합성한 $\text{LiMn}_2\text{O}_4$ 와 Tb를 도핑한 $\text{LiTb}_x\text{Mn}_{2-x}\text{O}_4$

### $[0 \leq x \leq 0.08]$ 의 전기화학적 특성과 구조

이동균 표명호<sup>1</sup>

순천대 인쇄전자공학과 <sup>1</sup>순천대 화학과

전기자동차와 소형 기기의 전원으로 사용되는 스피넬  $\text{LiMn}_2\text{O}_4$  는 다른 재료들에 비해 가격이 싸고, 열적 안정성이 매우 우수하다. 하지만 이러한 스피넬  $\text{LiMn}_2\text{O}_4$  는 충/방전 중에 Jahn-Teller distortion 에 의한 격자 자체의 변화와 전극/전해질 사이에서 망간이 소멸되어 심각한 용량감소가 일어난다. 본 연구에서는 리튬 아세테이트와 망간 아세테이트 (Tb 아세테이트) 그리고 citric acid 를 사용하여 분말을 만든 후  $450^\circ\text{C}$ 에서 2 시간 동안 열처리를 하고,  $800^\circ\text{C}$ 에서 16 시간 동안 소결하여  $\text{LiMn}_2\text{O}_4$  와  $\text{LiTb}_x\text{Mn}_{2-x}\text{O}_4[0 \leq x \leq 0.08]$ 를 성공적으로 합성하였다. 스피넬  $\text{LiMn}_2\text{O}_4$  의 경우 상온 1C, 5C 에서 높은 초기용량을 (124 mAh/g, 90 mAh/g) 가지나, 충/방전 50 사이클 후에 심각한 용량 감소가(107mAh/g, 63mAh/g) 발생하는 반면, Tb 을 소량 도핑한  $\text{LiTb}_{0.02}\text{Mn}_{1.98}\text{O}_4$  경우에는 비록 1C, 5C 에서  $\text{LiMn}_2\text{O}_4$  보다



낮은 초기 용량을 (117 mAh/g, 108 mAh/g) 가지나, 충/방전 50 사이클 후에는 가역용량이 1C, 5C 에서 111 mAh/g, 104 mAh/g 로  $\text{LiMn}_2\text{O}_4$  보다 더 높은 용량을 보였다. 고온( $60^\circ\text{C}$ )에서 전극퇴화가 빠르게 일어나는 문제점을 가지는  $\text{LiMn}_2\text{O}_4$  의 충/방전 테스트 결과, 알려진 바대로 심각한 용량 감소가 (1C; 130 mAh/g  $\rightarrow$  50 사이클 후 80 mAh/g) 일어났다. 하지만, Tb 을 소량 도핑한  $\text{LiTb}_{0.02}\text{Mn}_{1.98}\text{O}_4$  경우에는  $\text{LiMn}_2\text{O}_4$  보다 고온에서 더 안정한 결과를 보였다. (1C; 118 mAh/g  $\rightarrow$  101 mAh/g) 이와 같이 스피넬  $\text{LiMn}_2\text{O}_4$  에 Tb 을 도핑하여 뚜렷한 전기화학적 특성 향상을 확인하였으며, 구조 분석을 통하여 그 이유를 분석 중에 있다.



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## TMA (Trimesic acid)를 이용한 2차원 구조와 $Zn^{2+}$ 이온과의 결합 에 대한 STM 연구

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충남대 화학과 <sup>1</sup>충남대 화학과, 분석과학기술과

유기 단분자의 패터닝된 2 차원 network 은 손님 분자를 수용함으로써 기능성 부여, 센서 및 유기 전자소재 등을 위한 추가의 표면 변형에 이용될 수 있다. 자기조립 유기 단분자막의 형성은 분자간 수소 결합, 금속-리간드 배위결합 및 van der Waals 힘에 의하여 생성된다. TMA (trimesic acid)는 분자간 수소 결합에 의하여 Au 등의 표면에서 단분자층을 형성한다. 한편,  $Pd^{2+}$ 와  $Cu^{2+}$ 와 같은 금속 이온과의 배위결합을 통하여 2,2'-bipyridine 유도체는 단분자층을 형성하는 것으로 알려져 있다. 따라서 유기 단분자층의 응용을 위해서는 단분자층의 형성에 이용되는 화학결합을 이해하는 것이 필요하다. 본 연구에서는 TMA 자기조립 유기 단분자층에  $Zn^{2+}$  이온을 혼입하여 추후 metal organic framework 의 template 에 사용할 수 있는 가능성을 연구하였다.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Pt/CCG(chemically converted graphene)을 spin-coating방법으로 제조한 dye-sensitised solar cells(DSSC)의 counter electrode 제조

김원지 표명호<sup>1</sup>

순천대 기초의 화학부 <sup>1</sup>순천대 화학과

본 연구에서는 graphene oxide 에 PtNPs 을 화학적으로 합성한 Pt/CCG(chemically converted graphene)을 spin coating 하여 DSSC 의 counter electrode 을 제조하였다. 지금까지 보고된 graphene-modified counter electrode 제조방법으로는 electrophoretic deposition (EPD), transfer 방법(graphene film 을 만든 후 TCO 에 transfer 하는 방법), spin-coating 등이 있다. 본 연구에서는 이 제조방법 중 spin-coating 으로 counter electrode 을 제조했다. Pt/CCG 의 합성 시 Ethylene glycol 은 Pt 이온과 GO 를 모두 환원시키는 환원제로 활용했다. PtNPs 의 형성과 형성된 PtNPs 과 GO 간의 화학적 결합 및 고른 분산은 TEM 과 XRD 를 통해 확인하였다. Pt/CCG 가 spin-coating 된 counter electrode 의 촉매전극 효과를 PtNPs 만 deposition 된 electrode, GO 만 spin-coating 된 electrode 와 비교하기 위해서 I-/I3-의 cyclic voltammogram(CV)를

측정하였다. 그 결과 CV 에서 Pt/CCG 를 spin-coating 한 counter electrode 가 PtNPs 만 deposition 된 electrode 보다 current density 가 더 높게 나왔다. 하지만 electron transfer rate 와 관계가 있는 peak separation( $\Delta E_p$ )은 PtNPs 만 deposition 된 electrode 가 더 작게 나왔다. 앞으로 이것을 개선하기 위해서 더 연구할 계획이다.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Electrochemical Characteristics of Neuroglobin and Application to an Electrochemical Sensor

이영경 김유정 심윤보

부산대 화학과

Despite considerable interest, however, the electrochemical characterization of Neuroglobin (Ngb) is still challenge. In this paper, we report the electrochemical characteristics and electrocatalysis of Neuroglobin on the GCE/AuNPs/poly-TTBA/Ngb. A probe was constructed based on a conducting polymer [poly-2,2':5',2''terthiophene-3'-(p-benzoic acid)](poly-TTBA) formed on the Au nanoparticles; the probe was modified with biomaterials including Ngb, which reveals the direct electron transfer process. Ngb-modified electrode exhibited a pair of quasi-reversible and well-defined redox peaks in 0.1M phosphate buffer solution (pH 7.0) and the electron-transfer rate constants were calculated by Laviron's equation. The characteristics of the Ngb-modified electrode were investigated by cyclic voltammetry, quartz crystal microbalance, impedance spectroscopy and X-ray photoelectron spectroscopy. The applicability of this Ngb immobilized electrode was tested as biosensors. Keywords: Neuroglobin, direct electrochemistry, conducting polymer

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Fabrication of carbon-encapsulated magnetite clusters as an active material for improved Li-ion batteries

오항덕 이상화

경원대 화학생명공학과

이 실험은, 리튬 이온 전지에 사용되어지는 활성 전극의 물질로서 마그네타이트와 탄소의 코어-셸 구조의 복합체를 연구하고 있다. 첫째로, 잘 알려진 공침법으로 citrate 가 싸여있는 마그네타이트 클러스터를 만들었다. 그 다음에, 1,12-diaminododecane 을 이용하여 양쪽의 amine 그룹에 마그네타이트 클러스터의 carboxyl 그룹과 반응하여 일종의 코어-셸 구조를 지니게 된다. 이 생성된 물질을 질소 분위기하에 700 도에서 소결시켜 탄소막이 형성된다. 이 물질의 분석은 SEM (Scanning Electron Microscope), TEM (Transmission Electron Microscope), DLS (Dynamic Light Scattering), XRD (X-ray Diffraction)와 Raman spectroscopy 로 하였으며, 전기적 특성의 결과는 cyclic voltammetry 와 charge/discharge tests 로 도출되어졌다. Keyword: magnetite cluster, core-shell, Li-ion batteries

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Aptamer-functionalized Bioconjugate for Detection of Cancer Cells

Ye Zhu Pranjal Chandra **심윤보**

부산대 화학과

An electrochemical immunosensor was developed using for the detection of breast cancer cells. An aptamer-AuNP bioconjugate was synthesized. A probe was fabricated by covalently immobilizing the monoclonal antibody onto the nanocomposite composed of self-assembled 2, 5-di-(2-thienyl)-1H-pyrrole-1-(p-benzoic acid) (DPB) on AuNPs. In the detection process, antibody-immobilized probe, cancer cell, and the aptamer-AuNP bioconjugate form a sandwich format. The signal was generated and amplified by stripping of the metal labeled to achieve high sensitivity. The modification of the probe was demonstrated by SEM and XPS. The parameters that could affect the response were optimized. The dynamic range was determined between 0.1 pg/mL and 10 ng/mL biomarker with a detection limit of  $0.037 \pm 0.002$  pg/mL. Finally, the proposed strategy was applied to detect breast cancer cells and a detection limit of 26 cells/mL was obtained. Keywords: Immunosensor, Breast cancer; Cell detection; Conducting polymers

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발표코드: ELEC.P-1263

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Conducting polymer bonded collagen-antibody biocompatible matrix for the proliferation and detection of bone cancer cells

Ramjee Pallela Pranjal Chandra 심윤보

부산대 화학과

A collagen-antibody based biocompatible matrix was prepared by the simultaneous immobilization of bone cancer specific antibody and collagen on to the poly(2,2':5',2''-terthiophene-3'-(p-benzoic acid)) (poly-TTBA) electropolymerized layer. The probe layers were characterized by XPS, QCM, and AFM. Electrochemical response of the sensor was compared with and without collagen in terms of cell interfacing and proliferation. Various experimental parameters including pH, temperature, collagen : antibody ratio, and the reaction time were optimized and performance of the sensor was examined. Interaction between the sensor probe and cancer cells was observed with electrochemical impedance spectroscopy and the interference effect was also studied by using other cancer cell lines and normal cells. The strategy described in the present study is very simple and useful for the detection of bone cancer cells in vitro and in vivo.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The cyclic stability of Sn/graphene composite film prepared by electrophoretic deposition for anode of lithium ion batteries**

**배은경 표명호<sup>1</sup>**

순천대 인쇄전자공학과 <sup>1</sup>순천대 화학과

Many metallic systems as anode materials have been applied to lithium ion batteries (LIBs) with the purpose to improve the capacity and energy density. Among them, Sn-based materials also have been extensively studied because of its high specific capacity. However, the cycling performance of Sn is poor due to the large specific volume change during lithiation/delithiation. Graphene of single layer with two-dimensional honeycomb-structure has superior mechanical properties, excellent electrical conductivity, and high surface area. In this work, we prepared Sn/Graphene composite films on a Cu substrate by electrophoretic deposition (EPD) without binders or conductive additives. The thickness of the composites was controlled by concentration, potential, pH, and deposition time. The smooth and well adhered composite films were prepared and used for electrochemical performance test. We are now examining the effect of graphene on the cycling stability of Sn.

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발표코드: ELEC.P-1265

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Influence of Particle Size of Polypyrrole on Electrochemical Performance of Polypyrrole/Activated Carbon Composites**

**김대원 박수진**

인하대 화학과

In this work, polypyrrole has been synthesized by microemulsion polymerization and was used to prepare the polypyrrole/activated carbon (PPy/AC) electrode. Particle size of PPy was controlled using different stirring speeds by homogenizer. The effects of particle size of PPy on electrochemical performance of PPy/AC electrode were investigated. The structural characteristics of PPy were determined by X-ray diffraction (XRD). The surface morphology was characterized by scanning electron microscope (SEM). The thermal properties of PPy were measured by differential scanning calorimeter (DSC). The electrochemical performance of PPy/AC was determined by cyclic voltammetry (CV) and galvanostatic charge/discharge characteristics in 0.5 M H<sub>2</sub>SO<sub>4</sub> electrolyte. As a result, the specific capacitance of PPy/AC was improved with decreasing particle size of PPy. This was probably due to the high surface area and good conductivity of PPy.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Capacitance Performance of Pre-oxidized Petroleum Pitch-based Activated Carbons

김대원 박수진

인하대 화학과

In this work, pre-oxidized petroleum pitch-based activated carbons (ONP-AC) are obtained by the combination of a pre-oxidation at 300°C in oxygen atmosphere and a chemical activation with potassium hydroxide. The effect of pre-oxidation of petroleum pitch as precursor on the electrochemical performances of the ONP-AC was investigated. It was found that micropore volume ratio of ONP-AC was higher than that of the non-oxidized Pitch-based AC (P-AC). In addition, the electrochemical performance including the current density, charge-discharge, and specific capacitance of the ONP-AC was higher than those of P-AC. The highest specific capacitance (357 F/g) of the electrodes was obtained at a scan rate of 0.2 A/g for the ONP-AC compared to 285 F/g for the P-AC. This result suggested that the improved electrochemical performance of the ONP-AC could be attributed to high micropore volume ratio of ONP-AC, resulting from the active site formed by pre-oxidation.

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발표코드: **ELEC.P-1267**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and electrochemical properties of water-soluble Au<sub>25</sub> nanoparticles

곽규주 이동일

연세대 화학과

In recent years, the synthesis and characterization of thiolate-protected gold nanoparticles have drawn broad research interests because of their unusual physical and chemical properties. Au<sub>25</sub> nanoparticles, in particular, have been extensively studied because they are exceptionally stable and exhibit unique electrochemical and optical properties. In this poster, we present the preparation and electrochemical and spectroscopic characterization of Au<sub>25</sub> protected with mercaptopropionic sulfonate (MPS). The MPS-Au<sub>25</sub> nanoparticles were water-soluble, highly monodisperse and their chemical composition was identified as Au<sub>25</sub>(MPS)<sub>18</sub> using electrospray ionization mass spectrometry. The MPS-Au<sub>25</sub> nanoparticles also show the characteristic UV-vis absorption profile and photoluminescence properties. The electrochemical characterization of the water soluble MPS-Au<sub>25</sub> nanoparticles were carried out by transferring them into organic solvent, for example, dichloromethane, using a phase transfer agent. The

phase transferred MPS-Au<sub>25</sub> display the characteristic voltammetry of Au<sub>25</sub>, that is, well-defined voltammetric peaks with large electrochemical HOMO-LUMO gap.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Preparation and Characterization of Platinumium-ruthenium (Pt-Ru) Catalysts Supported on Porous Carbon Prepared from Activated Styrene-acrylonitrile (SAN) Carbon Precursor**

이지한 박수진

인하대 화학과

In this work, the activated styrene-acrylonitrile (SAN)-based porous carbons (ASANs) were prepared by potassium hydroxide (KOH) chemical activation, and used as a carbon precursor to prepare carbon support materials for Pt-Ru alloy nanoparticles. And then, the Pt-Ru supported porous carbon materials as catalyst for direct methanol fuel cells were prepared by ethylene glycol chemical reduction. Transmission electron microscopy (TEM), X-ray diffraction (XRD), and Brunauer-Emmett-Teller (BET) were used to characterize the carbon support materials and the Pt-Ru catalysts. The effects of Pt-Ru alloy content on the electrochemical behaviors of the Pt-Ru supported porous carbon were investigated by cyclic voltammetry (CV).

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장소: 일산KINTEX

발표코드: ELEC.P-1269

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **A study for the toxicity effect of endocrine disruptors on the i-NOS concentration in neuronal cells using an i-NOS immunosensor**

**Pranjal Chandra 노희복 심윤보**

부산대 화학과

The amperometric immunosensor has demonstrated the toxicity of endocrine disruptors (EDs) through monitoring the in vitro i-NOS concentration change, where the antibody of inducible nitric oxide synthase (i-NOS) was immobilized on the conducting polymer?gold nanoparticles composite. The performance of the sensor and the experimental parameters affecting the immunoreaction were optimized. Neuronal cells treated by EDs decreased in the in vitro i-NOS concentration. The effect of bisphenol A (BPA) on the i-NOS concentration released in the cells was investigated with different incubation times, and the interfering by nonspecific binding species present in a neuronal cell lysate was also examined. Of all the tested EDs, BPA showed the inhibitoriest effect and the minimum inhibitory concentration of BPA affecting the i-NOS concentration was  $0.09 \pm 0.005 \mu\text{M}$ . The result shows that monitoring of i-NOS in the neuronal cells treated by EDs will be a useful method to evaluate the toxic behavior of EDs. Keywords: Toxicity; Bisphenol A; Inducible nitric oxide synthase; In vitro immunosensor; Neuronal cells

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Ab initio study of the sodium intercalation and intermediate phases in $\text{Na}_{0.44}\text{MnO}_2$

김희진

KAIST EEWS

The  $\text{Na}_{0.44}\text{MnO}_2$  structure is a promising cathode material for sodium ion batteries due to a high capacity (~130mAh/g) and good cycle performance. In this work, we present the results of density functional theory (DFT) calculations on the structural and electrochemical properties of  $\text{Na}_{0.44}\text{MnO}_2$ , combined with experiments. Seven intermediate phases and the two-phase reactions among them were found, where the calculated voltage profile agreed well with experiments. We found that the S-shaped tunnel is not empty in the deintercalated  $\text{Na}_{0.22}\text{MnO}_2$  structure, but has a partial occupancy of sodium ions. The new sodium sites were found in a limited sodium composition range ( $x=0.44\sim0.55$ ) which is attributed to the electrostatic interactions between sodium ions and manganese atoms. The asymmetric lattice evolution in  $\text{Na}_{0.44}\text{MnO}_2$  as a function of sodium insertion/deinsertion is shown to be due to the Jahn-Teller effects. Based on this interpretation, we suggest that the Cr substitution will reduce the volume change significantly.



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발표분야: 전기화학

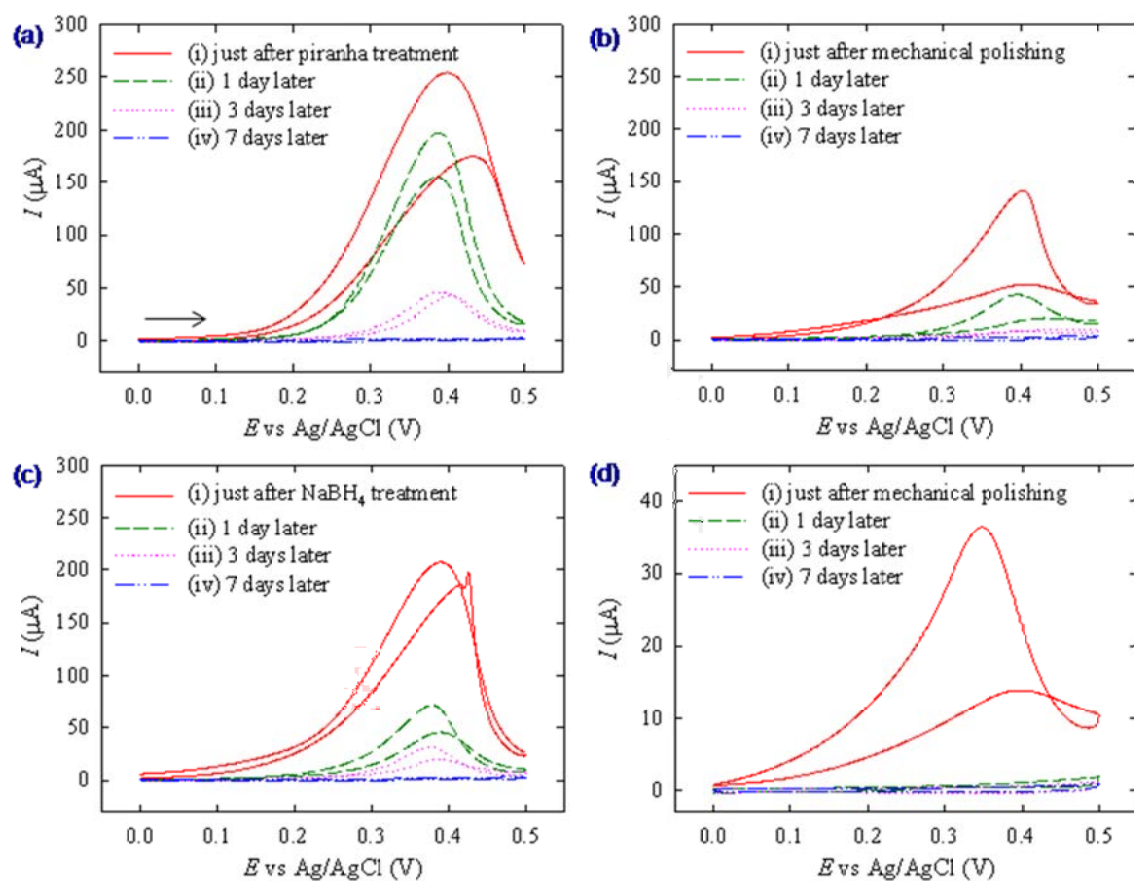
발표종류: 포스터, 발표일시: 수 18:00~21:00

**TIME-DEPENDENT DECREASE IN THE ENHANCED  
ELECTROCATALYTIC ACTIVITIES Observed after Three Different  
Pretreatments OF GOLD ELECTRODES**

이현우

부산대

The enhanced electrocatalytic activities of gold (Au) electrodes observed after piranha treatment, mechanical polishing, or NaBH<sub>4</sub> treatment deteriorate in a similar manner with aging under ambient conditions. The enhanced electrocatalytic activities toward p-benzoquinone reduction and glucose oxidation decrease significantly 7 days after the NaBH<sub>4</sub> treatment, even though there is no significant change in surface contamination during aging. The surface contamination does not seem to be a major factor affecting the decrease in activity with aging. The surface roughness of the Au electrodes is maintained during the NaBH<sub>4</sub> treatment, whereas it changes substantially during the piranha treatment and mechanical polishing.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of Fenton's Reagent on the Electrocatalytic Activity of Gold Nanoparticles

Dutta Gorachand

부산대 화학과

The effect of Fenton's reagent on gold nanoparticles (AuNPs) is investigated using indium tin oxide electrodes modified with electrodeposited AuNPs. The size of AuNPs and their total surface area do not change appreciably during treatment of the electrodes with Fenton's reagent, but the electrocatalytic activities of AuNPs for hydroquinone electrooxidation (and H<sub>2</sub>O<sub>2</sub> electrooxidation) decrease with an increase of the treatment period. This decrease is much more rapid than that occurring when AuNPs age in air, but it is slower than that occurring when bulk Au electrodes are treated with Fenton's reagent. Considering all results and our previous study, the fast deactivation of AuNPs might be due to the fast structural reorganization during treatment of Fenton's reagent.

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발표코드: ELEC.P-1273

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Metal-free Heteroatom Containing Nano-Carbon for Cell Imaging and Electrocatalysis

K.Sudhakara Prasad Ramjee Pallela 최영진 김동민 심윤보

부산대 화학과

We report a facile one-step microwave assisted synthesis of metal-free heteroatom containing photoluminescent carbon nanoparticle (PCNP) and electrocatalytically active nano-carbon (FNC). The as-prepared PCNP showed blue fluorescence under UV exposure and it was successfully used for bio-imaging applications. The PCNP enter into cells without any functionalization and exhibited good biocompatibility and optical properties. The heteroatom containing FNCs were characterized by X-ray photoelectron spectroscopy, transmission electron microscopy, cyclic voltammetry, and rotating disc electrode measurements. The FNC exhibited remarkable electrocatalytic activity towards clinically important biomolecules and oxygen reduction reaction in alkaline media.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and in vitro cytotoxic evaluation of some novel N- butyl Isatins derivatives

S.subba reddy Ramjee Pallela 심윤보

부산대 화학과

A series of novel 1-butyl-3-(phenylimino) indolin-2-ones (3a-h)/N-phenyl-3-(phenyl amino-3H-indol-2-amines (4a-h)/N-phenyl-3-(phenylimino)-3H-indol-2-amines (5a-h) were synthesized and characterized by FT- IR, <sup>1</sup>H & <sup>13</sup>C NMR, mass spectrometry, and elemental analysis. The newly synthesized compounds screened for in vitro cytotoxic evaluation against HeLa (human cervical cancer), SK-BR-3 (human breast adenocarcinoma) and MCF-7 (human breast adenocarcinoma) cells. It was observed from the results that the compounds 3a, 3c, 4a and 4b are showing significant anticancerous activity against HeLa cells than other compounds, and in turn, compound 4a showed highest cytotoxicity (with an IC<sub>50</sub> of  $1.78 \pm 0.16$   $\mu$ g/mL) than all the other compounds. The compound 3a is significantly active against HeLa, SK-BR-3 and MCF7 cells with IC<sub>50</sub> values of  $2.33 \pm 0.49$ ,  $6.18 \pm 0.97$ , and  $5.27 \pm 0.96$   $\mu$ g/mL, respectively. Among all the synthesized compounds, four compounds 5b, 5c, 5d and 5h did not show any cytotoxicity against all the cell lines even at the higher concentrations (100  $\mu$ g/mL).

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발표분야: 전기화학

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## Understanding the Improvement in Electrochemical Performance of Spinel $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ - Graphene Composite as a Cathode Material in LiB

S.J. Richard Prabakar 표명호<sup>1</sup>

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Among the various 5 V spinel  $\text{LiM}_x\text{Mn}_{2-x}\text{O}_4$  cathodes investigated,  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$  has drawn much attention because of its high capacity arising from the operation of  $\text{Ni}^{2+/3+}$  and  $\text{Ni}^{3+/4+}$  redox couples. However a large capacity fade is experienced which is believed to be due to the large lattice strain, low electronic conductivity and due to the corrosion reaction between the cathode surface and the electrolyte. Graphene has excellent electronic conductivity, mechanical properties and high surface area and it can be used as an ideal conductive additive. Graphene was used as a conductive additive to enhance the discharge capacity and rate capability of spinel  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ .  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$  and its composites with graphene (1-10 wt %) were prepared and their structural and morphological features of the prepared composites were investigated with powder XRD, SEM, TEM, and XPS. Characterization techniques depicted single-phase  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$  and the electrochemical studies on the composites by CV,

galvanostatic charge-discharge revealed well-defined redox peaks in contrast to the pristine  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ . Charge-discharge tests performed at different C rates indicated better electrochemical performance of  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ -graphene composite in terms of high discharge capacity, lesser charging time and good cyclic performance compared to  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ . The  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ -graphene composite with a much more stable surface chemistry improved the electrochemical performance significantly by decrease in the charge transfer resistance compared to the bare  $\text{LiNi}_{0.05}\text{Mn}_{1.5}\text{O}_4$ .



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## Facile fabrication of conducting polymer modified membrane with different dopant ions

PIAOHUSHAN

성균관대 화학과

A lot of membrane separation methods were introduced in recent years. Those are size based, charge based, hydrophobicity based separations. In this study, we went to perform a facile fabrication of conducting polymer modified membrane with various dopant ions. These modified membranes will be used for separation propose. 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. Many of dopant ions were adopted in this polymerization process. Conducting polymer with different dopant ions have different electrochemical properties and morphology. Characterizations of the conducting polymer modified membrane were performed with various electrochemical and spectroscopic methods. Those membranes have different properties will be chosen for proper application. 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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발표코드: ELEC.P-1277

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nanoporous Platinum Electrode Fabricated by Electrochemically Alloying-Dealloying Method

조혜진

성균관대 화학과

Platinum is a well known element that shows a significant electrocatalytic activity in many important applications. However, bare platinum electrodes are low sensitivity and poor selectivity in glucose detection. We presented this work that porous platinum electrode decreases such disadvantages. Nanoporous metals having very high surface area have attracted considerable amount of research work, because they have diverse possibilities of application, i.e. catalysis, fuel cells and sensors etc. In this report, we fabricated porous Pt by alloying-dealloying method. First, porous electrode was made of Pt wire which has electrochemically deposited zinc on its surface. Later then, Pt-Zn alloy was dealloyed electrochemically to obtain nanoporous surface structure. We proved that porous Pt is sensitivity by showing response of  $\text{H}_2\text{SO}_4$ , methanol and SEM images. 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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발표코드: ELEC.P-1278

발표분야: 전기화학

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## Various morphology controlled mesoporous carbon materials for anode material in Li ion battery

김민식 유종성

고려대 신소재화학과

In recent decades, Li ion batteries have been considered as a leading candidate for electric/hybrid vehicles and high-end consumer electronic products due to their high electromotive force and high energy density. However, presently many potential Li ion batteries electrode materials are experiencing slow Li ion diffusion and high resistance at the interface of electrode/electrolyte at high charge-discharge rates. Furthermore, rate capability, dominated mainly by the diffusion rate of Li ion and the electron transfer in electrode materials, must be improved considerably. To date, extensive research work has been done to improve transport of Li ion and electron. In order to improve the transport of Li ions within electrode, various nanostructured materials with high surface area, nanoscale size and/or nanoporous structure have been widely investigated. Particularly, nanostructured porous carbon materials have received great attentions. Nanostructured carbon materials have demonstrated good electrode properties in diversified energy storage and conversion systems, such as low temperature fuel cells, hydrogen storage systems,

solar cells, and lithium ion batteries as well. One of these nanostructured carbon materials, ordered mesoporous carbon (CMK-3) has demonstrated greatly enhanced Li storage capacity and/or improved the rate capability compared with commercial graphite anode. In this work, CMK-3 of different lengths was explored as anode in Li ion battery. Compared with the commercial graphite, the various CMK-3 not only demonstrates higher Li storage capacity, but also better cycling performance and rate capability. The enhanced capacity and improved cycling performance and so the rate capability are mainly attributable to the unique structural characteristics such as large surface area and mesopore volume of various CMK-3, facilitating fast mass transport. CMK-3 with different lengths serves as efficient Li storage and buffer reservoir, which not only shortens the diffusion path for Li ions but also reduces volume change during the charge/discharge cycling especially at higher rate.



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발표코드: ELEC.P-1279

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical and structural studies of anion site substituted olivine cathode material

신병철 이영일

울산대 화학과

There has been considerable interest in olivine structure as a cathode active material in Li-ion cells due to its superior cost, safety, stability and low toxicity. The main obstacle is the low electrical conductivity, which makes to use with carbon coating. Anion substitution at the phosphate ( $\text{PO}_4^{3-}$ ) site of the cathode active materials like  $\text{LiMPO}_4$  for lithium ion batteries are attractive to improve electrochemical properties. In this presentation, fluorine substituted  $\text{LiFeMnPO}_4$  will be discussed with studies of electrochemical properties, electrical conductivity, XRD, SEM, etc.

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장소: 일산KINTEX

발표코드: ELEC.P-1280

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and characterization of rodlike CMK-3 with different length

박진솔 김정호<sup>1</sup> 김민식<sup>1</sup> 송민영<sup>1</sup> 양대수<sup>1</sup> 최혁수 유종성<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

The shape and size of well-ordered two-dimensional hexagonal rodlike SBA-15 mesopore silica structure with p6mm space group were controlled by adjusting hydrochloric acid concentration in the range 0.1-5.0 M. The aspect ratio (length vs. diameter) of the rodlike structure was decreased with increasing HCl concentration. However, synthesis of unique SBA-15 structure with aspect ratios of 1 or less is turned out to be very difficult. A novel synthesis route for preparing highly ordered plate-like SBA-15 silica with short mesochannels (150 ~ 350 nm), which have aspect ratio of about 0.2 and large pore diameters up to 12 nm has been developed. In this work, a small amount of Zr(IV) ions along with trimethylbenzene (TMB) as the pore swelling agent was added to the conventional SBA-15 (SBA-15-c) synthesis mixture to prepare platelet SBA-15 (SBA-15-p) materials with expanded 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 a template and phenol as a carbon

source. The shape and size of CMK-3 can be tuned by controlling the morphology of SBA-15 for various specific applications such as fuel cell, lithium-ion battery, capacitor and so on.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Various Faceted Anatase TiO<sub>2</sub> Nano-crystals by controlled etching pH as Li-ion battery anode

최혁수 김민식<sup>1</sup> 유종성<sup>1</sup>

고려대 소재화학과 <sup>1</sup>고려대 신소재화학과

Here we report a facile hydrothermal approach to grow directly anatase TiO<sub>2</sub> nano-crystals (NCs) with exposed (0 0 1) facets on titanium foil substrate by controlling the pH of HF solution. The mechanistic role of HF for controlling growth of anatase TiO<sub>2</sub> crystal facets has been investigated. The results demonstrates that controlling solution pH controls the extent of surface fluorination of anatase TiO<sub>2</sub>, hence the size, shape, morphology, and (0 0 1) faceted surface area of TiO<sub>2</sub> crystals. Anatase TiO<sub>2</sub> crystals with exposed (0 0 1) facets can be directly fabricated on titanium foil by controlling the solution pH  $\leq 5.8$ . When pH was increased to near neutral and beyond (e.g., pH  $\geq 6.6$ ), the insufficient concentration of HF ([HF]  $\leq 0.04\%$ ) dramatically reduces the extent of surface fluorination, leading to the formation of anatase TiO<sub>2</sub> crystals with (1 0 1) facets and titanate nanorods/nanosheets. TiO<sub>2</sub> is studied for rechargeable and recycled energy like Li-ion battery as it is abundant, and low cost material. TiO<sub>2</sub> is also structurally stable during Li-insertion/ extraction and is intrinsically safe by avoiding Lithium

electrochemical deposition. These properties make  $\text{TiO}_2$  particularly attractive for large scale energy storage. Various anatase  $\text{TiO}_2$  NCs made by different pH were directly used as an anode for Li ion battery and shown good cycle performance at even very high charge/discharge rate.





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발표코드: ELEC.P-1282

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Pt?Ru?Co?W quaternary anode electrocatalysts for direct methanol fuel cell**

**권선영 김정호 김민식 양대수 송민영 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, ( $\text{CH}_3\text{OH}$  and  $\text{O}_2$ ) into electrical energy. Oxidation of methanol on Pt catalyst generates CO as an intermediate, which causes the poisoning of the active Pt surface. Thus, it is very important to oxidize CO adsorbed on Pt to  $\text{CO}_2$  to reinstate the catalytic activity of Pt catalyst. 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. In this work, new Pt-based multi-component quaternary Pt-Ru-Co-W alloy electro-catalysts are reported. Pt-Ru-Co-W quaternary alloy system was explored by a robotic dispenser and combinatorial optical screening method, and some active quaternary electrocatalysts were discovered for methanol oxidation in DMFC. The newly developed alloy catalysts were synthesized by several different synthesis methods such as impregnation-

NaBH<sub>4</sub> 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 electrocatalytic activity for methanol oxidation.



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Solid-state NMR study of soft carbon treated with $\text{H}_3\text{PO}_4$ as an anode material of lithium-ion batteries**

이경은 이영일

울산대 화학과

Graphite is commercially used as anode material of lithium ion batteries for portable electronic devices, but some new materials with high capacity have been explored to use for bulk size devices, such as electric vehicle. Soft carbon is an alternative, which has graphene layers neatly stacked but less-long order. Generally, it has excellent high performance, but low discharge capacity and low crystallinity. Recently researchers are being studied mixing-technology of soft carbon and graphite for improving both high capacity and high performance. By addition of phosphorous compounds during preparation provides soft carbon having higher electrochemical properties than that achieved with the conventional carboneous material. Herein, the soft carbon anode materials treated with phosphoric acid have been characterized by using  $^{31}\text{P}$  magic angle spinning (MAS) NMR. From  $^{31}\text{P}$  NMR spectra, it assumed that the two types of P are encapsulated. One may be in the graphite matrix shown broadened peak around 300 ppm and the other in the grain boundary shown strong and sharp peak around 0 ppm.

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발표코드: ELEC.P-1284

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Highly efficient supported PtFe cathode electrocatalysts prepared by homogeneous deposition for proton exchange membrane fuel cell

양대수 김민식 김정호 송민영 유종성

고려대 신소재화학과

A simple and efficient approach has been developed for synthesis of carbon-supported PtFe (50:50) electrocatalyst with high metal loading that combines homogeneous deposition (HD) of PtFe hydroxide complex species through generation of OH<sup>-</sup> ions realized by in situ hydrolysis of urea and subsequent uniform reduction by ethylene glycol (EG) in a polyol process, providing control over the size and dispersion of PtFe nanoparticles (NPs). Compared to PtFe catalysts prepared with other synthesis methods using NaBH<sub>4</sub> and EG and commercial PtFe catalyst, the supported PtFe catalyst prepared by the HD-EG method reveals more uniform homogenous dispersion of PtFe NPs with much smaller particle size, thus demonstrating excellent electrocatalytic ability and fuel cell performance. The structural properties and catalytic activities of Pt-Fe catalysts prepared in various synthesis methods were evaluated on the basis of the analysis of HR-TEM, HR-SEM, XRD, electrochemical surface area and fuel cell polarization performance.

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발표코드: ELEC.P-1285

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Effect of various carbon supported quaternary alloy PtRuIrNi/C catalysts for direct methanol fuel cell

김정호 김민식 양대수 송민영 최혁수<sup>1</sup> 김윤경<sup>1</sup> 권선영 박진솔<sup>1</sup> 박현열<sup>2</sup> 유종성

고려대 신소재화학과 <sup>1</sup>고려대 소재화학과 <sup>2</sup>고려대 세종캠퍼스 소재 화학과

PtRuIrNi quaternary alloy system is explored by a robotic dispenser and combinatorial optical screening method, and some active quaternary electrocatalysts are discovered for methanol oxidation in direct methanol fuel cells (DMFC). In combinatorial screening, the pH change allows one to differentiate active catalysts using fluorescent acid-base indicators. Combinatorial libraries of various nanostructured carbon-supported catalyst compositions containing Pt, Ru, Ir and Ni were screened. The newly developed PtRuIrNi/HCC and PtRuIrNi/CMK-3 catalysts exhibit superior electrochemical catalytic activity and better electrochemical stability toward methanol oxidation than Pt50-Ru50 binary alloy. A catalyst with Pt34Ru30Ir13Ni23 composition found to be the most active, demonstrating an enhancement in the activity of ca. 80 % compared with the commercial binary Pt50-Ru50 Johnson Metthery (J. M.) catalyst. The enhancement of catalytic activity can be explained by bifunctional mechanism, electronic effect, redox process and cooperative synergic effects of hierarchical nanostructures.

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발표코드: ELEC.P-1286

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Pt Nanoparticles Supported on Hollow Mesoporous Carbon as a Catalytic Counter Electrode for Dye-Sensitized Solar Cell**

송민영 김민식 김정호 양대수 박진솔<sup>1</sup> 유종성

고려대 신소재화학과 <sup>1</sup>고려대 소재화학과

Dye-sensitized solar cells (DSSCs) have attracted extensive attention as a highly efficient and environment friendly power generator due to their simple fabrication process and abundance of renewable solar energy. Counter electrode used in DSSC is generally Pt, which is very expensive and has limited natural resources on earth. Therefore, developing a practical and cost-effective alternative to minimize the Pt usage has been a research priority and is being extensively investigated for future development of DSSCs. In this work, highly dispersed Pt nanoparticles (NPs) supported on hollow mesoporous carbon (HMC) are explored as counter electrode in DSSC. Superior structural characteristics of HMC including large specific surface area and mesoporous volume, enable HMC to have highly enhanced catalytic activity toward the reduction of I<sup>3-</sup>, and to have considerably improved photovoltaic performance. The DSSC fabricated using Pt NPs supported on HMC as a counter electrode showed enhanced power conversion efficiency compared with that of the conventional Pt-based DSSC and HMC-based DSSC

under  $100\text{mW3cm}^{-2}$ , AM 1.5G sunlight illumination. The improvement of Pt/HMC counter electrode can be ascribed to interesting synergistic effect between Pt NPs and HMC, which helps to disperse Pt NPs homogeneously on the HMS with small particle size.



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발표코드: ELEC.P-1287

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **An aptamer biosensor for the detection of cardiac biomarker, B-type natriuretic peptide**

**구현우 이정봉 윤종해 차근식 남학현 신재호**

광운대 화학과

B-type natriuretic peptide (BNP) consisting of 32 amino acids is secreted by the ventricles of the heart in response to excessive stretching of heart muscle cells (e.g., cardiomyocytes). The level of BNP in blood is highly correlated with both the severity of symptoms and the prognosis in congestive heart failure. Therefore, BNP is one of the most important biomarkers to diagnose heart failure. The method to detect BNP has been well-known for immunoassay using antibodies. However, antibody is thermally unstable, and thus its utility in the immunosensor fabrication has been hindered. Moreover, production and purification of antibodies are costly and time-consuming. To overcome such disadvantages, immunosensors based on the use of aptamers as a new molecular recognition element have recently received tremendous attention. In comparison with antibodies, the aptamers (oligonucleic acid or peptide molecules) directly bind to a wide range of target molecules. Furthermore, they are more stable to biodegradation, easy to obtain, and adaptable to modification. Herein, we report on a new approach to



design an electrochemical aptamer sensor based on the label-free detection of BNP by utilizing ferrocene (Fc)-modified silica nanoparticles. The binding of target protein (i.e., BNP) to aptamer leads to change the electrochemical signal by blocking the access of the Fc-modified silica nanoparticles to the electrode surface. In this way, we investigate the utility of BNP aptamer sensor to determine BNP concentrations in biological samples (i.e., serum and blood).



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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **The Study on the Cyclability of Cobalt Oxide with Copper Nanowire as Anode for Lithium-Ion Batteries**

하성민 김원배

광주과학기술원 신소재공학부

Conversion-type active materials of transition metal oxides have been considered as attractive materials for Li-ion batteries due to larger capacity relatively. But the materials have major drawbacks such as large irreversible capacity and low energy efficiency. Many researchers have been studied to overcome these drawbacks through introducing nanostructured active materials and additives. In this work, we propose a novel structure of nanostructured conducting additive in active material for LIBs and investigate how change performance with nanostructure and the loading amount of active materials via sputtering. We introduce directly grown copper nanowires which have an average of ca. 80nm diameter and 3  $\mu\text{m}$  length on copper substrate vertically and densely via indirect vapor phase method and reduction.  $\text{Co}_3\text{O}_4$  as active materials which have the theoretical capacity of 890mAh/g is sputtered on them with various mass to confirm the loading amount effect.  $\text{Co}_3\text{O}_4$ /copper nanowires composites improve at least 25% compared with ordinary cobalt oxide anode after 50 cycles through the discharge-charge analysis with the

amount of 0.470mg approximately. Such enhanced property may be associated with nanoscale-modified electrode that has large surface area and strong facile stress stability. These advancements could be affected by increased reaction sites, faster charge transport, decreased electrochemical double-layer capacitance, and easy stress relaxation. Also, as the amount change of active materials, we expect they may effects on the kinetics of cell reaction. Because active materials deposited with the film morphology via sputtering, their actual contact area with conducting additives and electrolyte related with electron and lithium-ion conduction change with respect to loading amount. Therefore, Lower amount of them may increase their kinetics. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 20110016600 (Mid-career Researcher Program)), by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. R15-2008-006-03002-0), and by the Global Frontier R&D Program on Center for Multiscale Energy System funded by the National Research Foundation under the Ministry of Education, Science and Technology, Korea. (0420-20110157)



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발표코드: ELEC.P-1289

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation of ITO electrodes modified with functional materials and their electrochemical properties

백그린 S. Senthil Kumar<sup>1</sup> Lee Sera<sup>2</sup> 전철호 이동일

연세대 화학과 <sup>1</sup>Nanomaterials laboratory in India <sup>2</sup>Organo transition metal catalysis - hybrid materials laboratory in U.S.A

A facile method for the preparation of modified indium tin oxide (ITO) electrodes and their use in amperometric sensing of H<sub>2</sub>O<sub>2</sub> are described. ITO surface was first derivatized by acid-catalyzed grafting of N-hydroxysuccinimidyl-ester-functionalized methallylsilane at room temperature, followed by immobilization of functional materials such as gold nanoparticle and thionine by amide coupling reaction. The modification process was monitored using contact angle, scanning electron microscopy and electrochemical measurements, which revealed the controllability and high efficiency of this modification method. Thionine-modified ITO electrode exhibited excellent electrocatalytic activity towards the reduction and amperometric determination of H<sub>2</sub>O<sub>2</sub>, demonstrating the potential of this immobilization strategy in electrocatalysis and amperometric sensing. In addition, we present the preparation and characterization of aligned ZnO nanorods grown on ITO electrodes.

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발표코드: ELEC.P-1290

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Real-time monitoring nitric oxide and oxygen levels in myocardial ischemia and reperfusion injury in rat heart

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In recent years, endogenously produced nitric oxide (NO) has been studied broadly because of its role in numerous physiological processes including vasodilator, angiogenesis, neurotransmission, and phagocytosis. Nitric oxide is produced from L-arginine and oxygen (O<sub>2</sub>) by nitric oxide synthases (NOSs) in vivo. Since endogenously generated NO has been implicated in the control of O<sub>2</sub> consumption, it may be essential to monitor O<sub>2</sub> levels during NO measurement in physiological milieu. Nitric oxide and oxygen gas sensors based on the electrochemical techniques possess several advantages, including easy miniaturization, high sensitivity, and simple microfabrication for in vivo measurement. These characteristics are suitable for measurement in biological systems. However, the electrooxidation of NO requires a relatively high working potential (+0.8 V vs. Ag/AgCl); thus, other readily oxidizable biological species interfere selective detection of NO. Biofouling (initiated by protein adsorption) at the sensor's interface is another problem associated with biological measurement of in NO and O<sub>2</sub>. The

electrode surface is then modified with a xerogel membrane to improve the selectivity and prevent protein adsorption. It is well-known that amorphous and hydrophobic perfluoropolymers are highly permeable to various gaseous species including NO and O<sub>2</sub>. Applying a perfluorinated xerogel-derived gas permeable membrane is allowed to develop an amperometric NO sensor with dramatically improved selectivity, while maintaining high NO permeability. Herein, we demonstrate the utility of the perfluorinated xerogel-modified microsensor to monitor NO and O<sub>2</sub> levels in myocardial ischemia and reperfusion injury in vivo. The measurement reflects co-dynamic relationships between NO and O<sub>2</sub> contents in rat heart.



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## “Push-Pull” organic sensitizers for Dye-Sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) have been investigated extensively since Gratzel and coworkers reported a high solar energy-to-electricity conversion efficiency of >10%. Ruthenium complex dyes have actively been used to develop high efficiency DSSCs. However, metal free organic sensitizers have recently been received much attention due to their low-cost and high molar extinction coefficient while they do not need to use the precious metals that are in limited source. Furthermore, the organic dyes are easy to design to absorb selective solar spectral regions, and to synthesize with simple purification. In this study, push-pull structured  $\pi$ -conjugated organic sensitizers which contain triphenylamine moieties as a electron donor and cyanoacetic acid moiety as a electron acceptor are synthesized to prepare high efficiency DSSCs. Hierarchically structured TiO<sub>2</sub> (HS-TiO<sub>2</sub>) that are known to have enhanced electron diffusion coefficient and long lifetime are used as a photoelectrodes of DSSCs. The resulting DSSCs display the power conversion efficiency (PCE) of 6.38% under standard AM 1.5G sunlight (100mW/cm<sup>2</sup>)

with short circuit photocurrent density (JSC) of 11.73 mA/cm<sup>2</sup>, open circuit voltage (VOC) of 0.82 V and fill factor of 66%.





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## Highly sensitive mercury detection based on aptamer-thrombin interaction and enzymatic reaction

고현준 김규원

인천대 화학과

We present a highly sensitive detection of mercury(II) ions using thrombin and thrombin aptamer. Thrombin is a protein that plays many roles in the coagulation cascade-converting soluble fibrinogen into insoluble strands of fibrin as well as catalyzing many other coagulation-related reactions. Aptamers are oligonucleic acid or peptide molecules that bind to a specific target molecule. Aptamers are usually created by selecting them from a large random sequence pool. The aptamer folds into three-dimensional structures upon the exposure to target protein, which allow them to bind a specific protein. As a thrombin aptamer short single-stranded oligonucleotide including thymine (T)-rich sequence was employed in this study. Exposure of thrombin aptamer-modified surface to mercury ion(II) converts flexible aptamer into hairpin structure due to the formation of T-Hg<sup>2+</sup>-T pairs, which makes it difficult for thrombin to interact with aptamer. The estimation of the quantity of thrombin bound on the resulting surface will be

demonstrated by using various methods such as cyclic voltammetry, electrochemical impedance spectroscopy, surface plasmon resonance spectroscopy, and coagulation reaction of thrombin.



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## Graphene-based electrochemical detection of biomolecules

정한울 박혜진 김규원

인천대 화학과

In electrochemical biosensor applications, graphene, graphene oxide and reduced graphene oxide have usually been used as a platform for probe immobilization or an electrocatalyst for enhancing electrochemical signal. In this presentation we demonstrate graphene oxide as an electrochemical indicator as well as a platform of probe biomolecules, to probe target biomolecules such as DNA and protein. Bare gold film electrode was treated with mercaptopropionic acid to prepare negatively charged surface. A positively charged polymer was attached on the resulting surface through an electrostatic interaction. To immobilize graphene oxide, the positively charged polymer-immobilized gold electrode surfaces was exposed to graphene oxide solution. The graphene oxide-attached surface was modified with a probe DNA oligomer. We used the modified surfaces to detect target biomolecules such as thrombin. The electrochemical properties of graphene oxide were dependent upon the concentration of target biomolecules.

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## **Dopamine Detection Using Poly(dopamine) Formation on Bare Indium-Tin Oxide Electrode in the Presence of the Ascorbic Acid**

**김병권 양해식<sup>1</sup> 곽주현**

KAIST 화학과 <sup>1</sup>부산대 화학과

Dopamine is neurotransmitters which is important and widely investigated for the several decades. A deficiency of dopamine is associated with some physiological problems such as Parkinsonism, schizophrenia, and HIV infection. Therefore, the determination of the dopamine concentration is essential for disease diagnosis and for the study of physiological mechanisms. Dopamine can be easily electrooxidized owing to its high electroactivity. However, its selective detection in actual biological matrixes is limited by interfering molecules such as ascorbic acid. To solve these kinds of problems, various kinds of modified electrodes were suggested. These kinds of modified electrodes were showed good performance, but needed specific treatments and materials. Indium?tin oxide (ITO) electrodes have been widely used in displays and solar cells due to their high levels of optical transparency and conductivity. ITO electrodes have also been used in electrochemical sensors in an effort to utilize their low and reproducible capacitive background currents. The low electrocatalytic activities of ITO

electrodes are significantly increased after the modification of ITO electrodes with electrocatalytic materials. This change allows for facile discrimination between two states before and after the modification process. We present a sensitive electrochemical method capable of detecting dopamine in the presence of ascorbic acid. This method employs the spontaneous formation of electrocatalytic poly(dopamine) films on bare ITO electrodes in a solution of dopamine. The electrooxidation current of hydrazine is used for the determination of the dopamine concentration.



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## Synthesis of CdSe-ZnO and au-ZnO Composite by a Galvanic Replacement Reaction followed by Photoinduced Cathodic Deposition

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건국대 응용화학과

ZnO/CdSe composite was prepared via a combination of three techniques including electrodeposition, galvanic replacement and photoinduced cathodic deposition. ZnO nanowire arrays were electrodeposited on ITO or polycrystalline Au electrode and metallic zinc co-deposited with ZnO was galvanically replaced with Se in  $\text{Se}^{4+}$  containing aqueous solution, which resulted in ZnO/Se composite nanowire arrays. Then, Se in ZnO/Se composite was photoelectrochemically reduced to  $\text{Se}^{2-}$  when light was illuminated on the ZnO/Se composite, which reacted with  $\text{Cd}^{2+}$  in the electrolytes to produce ZnO/CdSe composite. The amount of metallic zinc increased with decrease of deposition potential, which was investigated with combined electrochemical quartz crystal microgravimetry with linear sweep voltammetry. The shape of electrodeposited ZnO nanowire arrays were maintained after galvanic replacement or light illumination, therefore ZnO/Se or ZnO/CdSe had the shape of nanowire arrays. ZnO, ZnO/Se, ZnO/CdSe were characterized by SEM, EDX and XRD. Photoelectrochemical experiments

revealed that electrodeposited ZnO nanowire arrays showed n-type semiconductor, which changed to p-type after deposition of Se. ZnO/CdSe composite showed anodic photocurrent upon light illumination which indicated n-type character. This study provides a facile method for the synthesis of CdSe sensitized ZnO composite photoelectrodes. Synthesis of Au-ZnO Composite is same reaction. First, Zn/ZnO electrode is deposited on the ITO electrode by electrodeposition. And then, Zn/ZnO electrode is soaked in solution included  $\text{Au}^{3+}$  ion. in that case Zn is substituted to Au by Galvanic Displacement Reaction. Created electrode is confirmed XRD, SEM, EDX, UV-VIS spectrometer.



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## Study of properties of silica sol-gel film prepared on electrode surface by electrochemical method

강호석 이호춘<sup>1</sup> 곽주현

KAIST 화학과 <sup>1</sup>대구경북과학기술원 에너지시스템공학

Silica sol-gel film was prepared on indium tin oxide (ITO) electrode by electrochemical method. The hydroxyl ions generated by negative potential initiated condensation process of hydrolyzed sol solution containing aqueous silica precursor on electrode surface. Silica deposited and formed porous film on electrode surface. As silica precursors, tetraethylorthosilicate (TEOS) and tetramethylorthosilicate (TMOS) were investigated. The thickness and porosity depending on the species of silica precursor and electrochemical treatment were demonstrated by electron microscope and electrochemical analysis. Cyclic voltammetry (CV) of  $\text{Fe(CN)}_6^{3-/4-}$  and  $\text{Ru(bpy)}_3^{2+/3+}$  redox reactions was conducted and ion permeability of silica film was analyzed.



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## Electrodeposition and Compositional Analysis of $\text{Cu}_2\text{Se}$ Thin films

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건국대 응용화학과 <sup>1</sup>고려대 신소재화학과

Combined stripping voltammetry and electrochemical quartz crystal microgravimetry were employed for the compositional analysis of electrodeposited copper selenide thin films. Electrodeposited films contain free Cu and free Se in addition to the targeted  $\text{Cu}_2\text{Se}$  compound and the amount of these “impurity” phases depends on the electrodeposition variables. Thus the free Se content was determined using the reduction peak of Se to  $\text{Se}^{2-}$  obtained during the cathodic scan of films in 0.1 M  $\text{Na}_2\text{SO}_4$  blank electrolyte. The Se content obtained during the cathodic stripping of  $\text{Cu}_2\text{Se}$  to  $\text{Cu} + \text{Se}^{2-}$  was used for the determination of  $\text{Cu}_2\text{Se}$  content using the assumption of 2:1 compound stoichiometry. Finally, the total Cu content was obtained from the anodic scan and the free Cu content was calculated from the difference between total Cu and the Cu present in  $\text{Cu}_2\text{Se}$ . The compositional assays thus obtained from the combined use of stripping voltammetry and EQCM are presented as a function of electrodeposition potential.

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## Enhancement of photocurrent of p-type $\text{Cu}_2\text{O}$ by platinum deposition

채상윤 최종호 주오심<sup>1</sup>

고려대 화학과 <sup>1</sup>KIST 청정에너지센터

$\text{Cu}_2\text{O}$  is one of the best materials as a p-type semiconductor for photochemical application because of its band gap and band edge. Unlike other p-type semiconductors,  $\text{Cu}_2\text{O}$  can be easily prepared by electrodeposition method. In this study, platinum was deposited on  $\text{Cu}_2\text{O}$  by photodeposition. The photocurrent of  $\text{Cu}_2\text{O}$  was enhanced by platinum in aqueous condition. Effect of hole scavenger during photodeposition also was investigated. Scanning Electron Microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Linear sweep voltammetry technique were conducted to characterize  $\text{Cu}_2\text{O}$  films.

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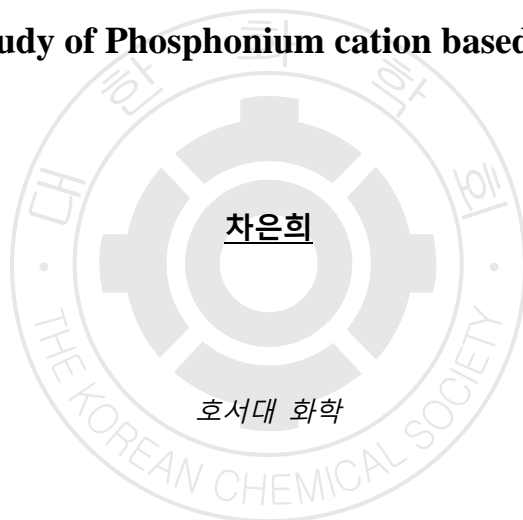
장소: 일산KINTEX

발표코드: ELEC.P-1299

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## Corrosion study of Phosphonium cation based Ionic Liquid



Tetradecyl trimethyl phosphonium bis(2-ethyl hexyl) phosphate was synthesized and analyzed to determine their characteristics and properties. The low conductivity and high viscosity(424.7mpaS) of Tetradecyl trimethyl phosphonium bis(2-ethyl hexyl) phosphate were exhibited. Phosphonium cation based ionic liquids (ILs) have become of interest due to their unique chemical and electrochemical stability as well as their promising tribological properties. At the same time, interest has also grown in the use of phosphate based ionic liquids for corrosion protection of reactive metals. In this paper, corrosion behavior on Al current collector was tested at room temperature. Tetradecyl trimethyl phosphonium bis(2-ethyl hexyl)phosphate is a good protecting candidate of Al corrosion was measured. Key words: Tetradecyl trimethyl phosphonium bis(2-ethyl hexyl) phosphate, corrosion, Al, ionic liquid

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발표종류: 포스터, 발표일시: 수 18:00~21:00

**Highly sensitive and selective detection of dopamine at  
poly(chromotrope 2B) modified anodized glassy carbon electrode in  
the presence of uric acid and high concentration of ascorbic acid**

**LIXIAOBO**

건국대 응용화학과

A polymerized  $\pi$ lm of chromotrope 2B was prepared on preanodized glassy carbon electrode (GCE) in neutral buffer solution by cyclic voltammetry (CV), and the electropolymerization mechanism of chromotrope 2B was proposed. The poly(chromotrope 2B)  $\pi$ lm-coated GCE exhibited excellent electrocatalytic activity towards the oxidation of dopamine (DA) in the presence of uric acid (UA) and high concentration of ascorbic acid (AA). The electrochemical oxidation signals of DA, UA, and AA were well resolved into three distinct peaks with peak potential separations of 172, 132 and 304 mV between AA-DA, DA-UA, and AA-UA in differential pulse voltammograms (DPVs), respectively. A linear range of 1 to 40  $\mu$ M and a detection limit of 40 nM were observed in pH 7.0 phosphate buffer solutions (PBS). Moreover, the poly(chromotrope 2B) modified electrode efficiently eliminated the interference of UA and a high concentration of AA in the determination of DA with high sensitivity, selectivity, and good reproducibility. The modified electrode was also successfully applied for the

determination of DA in human urine samples with satisfactory results. The proposed method provides a significant method for selective detection of DA from the interferences by AA and UA.



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## Recovery of rhodium(III) from wastewater coupled with power generation using a microbial fuel cell

최찬수

대전대 응용화학과

A recovery efficiency as high as 98%-99% of Rh(III) from wastewater was achieved for initial concentrations from 50 ppm to 200 ppm while generating electric power after 40 hours reactions in the catholyte containing 1 M KCl at pH 2. A maximum power of 2.44 W/m<sup>2</sup> cathode area with a fill factor of 0.675 was achieved in the 500 ppm Rh(III) (as [RhCl<sub>6-n</sub>(H<sub>2</sub>O)<sub>n</sub>]<sup>n-3</sup>) catholyte solution. The Cl<sup>-</sup> ion concentration in the catholyte greatly affected the formation of different rhodium ion species and the performance of MFC.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Electrochemical Sensor for Underwater Biofilm Detection using Amperometry

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Biofouling causes many problem in industrial processes, medical health industries and our daily life. Detecting of bacterial infection on the surfaces is very important to prevent those problems. In this study, we suggest an electrochemical sensor for detecting biofilm. It was investigated the current change of electrochemical sensor by increase of biofilm. As a result, it was observed that the decrease of the current occurs by the biofilm grew on the surface of electrochemical sensor compared to the sensor without biofilm on the surface. We expect that this work can be applied for water service utilities.

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## Spectroscopic and electrochemical characteristics of carboxylated graphene manganese oxide nanocomposites

박경원 정종화

경상대 화학과

Graphene oxide-COOH - $\text{Mn}_2\text{O}_3$  (GO-COOMn) composites grown  $\text{Mn}_2\text{O}_3$  nano-wire onto graphene sheets by a one-step thermal method using graphene oxide-COOH (GO-COOH) and  $\text{Mn}(\text{NO}_3)_2$ . The graphene oxide (GO) prepared by Hummer's method using graphite flakes was used as a starting material. The GO-COOH sheets were synthesized by GO and chloroacetic acid ( $\text{Cl-CH}_2\text{-COOH}$ ). The GO, GO-COOH and GO-COOMn were characterized by XRD, AFM, SEM, TEM, FT-IR,  $^{13}\text{C-NMR}$ , and Raman spectroscopy. The electrochemical performances of the GO-COOMn supercapacitor were tested by cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge-discharge tests. The results show that the asymmetric supercapacitor has electrochemical capacitance performance within potential range 0 ~ 0.7 V. The supercapacitor delivered a specific capacitance of  $\sim 300 \text{ F g}^{-1}$  at a current density of  $50 \text{ mA/cm}^2$ . This method provides an easy and straightforward approach to deposit  $\text{Mn}_2\text{O}_3$



nano-wire s onto the graphene sheets, and may be readily extended to the preparation of other classes of hybrids based on GO sheets for technological applications.



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## 중등화학교사 임용시험 출제경향 분석연구

하동수 이강범 김민아<sup>1</sup>

순천대 화학교육과 <sup>1</sup>순천대 화학교육

본 연구는 질 높은 교사를 임용하기 위하여 2008년 9월 30일에 고시된 2009학년도 개정안의 시행에 대해 개정안의 실시배경과 개정된 사항, 개정안의 세부 항목을 파악하여 개정안 시행 여무를 확인함으로써 임용시험을 준비하고 있는 예비 화학교사에게 정보를 제공하여 임용시험을 준비하는 데에 도움을 주기 위해 진행되었다. 현행 중등 화학교사 임용시험을 연도별로 전공영역교과목 출제 문항 수와 배점을 분석하였고, 2009년도 개정을 기준으로 잡아 전·후의 각 교과목 별 세부 영역을 분석하였다. 그리고 출제 비율과 미출제 영역을 비교·분석함으로써 개정안 시행에 따른 변화를 연구하였다.

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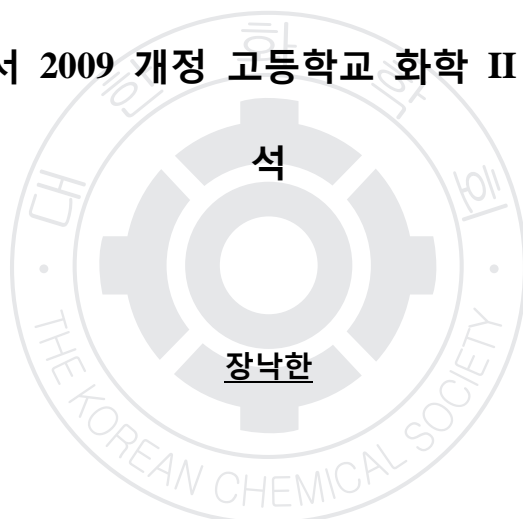
장소: 일산KINTEX

발표코드: EDEC.P-1305

발표분야: 초중등교사 · 화학교육

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## 열역학적 관점에서 2009 개정 고등학교 화학 II 교과서에 대한 분



공주대 화학교육과

2009 개정 고등학교 화학 II 교과서를 열역학적 관점에서 분석하고, 엔탈피, 엔트로피 및 깁스 자유 에너지에 대한 개념 도입과 연계 과정을 분석하였다. 2009 개정 화학 II에서는 기존의 7 차 교육과정 교과서와 달리 처음으로 엔트로피와 자유 에너지를 다루는 반응의 자발성 영역이 도입되었다. 또한 7 차의 화학 II 교과서에서는 화학 평형을 반응속도론적으로 다루는데 반해, 2009 개정 화학 II에서는 화학 평형을 열역학적 관점에서 다루고 있다. 그러나, 처음으로 도입된 엔트로피가 에너지 개념이 아닌 무질서도 개념으로 도입되어 자유 에너지와 연계성이 부족하며, 그 결과 자유 에너지 변화를 통한 화학 전지를 설명하는데 어려움이 있다. 따라서 엔트로피에 대한 개념을 도입할 때 에너지 관점에서 다양한 사례를 보여주고 이를 활용할 수 있는 예를 설명할 필요가 있다고 생각된다.

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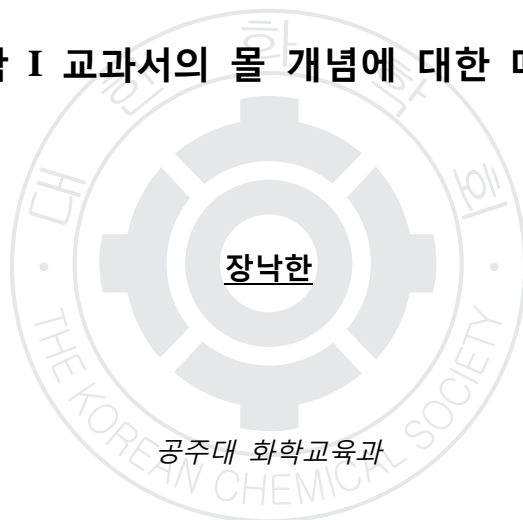
장소: 일산KINTEX

발표코드: EDEC.P-1306

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 2009 개정 화학 I 교과서의 물 개념에 대한 메타인지적 분석



2009 개정 화학 I 교과서 4 종에서 물 개념 학습에 필요한 메타지식인 원자, 분자, 전자, 이온 등의 입자적인 지식과 원자량, 분자량, 화학 반응식 등의 화학 반응적인 지식에 대한 기술 및 연계성을 조사하고 분석하였다. 대부분의 교과서에서 원자와 분자의 입자적 개념에 의해 물의 개념을 기술하기 보다는 화학 반응식에서 양적인 관계에 의한 정의적 개념으로 물의 개념을 기술하였다. 이것은 학생들에게 물이 화학 양론의 기본적인 개념이 아닌 변환적인 지식으로 생각할 수 있도록 할 수 있다. 따라서 교사가 물의 개념을 지도할 때 학생들의 이해를 돕기 위해 입자적 개념을 도입하여 수업을 진행하는 것이 필요할 것으로 생각된다.

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발표코드: EDEC.P-1307

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## SSC(Small-Scale Chemistry) 실험 수업이 성별에 따른 과학 불안 및 실험활동에 대한 태도에 미치는 영향

유미현

아주대 교육대학원

SSC(Small-Scale Chemistry) 실험이 국내에 도입된 지도 10 여 년이 되었다. 그 동안 여러 가지 SSC 실험이 개발되어 학교 현장에 적용되었으며, SSC 실험 수업의 적용 효과에 관한 연구도 다양하게 이루어지고 있다. 그러나 SSC 실험 수업의 효과가 성별에 따라 어떻게 달라지는지에 대한 연구는 거의 이루어지지 않았다. 본 연구에서는 고등학교 2 학년 자연계열 남학생 학급과 여학생 학급을 대상으로 4 주간 화학 I 물 단원에서 SSC 실험 수업을 실시하고 성별에 따른 효과의 차이를 비교 분석하였다. SSC 실험 전후 과학진로지향도, 과학 불안도, 과학실험 활동에 대한 태도 검사를 실시하였다. 얻어진 데이터는 공변량 분석(ANCOVA)을 통해 분석하고, 그에 따른 연구 결과를 논의하였다.

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발표코드: EDEC.P-1308

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 고등학교 화학실험 수업에서 자기조절 학습 전략이 과학탐구 능력, 과학적 태도 및 학업성취도에 미치는 효과

정시화<sup>1</sup> 곽옥금<sup>1</sup> 김봉곤<sup>1</sup> 박종근<sup>1</sup>

경남과학고 교무기획부<sup>1</sup> 경상대 화학교육과

본 연구는 과학계고등학교 11학년 ‘산화-환원’ 단원에 대해 자기조절 학습전략을 활용한 실험수업을 실시한 후, 과학탐구 능력, 과학적 태도 및 학업성취도에 대한 교수-학습 효과를 분석하였다. 통제집단에 대해 교과서 및 교사용 지도서에 따라 실험수업을 실시하였으며, 실험집단에 대해서는 자기조절 학습전략을 활용한 실험수업을 실시하였다. 사전 검사에서 두 집단 간에 유의미한 차이가 없었으나, 사후검사에서 실험집단의 평균값이 유의미하게 높았다.

‘산화-환원’ 단원에 대해 자기조절 학습전략을 활용한 실험수업을 처치한 후, 자기조절 학습 전략에 대한 변화의 사후 검사에서는 유의미한 차이가 약간 나타났다. 그러나 행동조절 학습요소에서 두 집단 간에는 유의미한 차이가 없었다. 과학탐구 능력에 대해 두

집단사이에 유의미한 차이가 약간 크게 나타났다. 추리 및 예상 등 기초탐구능력에서 두 집단사이의 차이는 없었다. 반면, 통합탐구에서 실험집단의 평균값이 약간 높게 나타났으며, 변인통제에서 가장 크게, 나머지 세부요소에서는 비슷하게 나타났다. 전체적인 결과에 대한 경향성은 각 모둠마다 비슷할지라도, 절대값 차이가 약간 발생하였다. 자기조절 학습과 과학탐구 능력 사이에 상관성이 유의미하게 나타났으며, 동기조절, 행동조절 및 인지조절 중 두 변인 간에 상관성을 나타내었다. 동기조절이 높은 상관관계를 보였다. 인지조절이 과학탐구 능력과 가장 낮게, 특히 메타인지 요소는 더 낮은 상관관계를 나타내었다. 과학적 태도에서 두 집단 간에 평균값의 차이가 약간 유의미하게 나타났다. 신중성과 협동성에서 비교적 크게, 자진성에서 적게 평균점 차이가 나타났다. 자기조절 학습 전략과 과학적 태도 사이에 유의미한 상관관계가 나타났으며, 인지조절 전략이 과학적 태도와 가장 큰 상관성을 나타내었다. 그 다음으로 동기조절과 행동조절 순으로 나타났다. 과학적 태도의 하위변인에서 ‘계속성’, ‘객관성’ 및 ‘호기심’이 자기조절 학습과 가장 높게 상관성을 나타내었다. 학업성취도에 대해 실험집단의 평균점수가 약간 높게 나타났다. 자기조절 학습과 학업성취도 사이에 유의한 상관성이 나타났으며, 학업성취도와 인지조절이 가장 높게, 그 다음으로 동기조절과 행동조절이 유의미한 상관관계를 나타내었다.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## ‘디자인적 사고 과정’ 기반 STEAM 과학교육 모형 개발 연구

이도현 강성주

한국교원대 화학교육과

이 연구의 목적은 ‘디자인적 사고 과정 기반 STEAM 과학교육 모형’을 개발함으로써 학생들의 융합적 · 창의적 사고 신장을 증진시키려는 것이다. 따라서 문헌연구를 통해 디자인적 사고의 개념을 정립하고, STEAM 과학교육에 적용 방안 모색하여 ‘디자인적 사고 과정 기반 STEAM 과학교육 모형’을 도출하였다. 도출된 모형을 토대로 ‘디자인적 사고 과정 기반 STEAM 과학교육 프로그램’을 개발하기 위해 초 · 중등 교육과정을 분석하고 학교 현장에서의 활용도를 높일 수 있는 소재를 선정하여 프로그램을 개발하였다. 이와 같은 모형을 활용함으로써 과학, 기술·공학, 미술, 수학의 내용의 융합을 통해 흥미를 증진시키는 것 뿐 만 아니라, 사고과정의 융합을 통해 학생들은 융합에의 필요성을 느낄 수 있어 보다 효과적인 STEAM 교육이 가능할 수 있을 것으로 기대된다.



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발표코드: EDEC.P-1310

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 중학생이 작성한 자유 탐구 보고서의 특징과 탐구 수행에 대한

### 학생들의 인식

김인환 차정호 박미현

대구대 과학교육학부

이 연구에서는 대구 지역 중학교 2학년 165 명이 작성한 자유 탐구 보고서를 주제 영역, 탐구 가설, 그리고 탐구 변인의 측면에서 분석하였다. 여름방학이 시작되기 전 2 시간 동안 오리엔테이션을 진행하면서 탐구 과정에 대해 소개하고, 주제를 탐색하도록 하였다. 여름방학 동안 학생들은 주제 선정, 실험설계 및 수행, 자료 수집 및 분석, 결과 보고서 작성 등의 과정을 스스로 진행하였다. 여름방학 후, 결과보고서를 제출받으면서 학생들이 주제 선정에서 활용한 자료의 출처, 가설의 정의, 그리고 탐구 과정에서 가장 어려운 단계에 대한 인식도 조사하였다. 보고서의 주제 영역은 물리, 화학, 생물, 지구과학, 생활 영역으로, 보고서에 기술된 가설은 예측 가설과 설명 가설로 분류하였고 가설의 정의에 대한 학생들의 인식과 비교하였다. 탐구 주제, 탐구 가설, 실험 설계 부분에 제시된 탐구 변인을 분석하여

범주형, 연속형, 불확실 유형으로 분류하였다. 연구 결과, 주제 영역 중 화학 영역의 보고서가 가장 많았고, 다음으로 생물과 생활 영역이 많았다. 전체 165 개 보고서 중 130 개에 탐구 가설을 포함하고 있었는데, 이들 중 대부분은 예측 가설에 해당하였다. 보고서에 제시된 탐구 변인을 분석한 결과, 탐구 주제와 탐구 가설에 기술된 독립 변인과 종속 변인은 불확실 유형이 많았다. 그러나 실험 설계 부분에 기술된 변인들은 불확실 유형이 많이 줄어들었고, 범주형 변인이 증가하였다. 탐구 수행 과정에서 가장 어려운 단계에 대한 질문에 학생들은 주제 선정 단계를 가장 많이 선택하였다.



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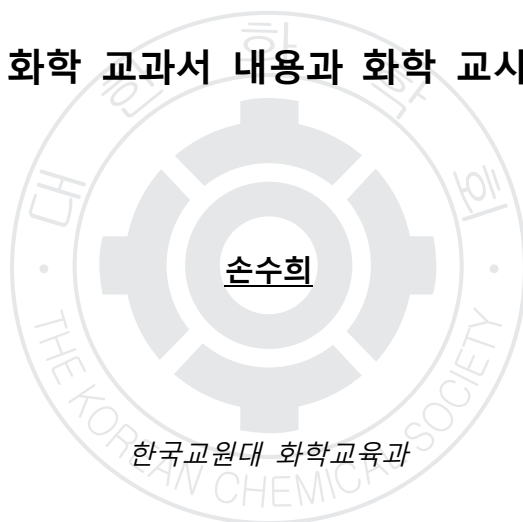
장소: 일산KINTEX

발표코드: EDEC.P-1311

발표분야: 초중등교사 · 화학교육

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## 강산에 대한 화학 교과서 내용과 화학 교사의 이해 분석



이 연구에서는 중등학교 화학 교사 50 명을 대상으로 강산의 이온화도와 세기, 이온화 상수에 대한 이해 정도를 알아보고, 개념 형성의 주된 근거가 무엇인지를 설문과 면담을 통하여 알아보았다. 그리고 교수요목기의 교과서부터 2009 개정 교육과정 화학Ⅱ 심의용 교과서까지의 서술 내용을 5 개국의 외국 교과서, 일반화학·분석화학 및 유기화학 등 대학 교재, 화학 자료집 등의 서술 내용과 비교·분석하였다. 연구 결과, 대부분의 화학 교사들은 강산의 이온화도와 이온화 상수에 대해 이해 정도가 매우 낮았고 이온화도와 이온화 상수 값이 호환되지 않는 현상에 대해 혼란스러워 하고 있었다. 교과서 서술 내용 오류는 첫째로 강산의 이온화도를 지나치게 낮게 제시하고 있었다. 대부분의 교재에서는 강산은  $\text{H}_3\text{O}^+$ 보다 산의 세기가 커서 수용액에서 100% 이온화되는 산으로 정의하고 있었는데 화학 교과서에서는 0.1 M, 25℃에서 강산의 이온화도를  $\text{HCl}$ -0.94,  $\text{HNO}_3$ -0.92,  $\text{H}_2\text{SO}_4$ -0.62 등으로 제시하였다. 둘째로 강산의 이온화 상수 값을 잘못 제시하고 있었다. 강산은  $\text{H}_3\text{O}^+$ 보다 산의

세기가 크므로 그 종류와 무관하게 물속에서 평준화 효과에 의해 산의 세기가 같아진다. 그러나 화학 교과서에서는 별다른 부연 설명 없이 제시한 강산의 이온화 상수( $\text{HCl}$ -107,  $\text{H}_2\text{SO}_4$ -102,  $\text{HNO}_3$ -20)를 그대로 믿는다면 강산의 평준화 효과와 모순되기에 과학적으로 신빙성 있는 자료로 보기 어렵다. 이러한 결과로부터 화학 교사들이 강산에 대해 올바른 개념을 가지기 위해서는 화학 교과서에 보다 정확하고 검증된 자료가 수록되어야 하고 교사들의 오개념을 과학자적 개념으로 수정하기 위한 화학 교사의 재교육이 필요함을 알 수 있다.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 초등교사와 학생의 과학 학습 평가에 대한 인식 비교

강석진

전주교육대 과학교육과

이 연구에서는 과학 평가에 대한 초등학교 교사와 학생의 인식을 조사하고 비교했다. 전라북도 소재 초등학교에서 173 명의 교사와 초등학교 6 학년 학생 183 명이 연구에 참여했다. 과학 평가에 대한 인식 검사는 35 개의 리커트 문항으로 구성했는데, 교사용과 학생용의 두 종류로 제작했다. 평가에 대한 인식 검사는 학습 내용과의 일치, 현실성, 학생의 참여, 투명성, 다양성 등의 5 가지 하위 범주로 구성했다. 교사와 학생의 성별, 교사의 교육 경력, 교사의 최종 학위 등과 같은 배경 변인도 조사했다. t-검정 결과, 평가에 대한 인식 검사에서 교사의 점수가 학생에 비해 유의미하게 높았고, 그 차이는 학생의 참여와 투명성 범주에서 두드러졌다. 남교사가 여교사에 비해 평가에 대한 인식 검사 점수에서 유의미하게 높았고, 그 차이는 학생의 참여, 투명성, 다양성 범주에서 두드러지게 나타났다. 그러나 교사의 교육 경력이나 교사의 최종 학위에 따른 차이는 유의미하지 않았다.

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발표코드: EDEC.P-1313

발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 과학교사의 현직 교사교육과 멘토링에 관한 인식 및 요구조사

남정희 이동원<sup>1</sup> 고미례<sup>2</sup>

부산대 화학교육과 <sup>1</sup>부산대 대학원 과학교육과 화학교육전공 <sup>2</sup>부산대 과학교육과 화학교육  
전공

교사의 교수실행에 있어서의 전문성 발달이 교육의 질적 향상과 결부됨은 더 이상의 논의가 필요 없으며, 교사의 지속적인 전문적 신장은 학생들에게 수준 높은 교수를 제공하는 확실한 방법이 될 것이다. 교사 전문성 발달을 위한 새로운 교사교육 방법의 하나로 1980년대 이후 광범위하게 논의되고 있는 것이 바로 멘토링(mentoring)이다. 그러나 단순히 멘토링 제도만의 도입으로는 그 효과를 기대하기 어렵다고 볼 수 있다. 특히 문화적·사회적 배경이 다르고 교사들의 인식론적 배경도 서양과는 다른 우리나라 학교상황에 대한 고려 없이 도입 적용되는 멘토링 프로그램은 좋은 효과를 기대하기 어렵다고 볼 수 있다. 따라서 멘토링이 교사의 전문성 신장을 위한 주요 방안으로 모색되고 있는 시점에서, 공교육기관에서 초임교사 뿐만 아니라 지원을 필요로 하는 경력교사를 위한 멘토링 프로그램을 설계하여 운영하는데 필요한 지적 토대를 마련할 연구들이 수행되어야 한다고

본다. 이 연구에서는 이러한 멘토링 프로그램의 개발에 앞서 현직 교사들의 현직 교사연수 프로그램 및 멘토링 관련 요구조사를 실시하여 그 결과에 대한 분석을 토대로 새로운 멘토링 프로그램을 개발하였다.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 중등 과학영재교육에서 초임 교사의 수업 전문성 제고 전략으로

### 씨의 멘토링 적용 사례연구

노태희 강석주 강훈식<sup>1</sup>

서울대 화학교육과 <sup>1</sup>춘천교육대 과학교육과

이 연구는 중등 과학영재교육에서 초임 교사의 수업 전문성 제고 전략으로써의 멘토링 적용에 관한 사례연구로, 멘토링 과학영재수업의 특징을 수업 계획, 수업 진행, 수업 평가, 멘토링 적용 후 단계로 나누어 분석했다. 한 명의 멘토와 두 명의 멘티를 선정한 후, 멘티별로 중등 과학영재수업 중에서 총 3 회에 걸친 9 차시의 수업에 대해 멘토링을 실시했다. 모든 수업을 관찰했고, 수업 촬영 동영상과 수업 자료, 멘토링 및 면담 녹음 자료, 참관 노트 등을 분석했다. 연구 결과, 멘토링 과학영재수업의 특징으로 수업 계획 단계에서는 좀 더 체계적인 과학영재수업 구성, ‘과학영재수업=약간 어려운 실험수업’이라는 도식의 탈피와 다양한 교수전략 도입, 과학영재교육 프로그램 개발에 대한 심리적 부담감에 영향, 과학영재수업 준비 시간의 증가 등이 나타났다. 수업 진행 단계의 특징으로는



과학영재수업의 질 향상, 수업 진행에 대한 심리적 부담감에 영향, 수업 진행의 혼선 초래 등이 있었다. 수업 평가 단계의 특징은 수업에 대한 심도 깊은 반성 기회 제공, 실제적인 수업 개선의 동력 제공으로 분류할 수 있었다. 멘토링 적용 후 단계의 특징으로는 멘티의 과학영재수업에 대한 자신감 증가, 멘토의 수업 전문성 및 멘토링 기술 일부 향상 등이 나타났다.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 중등 과학영재교육에서 코티칭을 통한 초임 교사의 수업 전문성 변화에 관한 사례연구

노태희 양찬호 김영훈 강석주 강훈식<sup>1</sup>

서울대 화학교육과 <sup>1</sup>춘천교육대 과학교육과

이 연구는 중등 과학영재교육에서 코티칭을 통한 초임 교사의 수업 전문성 변화에 관한 사례연구로, 그 변화 과정을 PCK 측면에서 심층적으로 조사했다. 과학영재교육 경력 5년 미만인 초임 교사 2인을 선정하여 총 3회에 걸친 9차시의 과학영재수업을 공동으로 계획, 진행, 반성하도록 했다. 두 교사들의 모든 코티칭 수업을 참관했고, 수업 촬영 동영상과 수업 자료, 대화 및 면담 전사본, 반성일지, 관찰노트 등을 지속적 비교 방법을 사용하여 분석했다. 연구 결과, 다소 제한되기는 했지만 코티칭 경험을 통해 두 교사들의 과학영재 교육과정, 과학영재 교수전략, 과학영재교육 평가, 과학영재학생, 과학내용에 관한 실천적 지식이 긍정적으로 변화하는 것으로 나타났다. 이런 결과는 과학영재교육에서 코티칭이

초임 교사의 수업 전문성을 제고하는 데 유용할 수 있음을 시사하며, 그 효과적인 활용 방안을 모색하는 데 실질적인 시사점을 제공할 수 있다.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Analysis of the Cause of Students' Misunderstanding About the Law of Definite Proportions Experiment and Improving the Experimental Equipment by Measuring the Mass

김순근

경기과학고 화학생명과학부

In the 7th national science curriculum of 9th grade, we generate lead iodide to explain the law of definite proportions. However, most of high school students were not able to understand the law by using current method. Thus, we tried to identify why students couldn't understand it properly by an experiment, and concerned about new method to understand the law by an experiment. Following the reference, we observed the change which might occur when potassium iodide aqueous solution is added into lead nitrate aqueous solution. As excess lead potassium iodide solution was added in to lead nitrate aqueous solution, the state of the deposit in the solution has been changed. Also, we tried to make a new experimental equipment which can measure a mass of deposit rather than a volume of that. The mass of the deposit was measured accurately by using 0.2  $\mu\text{m}$  syringe filter and 10mL syringe. By this research, we learned why

students was not able to understand the law, and, because it is possible to explain the law of definite proportions by the concept of the mass, students could understand it more easily and accurately.



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발표분야: 초중등교사 · 화학교육

발표종류: 포스터, 발표일시: 수 18:00~21:00

## 교육과정 수시 개정에 따른 과학 교과 물질 영역의 학습 내용 중

### 복 및 누락 분석

김정수 김현경<sup>1</sup> 차정호<sup>2</sup> 조형훈<sup>3</sup>

인천만수고 과학부 <sup>1</sup>한국교육과정평가원 교육평가본부 <sup>2</sup>대구대 과학교육학부 <sup>3</sup>정의여자고 3  
학년부

이 연구는 과학 교과 물질 영역을 배우는 초등학교 및 중학교 학생들이 교육과정 수시 개정으로 서로 다른 교육과정을 경험하게 되면서 교과 필수 학습 요소가 중복되거나 누락되는 경우를 교육과정 이행 유형에 따라 분석하였다. 연구 결과에 의하면 2001 학년도부터 2012 학년도까지 초등학교에 입학하는 학생들은 세 가지 유형으로 교육과정의 변화를 겪고 있다. 유형 A는 제 7 차 교육과정으로 과학을 배우기 시작한 학생들이 2009 개정 교육과정에 따른 교과 교육과정으로의 변화를 경험하는 학생들로 2001~2003 학년도에 초등학교에 입학한 학생들이 이 유형에 해당한다. 유형 B는 제 7 차 교육과정으로 과학을 배우기 시작한 학생들이 2007 개정 교육과정으로의 변화를 경험하는

학생들로 2004~2007 학년도에 초등학교에 입학한 학생들이 이 유형에 해당한다. 유형 C 는 2007 개정 교육과정으로 과학을 배우기 시작한 학생들이 2009 개정 교육과정에 따른 교과 교육과정으로의 변화를 경험하는 학생들로 2008~2012 학년도에 초등학교에 입학한 학생들이 이 유형에 해당한다. 각 유형별 물질 영역의 교과 필수학습 요소의 이행 과정을 비교하여 교육과정 개정으로 인해 교과 필수학습 요소를 중복 학습하거나 누락하게 되는 경우를 찾아내었다. 이러한 연구 결과는 교육과정 수시 개정 체제에서 교육과정 개정 시기를 결정하거나 교육과정 수시 개정에 따른 학습 결손 보충 자료를 개발하는데 시사하는 바가 클 것으로 기대한다.



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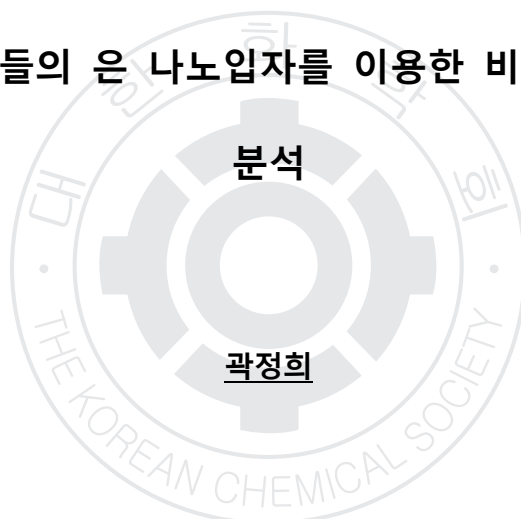
장소: 일산KINTEX

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발표분야: 초중등교사 · 화학교육

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## 고등학교 탐구자들의 은 나노입자를 이용한 비타민 음료의 성분



대진고 교무기획부

현대의 과학 교육은 과학의 기본 개념과 아울러, 논리적 사고와 창의성 개발을 위해 학생들이 스스로 탐구할 수 있도록 하는 일련의 과정을 중요시하고 있지만, 현재 우리 과학교육 여건은 다인 수 학습이라는 제약과 입시 준비 교육의 풍토 등 많은 장애 요인으로 실제적인 과학 탐구교육이 이루어지지 못하는 실정이다. 따라서 본 연구는 학생들이 스스로 기구를 다루며 구체적 경험을 하게끔 하여 탐구하는 과정에서 실험설계, 가설설정, 자료분석, 추리, 결론유도 등 형식적 사고의 신장을 도울 수 있는 과정을 경험하게 하여 과학 하는 방법과 사고과정을 배우는 것, 즉 과학적 탐구능력 증진을 목표로 하였다. 과학적 탐구 능력이 많은 과학 학습 프로그램에서 강조되고 있는 이유도 바로 탐구과정을 통해서 과학적 사고를 신장시킬 수 있을 뿐만 아니라, 지식을 획득하게 되고, 또 그를 통해서 과학적 태도를 기를



수 있기 때문이다. 학생들은(사봉준, 국원준, 이산하, 김현일, 류석수, 정상진, 정명훈, 남궁준-이상 8 명 1 학년, 선지웅-2 학년) 은 나노입자를 흡착한 샤프심 전극을 이용하여, 시중에 판매되는 비타민 음료에서의 ascorbic acid 를 전기화학적 방법으로 정량하는 연구를 진행하였다. 전극은 간단한 공정인 액상 환원법으로 제조하였는데, 이는 은 이온( $\text{Ag}^+$ ) seed 를 샤프심에 형성한 후  $\text{NaBH}_4$  를 첨가하여  $\text{Ag}^+$  을 환원시켜 은( $\text{Ag}^0$ )으로 형성시키고, 여분의  $\text{BH}_4^-$ 이 은 나노입자를 둘러싸게 되어 정전기적 반발에 의해 안정한 형태가 되는 방법이다. 이렇게 형성된 전극은 단위부피당 큰 표면적을 가지고 있어 높은 전기화학적 감응 능력을 보인다. 전기화학은 전기적인 측면과 화학적인 측면을 관련 지어 연구하는 화학의 한 분야로써, 주로 산화-환원 반응으로 인한 전기적 에너지의 발생에 대해 다루기 때문에 학생들의 이해가 용이한 분석 방법이다. 사용한 검출 방법은 cyclic voltammetry 를 사용하였고, 이는 조작이 쉽고 간단하여 고도의 기술이 필요하지 않으며 전기적인 신호를 단시간에 얻어낼 수 있다는 데 장점이 있다. 학생들은 본 연구를 통해 은 나노입자를 이용한 전극의 제조 기술과 원리에 대해 흥미를 갖고 주도적으로 참여하여, 평소 의구심을 가졌던 비타민 음료 속의 ascorbic acid 을 전기화학적 검출 방법으로 정량하고 결과를 도출하는 과정에서 탐구의 중요성을 깨달았으며 과학적 사고와 태도 및 탐구능력을 향상할 수 있었다.



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## 광합성 실험에서 BTB 지시약의 변색에 대한 예비 교사의 인식

조사 및 실험 개선

윤희숙

강원대 과학교육학부

광합성은 생명현상을 파악하고 생물을 학습하는데 기본적인 개념으로 여러 차례의 교육과정의 개정에도 불구하고 과학과 교육과정에서 꾸준히 제시되고 있다. 특히 중학교 2학년의 ‘광합성에 필요한 물질’, ‘광합성과 호흡의 기체 교환’ 영역에서는 광합성과 호흡에서의 이산화탄소의 출입을 BTB 용액의 변색을 통해 확인하도록 하고 있다. 그러나 광합성 실험에 대한 중고등학생들의 실험 과정 이해도를 조사한 연구(문경원, 김선수, 2008)에 의하면 상당수의 학생이 BTB 용액의 색깔 변화를 이산화탄소의 농도 변화와 관련하여 이해하는 것을 어려워하고 있으며, BTB 용액의 변색에 대한 의문과 색깔 관찰에 대한 어려움 등을 가지고 있는 것으로 보고되고 있다. 즉, 실험을 통해 생명현상인 광합성과 호흡을 이해하기 위해서는 실험상황에 대한 화학적 이해가 바탕이 되어야 함에도 불구하고,

이산화탄소가 녹은 용액의 액성과 BTB의 색변화에 대한 화학적 이해가 어렵다는 것이다. 광합성 실험은 생명현상을 이해하기 위한 것이지만 이산화탄소가 녹은 용액의 액성과 BTB의 색변화에 대한 화학적 이해가 필요한 생물과 화학의 통합적 실험이라고 할 수 있다. 따라서 화학적인 관점으로 기존의 광합성 실험에서 BTB 용액의 변색과 관련된 문제들을 분석해보고, 개선점을 제안할 필요가 있다. 이러한 맥락에서 본 연구에서는 BTB 용액의 색변화에 대한 예비교사 또는 교사의 인식을 조사하여 광합성 실험에서 BTB 용액의 변색과 관련한 실험의 문제점을 파악하고, 이의 개선을 위한 실험을 제안하고자 한다.



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## Study of Evaporation of Sulfur Mustard on Various Substance Materials

정현숙

국방과학연구소 화생방부

Sulfur mustard (bis(2-chloroethyl)sulfide, abbreviated HD) is a blister chemical agent to form blisters on exposed skin, which is regulated under the 1993 Chemical Weapons Convention (CWC). Environmentally, HD persists for 4 years after it is deposited in soil. While it remains in soil, some HD is adsorbed and degraded. Others are re-evaporated into air, which can cause a lethal problem to human and environment. However, there is very little known in open literature regarding how HD is evaporated upon deposition. Here we studied the evaporation characteristics (initial evaporation rates and process) of a sessile drop of HD on various substance materials such as glass, stainless steel, and aluminum. We use a laboratory-sized wind tunnel, gas chromatograph mass spectrometry, and drop shape analysis. It was found that the initial evaporation rates of HD increased from stainless steel and aluminum to glass. The evaporation process will be discussed based upon data from drop shape analysis.

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## The Photovoltaic Performance with gel electrolytes for Dye-sensitized solar cells

이경주

현대하이스코 환경에너지연구팀

Dye-sensitized solar cells (DSSCs) have attracted great interest in the last decade and are anticipated to be a potential alternative to silicon-based solar cells. High-efficient DSSCs with conversion efficiency up to 11% have been achieved using a liquid electrolyte containing triiodide/iodide redox couple. However, the volatile nature of the organic solvents (e.g., acetonitrile and 3-methoxypropionitrile) used in the liquid electrolytes triggers the leakage and evaporation of the solvents under long-term use. Therefore, critical sealing techniques are required in assembling the liquid-type DSSCs. To solve these drawbacks, several attempts have been taken by replacing the liquid electrolytes with gel-type polymer electrolyte, room temperature ionic liquid, hole-transporting materials based on organic or inorganic semiconductors, and liquid electrolytes solidified by cross-linked gelators. However, the energy conversion efficiencies of DSSCs using these materials are lower than that achieved by the liquid electrolyte, ascribed to the lower conductivity of charge in the solid and gel electrolytes compared to that in the liquid electrolyte. Among

various alternatives for liquid electrolytes, polymer gel electrolyte (PGE) appears to have superior properties in terms of ionic conductivity and cell performance. For the PGE, the liquid electrolyte was trapped in a polymer matrix. Although the polymer network may hinder the ion transfer, the ions can move freely in the cages of polymer network which is helpful to the ion conductivity of a PGE. For the practical application of PGEs, the high viscosity of gel-electrolytes makes it difficult for them to penetrate into the pores of mesoporous  $\text{TiO}_2$  electrodes. In this study, we prepared gel type polymer electrolytes. We analyzed the characteristics of gel electrolyte with the different amount of the polymer materials in electrolytes. The measurement was carried out after the open circuit voltage was stabilized.



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발표분야: 환경에너지

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## Effect of KOH Activation on Carbon Dioxide Capture Behaviorsof Mesoporous Carbons Synthesized from One-pot Method

유혜민 박수진

인하대 화학과

In this work, we prepared the activated mesoporous carbons (A-MCs) *via* chemical activation with KOH/MCs ratios in a range of 1:1 to 1:4. Mesoporous carbons (MCs) have been prepared by the one-pot method which is the organic-organic self-assembly using resorcinol and triblock copolymer Pluronic F127. The textural properties of the A-MCs were investigated by N<sub>2</sub>/77 K adsorption isotherms using a Brunauer-Emmett-Teller (BET) equation. The structural properties of the A-MCs were measured from X-ray diffraction (XRD). The CO<sub>2</sub> capture behaviors were measured by CO<sub>2</sub> isothermal adsorption at 298 K and 30 atm. From the results, it was found that the KOH/MCs ratios have a major influence on CO<sub>2</sub> capture behavior, resulting from the specific surface area and total pore volumes of A-MCs.

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## Synthesis and Characterization of Dual-pore Carbons for Carbon Dioxide Adsorption

유혜민 박수진

인하대 화학과

In this work, we prepared the dual-pore carbons (DPCs), containing mesopores synthesized by templating method co-exist with micropores formed by pyrolysis, in order to investigate the relationship between meso/micropore volume ratio and CO<sub>2</sub> adsorption. The textural properties were investigated by N<sub>2</sub>/77 K adsorption isotherms. The structural properties were measured from transmission electron microscopy (TEM) and X-ray diffraction (XRD). The CO<sub>2</sub> adsorption behaviors were measured by CO<sub>2</sub> isothermal adsorption at 298 K and 1 atm. Consequently, the CO<sub>2</sub> adsorption capacity was strongly affected by microporosity of DPCs, resulted in the enhancement of CO<sub>2</sub> adsorption capacity.



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## Influence of Dissolved Organic Ligands on the Reactivity of Nano Zero Valent Iron(nZVI) for persistent explosive compounds degradation

송시욱 김동욱

육군사관학교학교 화학과

나노 입자에 대한 연구는 현재 모든 분야에서 가장 주목받고 있는 연구분야 중의 하나이다. 환경분야에서도 나노소재를 사용한 수처리 또는 토양오염처리가 큰 관심의 대상이다. 이중 가장 각광을 받고 있는 소재는 영가철로 비소, chlorinated organic contaminants(e.g., TCE and PCE), explosive nitroaromatic compounds(e.g., TNT, modified nitrobenzene, and RDX 등)의 다양한 오염물질과의 반응성이 매우 높을 뿐 아니라 친환경적이며 상대적으로 처리비용이 저렴한 장점 등을 가지고 있어 오염물 제거를 위한 가장 좋은 물질중의 하나로 사용되어 왔다. 나노영가철(nZVI)은 기존의 영가철(ZVI)에 비해 반응성이 월등하고 필요한 경우 지하의 오염원에 직접 주입하여 깊은 심도에 존재하는 오염물질을 처리할 수 있는 장점이 있고, 표면적이 다른 영가철(ZVI)에 비해 수십 배에서 수백 배까지 넓어 오염물과 접촉하는 면적이 늘어나게 되면서 다른 영가철(ZVI)의 반응성과 비교할 경우 처리효율이 높다. 하지만 나노영가철(nZVI)은 입자 표면에 형성되는 산화철 피막에 의해 반응성이 감소되는

문제점이 제시되어 왔었다. 본 실험에서는 RNIP(Core : nZVI, Shell : 산화피막)의 반응성 및 반응정도에 유기리간드가 미치는 영향에 대해 조사하였다. RNIP 존재하 반응 속도와 반응정도가 대조군의 반응 속도와 반응정도에 미치는 영향이 리간드의 종류에 따라 달랐으며, 또한 pH 에 따라 달라지는 것을 확인하였다. pH 변화에 따른 반응성 및 반응정도의 변화를 포스터에서 토의될 예정이다.



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## Behavior of cationic cetylpyridinium chloride adsorption on pyrite surface in variety of pH ranges

배성준 이우진

KAIST 건설 및 환경공학과

Adsorption mechanism of cetylpyridinium chloride (CPC), a cationic surfactant, on pyrite surface was identified in variety of pH ranges in this study. The adsorption capacity increased as the pH increased 5 to 7 and decreased as it increased 7 to 9. At pH 5 and 6, zeta potential ( $\zeta$ ) of pyrite suspensions showed increasing positive values (i.e., 5 to 13.5 mV at pH 5 and 8.12 to 22 mV at pH 6) as CPC adsorption proceeded, which indicated that hydrophobic adsorption of CPC is predominant in the pyrite suspensions at this pH range. At pH  $\geq 7$ ,  $\zeta$  changed from negative to positive value (i.e., -5 to 36 mV at pH 7, -10 to 30 mV at pH 8, and -15 to 20 mV at pH 9), indicating that both hydrophilic and hydrophobic adsorptions were responsible for CPC adsorption on pyrite surface at pH 7-9. The adsorption mechanism of surfactant on pyrite can be used to the development of adsorption technologies to clean surfactants in groundwater in the broad pH range and applied to the operation of effective pyrite Fenton system to treat surfactant-washed wastewater after soil washing process.

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## Reaction mechanism study in catalytic nitrate reduction with maghemite supported bimetallic catalyst

정준영 배성준<sup>1</sup> 이우진<sup>1</sup>

KAIST 건설및환경공학과 <sup>1</sup>KAIST 건설환경공학과

We have verified reaction mechanism of catalytic nitrate reduction by bimetallic catalyst (Cu/Pd) supported with maghemite (Maghemite/Cu/Pd). Scanning electron microscopy/energy dispersive X-ray spectroscopy and transmission electron microscopy analysis were conducted to characterize morphology of Maghemite/Cu/Pd and distribution of Cu and Pd on maghemite surface. Maghemite/Cu/Pd exhibited remarkable nitrate reduction efficiency (100%) in 90 min under constant supply of hydrogen gas (100 cc/min). Selectivity of nitrogen gas was 43% while selectivity to nitrite and ammonium were 3% and 54% respectively. X-ray photoelectron spectroscopy (XPS) analysis was carried out to investigate the changes in oxidation state of Cu and Pd on maghemite before and after catalytic nitrate reaction. Cu(0) was oxidized to Cu<sub>2</sub>O and CuO during the reaction while Pd(0) did not change. Reaction mechanism of catalytic nitrate reduction revealed via XPS was that nitrate reduction to nitrite was coupled with

oxidation of Cu(0) and nitrite reduction to nitrogen gas or ammonium was induced by hydrogen adsorbed on active site of Pd(0).



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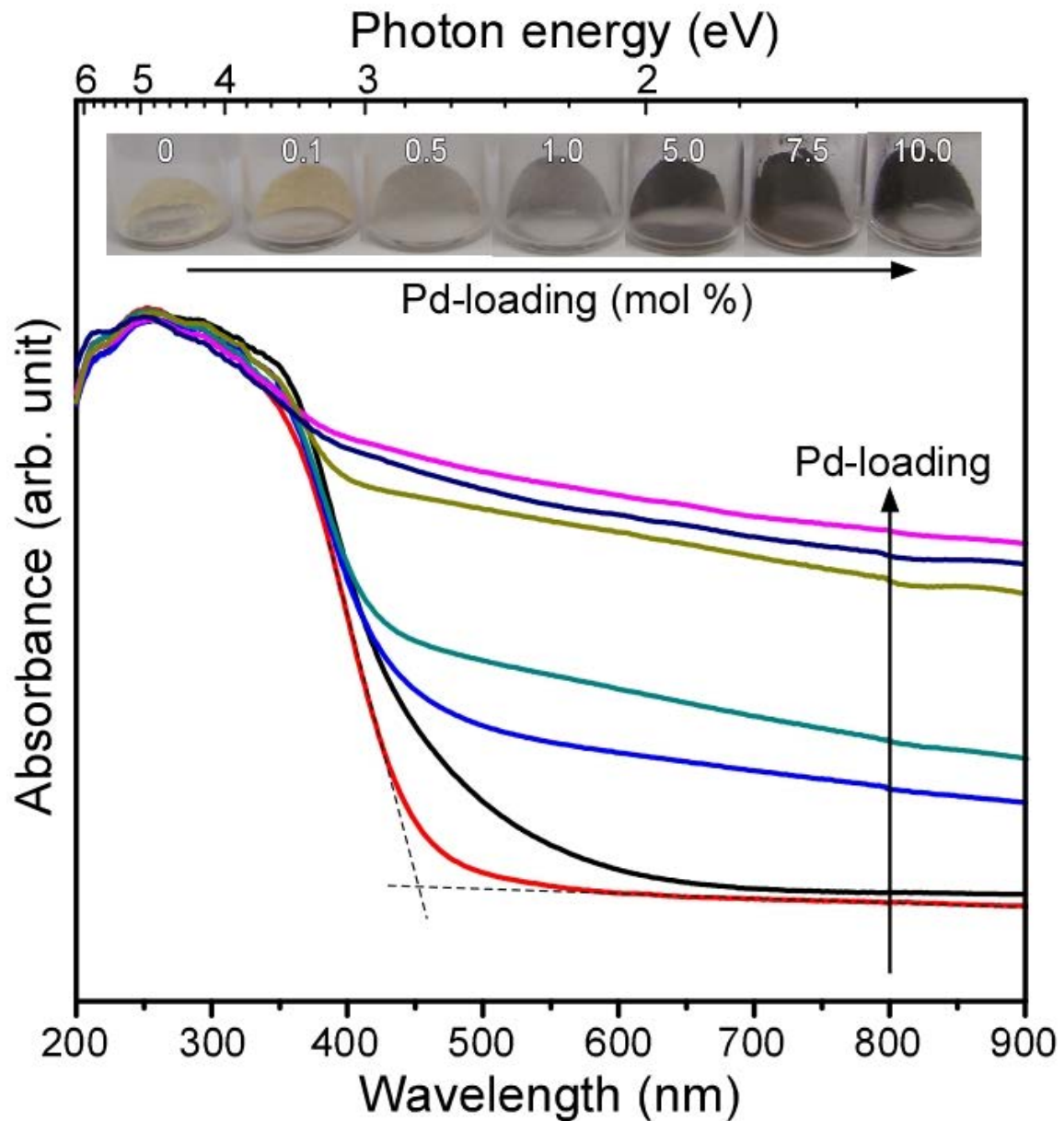
## **Pd, Ag, Au-loaded CeO<sub>2</sub> catalysts; Oxidation Reaction Performance vs. Hybrid, Morphology, Size, Element, and Volume Effects**

**박요한 손영구**

영남대 화학과

촉매는 환경, 화학산업 등 다양한 분야에서 필수적으로 사용되는 것으로 현재 사용되고 있는 촉매의 성능을 향상시키고 성능향상과 저하의 원인을 찾아 촉매개발 산업 및 학문적 발전에 기여하고자 이 연구를 수행하였다. 모델로 사용된 촉매는 다양한 구조를 가지는 CeO<sub>2</sub> (ceria)를 지지체로 사용하고 다양한 금속들(Pd, Ag, Au 등)을 도핑시킨 물질을 가지고 유기물질(예, 알코올)의 산화반응(예, 에탄올 → 알데하이드)에 대하여 다음과 같은 5 가지 내용을 주제로 논의를 하고자 한다. 촉매성능의 향상과 저하의 원인으로 1) 하이브리드, 2) 구조, 3) 사이즈, 4)하이브리드 원소, 5) 상대적 첨가 양 효과들로 결정지을 수 있을까? 하는 의문에 대해 논의하면서 최적의 조건을 찾는 초성능 촉매를 얻고자 한다. 이 논의를 돕기 위해 GC-MS 분석, SEM(scanning electron microscopy), TEM(transmission electron microscopy), XRD(X-ray diffraction), XPS(X-ray-photoelectron spectroscopy), UV-visible absorption 결과들을 보여줄 것이다. 이 연구진행은 촉매개발로 가는 기초와 응용을 결합된 것으로 향후

경제발전뿐만 아니라 학문발전에도 큰 기여를 하리라 기대한다. 참고문헌 1. L.O.O. Costa, A.M. Silva, L.E.P. Borges, L.V. Mattos, F.B. Noronha, Catal. Today 138 (2008) 147-151.2. J. -Y. Luo, M. Meng, J. -S. Yao, X. -G. Li, Y.-Q. Zha, X. Wang, T. -Y. Zhang Appl. Catal. B 87 (2009) 92-103.3. N. Zhang, S. Liu, X. Fu, Y. -J. Xu, J. Phys. Chem. C 115 (2011) 22901-22909.연구지원기관한국연구재단(NO. 2011-0025386)/과학기술국제화 사업



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장소: 일산KINTEX

발표코드: ENVR.P-1328

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Quantitative analysis of heavy metals in water by dual-pulse laser-induced breakdown spectroscopy

이동형 김태형 윤종일<sup>1</sup>

KAIST 원자력및양자공학과 <sup>1</sup>KAIST 원자력 및 양자공학과

Dual-pulse laser-induced breakdown spectroscopy has been applied to the quantitative analysis of heavy metals such as Pb and Cd in water. The laser-induced plasma was generated by two sequential Nd:YAG lasers at 355 nm (first laser pulse) and 532 nm (second laser pulse) wavelengths on the surface of liquid in the homemade water jet configuration and plasma emission lines were detected by a high resolution echelle spectrometer. The influence of lens-to-sample distance, interpulse delay time, and detection gate delay on the emission signals was investigated for the optimization of DP-LIBS. Under the optimized conditions, the limits of detection for Pb and Cd were achieved in the range of some ppm. Determination of the electron density and plasma temperature were performed by utilizing H and Eu emission lines, respectively. This study showed that DP-LIBS is ample for the online determination of toxic metals in water due to its rapid and noncontact assay, and no/little sample preparation.



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장소: 일산KINTEX

발표코드: ENVR.P-1329

발표분야: 환경에너지

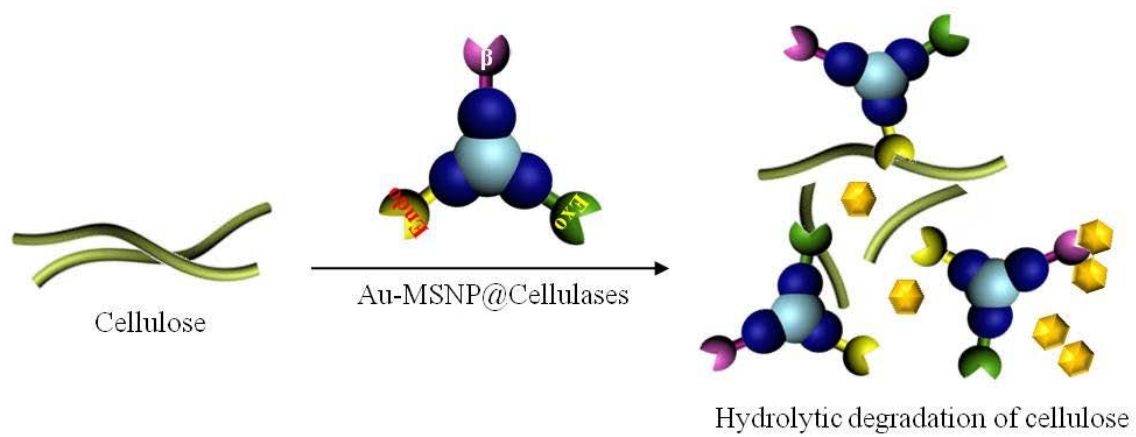
발표종류: 포스터, 발표일시: 수 18:00~21:00

## Co-Immobilization of Three Cellulases on Au-Doped Magnetic Silica Nanoparticles for the Hydrolytic Degradation of Cellulose

조은진 정세라<sup>1</sup> 김호명 배현종

전남대 바이오에너지공학과 <sup>1</sup>전남대 임산가공학과

Three main cystein-tagged cellulases co-immobilized on AuNP and Au-MSNP for the hydrolytic degradation of cellulose. The biochemical properties, stabilities, and activities of these co-immobilized systems were compared to those of mixtures of free cellulases. The co-immobilization on Au-MSNP enhanced enzyme efficiency, activity, and stability. In addition, cellulases co-immobilized on Au-MSNP were able to withstand over seven times while retaining significant residual activity.



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장소: 일산KINTEX

발표코드: ENVR.P-1330

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Extraction of Porosity Silica from Rice Husk Ashes

박상수 이상균<sup>1</sup> 진성일<sup>2</sup> 박찬량<sup>2</sup>

원익머트리얼즈 개발팀 <sup>1</sup>(주)대흥기업 기술연구소 <sup>2</sup>국민대 화학과

A rice crop produces a huge amount of rice husks, which is mainly reused as a fertilizer with domestic animal feces or lagging materials on the soil. Recently, the rice husks are also utilized as a thermal energy source by combustion, which, however, causes severe air pollution by flying off a lot of ashes in the air. In this study, we introduce a extraction method of porosity silica(PS) from rice husk ashes. Morphologies and compositions of the extracted silica are studied using XRD, SEM, TEM, and ICP. Adsorption properties of porosity silica toward various transitional metal ions in water are also measured for the application to the heavy metal remover.

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장소: 일산KINTEX

발표코드: ENVR.P-1331

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Direct Solar Conversion of CO<sub>2</sub> into Longer Hydrocarbons using Nafion Coated Pd-TiO<sub>2</sub>

김우열 최원용

포항공과대 환경공학부

Direct solar conversion of CO<sub>2</sub>, the most abundant green house gas, and water into hydrocarbon is one of the most challenging issues to reduce excess CO<sub>2</sub> present in the atmosphere, and simultaneously produce solar fuels (e.g. CO, CH<sub>4</sub> and CH<sub>3</sub>OH) by means of an environmental friendly approach (i.e., artificial photosynthesis). Intensive efforts have been made to achieve this goal for the last 30 years. Among them, titanium dioxide (TiO<sub>2</sub>) is one of the most frequently studied photocatalyst due to its durability, non-toxicity, and low cost; however, the overall efficiency of the process in aqueous suspensions is still very low. There are four major reasons: (i) the strong oxidation power of photogenerated valence band holes (or surface OH radicals) that can react with stable intermediates (formate, formaldehyde, and methanol in reactions 1-4), (ii) the highly undesirable one electron reduction to form CO<sub>2</sub>??, (iii) the low solubility of CO<sub>2</sub> in water (33 mM @ normal conditions), and (iv) the competition with H<sub>2</sub> formation. For overcoming the high one electron redox potential of CO<sub>2</sub>, an alternative and more favorable pathway is to

reduce CO<sub>2</sub> through proton-coupled multielectron transfer (PCET) (reactions 1-4). In this study, introducing a thin Nafion overlayer on Pd-TiO<sub>2</sub> significantly increased the UV and solar light induced activity for CO<sub>2</sub> reduction. The main role of the Nafion overlayer is thought to maintain high proton concentration for PCET and to retard the direct contact between the negatively charged major intermediates and the surface trapped h<sup>+</sup> (or ·OH).Reference W. Kim, T. Seok, W. Choi, Energy Environ. Sci., 2012 in press.



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장소: 일산KINTEX

발표코드: ENVR.P-1332

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Transient Absorption Spectroscopic Study for TiO<sub>2</sub> Thickness Effect on Performance of Dye-sensitized Solar Cell

황경준 조대원<sup>1</sup> 임찬<sup>2</sup>

건국대 건국프라운호퍼 차세대태양전지 연구소 <sup>1</sup>건국대 건국대-프라운호퍼 태양전지 연구소  
<sup>2</sup>건국대 화학과

We have investigated the photovoltaic performance of dye-sensitized solar cell (DSSC) consists of N719 on TiO<sub>2</sub> nanocrystalline semiconductor and the interfacial electron transfer dynamics using various time-resolved transient absorption spectroscopic methods. We examined the effect of the thickness of TiO<sub>2</sub> electrode. Upon 540 nm pulse excitation, the electron injection from N719 to TiO<sub>2</sub> takes place, generating N719 cation radical (N719<sup>+</sup>) which have a transient absorption band at around 830 nm. The electron injection process is very fast within few picoseconds. The charge recombination process for bare TiO<sub>2</sub> film in CH<sub>3</sub>CN became rapid according to increasing of TiO<sub>2</sub> thickness. Upon the addition of electrolyte (I/I<sub>3</sub><sup>-</sup>), the rates of charge recombination and regeneration processes increased according to increasing of TiO<sub>2</sub> thickness. The efficiencies of DSSC were affected by the thickness of TiO<sub>2</sub> film.

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발표코드: ENVR.P-1333

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Transient Absorption Spectroscopic Study of Nanoporous TiO<sub>2</sub> Electrode Prepared by Mesoporous Silica Template

황경준 조대원<sup>1</sup> 임찬<sup>2</sup>

건국대 건국프라운호퍼 차세대태양전지 연구소 <sup>1</sup>건국대 건국대-프라운호퍼 태양전지 연구소  
<sup>2</sup>건국대 화학과

A bilayer structured electrode was constructed by employing a nanoporous TiO<sub>2</sub> overlayer above TiO<sub>2</sub> nanoparticles underlayer. The nanoporous TiO<sub>2</sub>, prepared from different mesoporous silica templates including SBA-15, KIT-6 and MSU-H, possessed highly ordered pore size and well inter-connected network structure, both beneficial for dye adsorption and electron transfer. The dye adsorption capability of the nanoporous TiO<sub>2</sub> was nearly one and half times that of the TiO<sub>2</sub> nanoparticle. In the photoelectrode, the nanoporous TiO<sub>2</sub> film enhanced both dye adsorption and light harvest, to increase photocurrent ( $J_{sc}$ ) and fill factor (FF). Compared to the TiO<sub>2</sub> nanoparticle film, the synergy of the nanoporous TiO<sub>2</sub> and the TiO<sub>2</sub> nanoparticle films in the photoelectrode resulted in a 20% improvement in light-to-electricity conversion efficiency ( $\eta_{eff}$ ). This bilayered electrode provides an alternative approach for further developing a photovoltaic device with better cell performance. We also have investigated the

photodynamic properties for charge-recombination and dye-regeneration processes using the transient absorption measurement.





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발표코드: ENVR.P-1334

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Enhanced Photovoltaic and Photodynamic Properties of TiO<sub>2</sub> Film Prepared by Polycondensation in Sol Reaction

황경준 조대원<sup>1</sup> 임찬<sup>2</sup>

건국대 건국프라운호퍼 차세대태양전지 연구소 <sup>1</sup>건국대 건국대-프라운호퍼 태양전지 연구소  
<sup>2</sup>건국대 화학과

A TiO<sub>2</sub> film of dye-sensitized solar cells was fabricated using a TiO<sub>2</sub> sol prepared from titanium isopropoxide as a starting material. The effect of polycondensation time and temperature on physical and chemical properties of TiO<sub>2</sub> film shows that the crystallinity, particle size, roughness, and surface area of TiO<sub>2</sub> film can be successfully controlled by adjusting the polycondensation time and temperature in the synthesis process of the TiO<sub>2</sub> sol. Adsorption properties (adsorption equilibrium, isosteric enthalpies of adsorption, and adsorption energy distributions) of N719 dye molecules on the prepared TiO<sub>2</sub> film revealed that the short circuit current ( $I_{sc}$ ) and overall conversion efficiency ( $\eta_{eff}$ ) are highly dependent on the crystallite size and the N719 dye adsorption properties. The TiO<sub>2</sub> film has a pure anatase phase, high surface area including pore volume, and large anatase crystallite size and is capable of enhancing the photovoltaic performance. The energy conversion efficiency of the dye-sensitized solar cells is highly

dependent on the physical and chemical properties of  $\text{TiO}_2$  films. We have investigated the charge-recombination and dye-regeneration properties using ns-transient absorption measurement.



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발표코드: ENVR.P-1335

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Nano-scale surface study and reaction mechanism: Interaction between U(VI) and nZVI

신영호 이우진

KAIST 건설 및 환경공학과

Uranium (U) usually exists as soluble U(VI) and insoluble U(IV) in the nature. Oxidation-reduction processes can significantly affect the mobility, transport, and fate of U. Iron(Fe(II)/Fe(III)) plays an important role in the determination of uranium oxidation state in the subsurface. Recently it was reported that Fe(II) on ZVI surface can reduce U(VI) into U(IV) as reactive reductant. Furthermore ZVI, among other iron sources in nature, has received much attention in study of reductively degradation of chlorinated compounds and reduction of heavy-metal. Since ZVI has been used major material in soil/ground water remediation technology(e.g., PRB) and has been used as base material of canister for storage of radioactive wastes, it is important to understand interaction mechanism between ZVI and U(VI) for the successful remediation of radioactively contaminated sites and managing radioactive waste safely. In this study, nano-sized ZVI(nZVI) was reacted with aqueous U(VI) under anaerobic condition. The U(VI) fate in aqueous phase was monitored by laser-spectroscopy and surface reaction on nZVI was

analyzed by x-ray spectroscopy to verify nano-scaled interaction mechanism. As a result of quantification of aqueous Fe(II)/Fe(III) concentration with reaction time, U(VI) accelerated Fe(II) dissolution from nZVI surface indicating U(VI) can be removed from aqueous phase by cation exchange with Fe(II) on nZVI surface.



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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Remediation of contaminated soil with Diesel by chemical oxidation

배선영 방예진 이승선

서울여대 화학과

Oxidation technique has been used to remediate the organic compounds from the contaminated soils with petroleum hydrocarbons due to its high oxidation capacity. Among various oxidizing chemicals, SOREM™ (Potassium monopersulfate & Sodium persulfate compound, Kings field Inc.) which produced SO<sub>4</sub> radical in water has received a great attention. This radical has shown high remediation efficiency than OH radical produced by hydrogen peroxide. In this study, soil contaminated with total petroleum hydrocarbon (TPH) was treated with SOREM™. Various amounts of SOREM™ (0.5, 1, 3, 5%) were applied to soil spiked with 20,000ppm diesel (equivalent to 313.4 ppm TPH) for 10, 30, 60, and 120 min, respectively. The residual TPH in soil after treatment of SOREM™ was extracted with a mixture of methylene chloride and acetone (1:1). Aliquot of extraction was analyzed by GC-FID (Hewlett-Packard, 5890 II) with a capillary column (Ultra-2, 25 m × 0.20 mm × 0.33 μm). The temperature programming was used at 45 °C for 2 min increased at the rate of 10 °C / min to 310 °C for 25 min and the injector temperature was 280 °C. The soil used in this study was consisted of sand (54.55%), silt (31.83%), and

clay (0.03%). The best efficiency on TPH removal was achieved using 0.5% SOREM™ for 60 min and its efficiency was ranged of 79.4~87.9%. Based on our preliminary study, SOREM™ will be combined with thermal desorption treatment for the contaminated soil with TPH. Key words : TPH, Diesel, Oxidation, Soil remediation, SOREM™



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발표코드: ENVR.P-1337

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Biodiesel production and etherification of glycerol

배선영 채유리<sup>1</sup> 심지연

서울여대 화학과 <sup>1</sup>서울여대 화학

Biodiesel, which is renewable as diesel fuel, has been receiving more dramatic increasing attention all over world shortage of fossil fuels and environmental concerns. Among various feedstocks for biodiesel production, the used canola oil was investigated. The pure canola oil as a control was converted to biodiesel by transesterification using homogeneous based catalyst. The pure canola oil had the acid number about 0.03261 ( $\pm 0.0058$ ). The basic catalyst that was used in this was potassium hydroxide (KOH) and reaction temperature was  $55 \pm 5$  °C and the ratio of methanol : canola oil was 9:1. Biodiesel conversion was 76.34wt% ( $\pm 2.84$ ), and glycerol yield was 11.3wt% ( $\pm 1.1$ ) of oil. In continuous study, purified glycerol converted to dimer, trimer, oligomer of glycerol by etherification using cesium bicarbonate( $\text{CsHCO}_3$ ) catalyst and reaction temperature 260 °C 6h under Ar gas flow. Properties of productions by GC-FID, GC-MS, H-NMR and C-NMR. Key word : Biodiesel, Transesterification, Yellow grease, Glycerol, Etherification

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발표코드: ENVR.P-1338

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Preparation magnetic biochar and its sorption capacity of Zn and Pb

배선영 한수정 박효선

서울여대 화학과

Biochar derived from food waste is recognized as a substance for living and environmental applications. The conversion from food waste to biochar can be achieved through thermal, biological process, and hydrothermal treatment. In this study, biochar was prepared via hydrothermal carbonization (HTC) using a tubular reactor (patent applied) at 220 °C for 0.5 hr, 1 hr, 1.5 hr, and 2 hr. The food waste as feedstock for biochar preparation was made of cabbage, apple skin, the cooked rice, and fish, which contained the moisture content about 78(±5)%. In addition, magnetic biochar was prepared by chemical co-precipitation of Fe solution( $\text{Fe}^{2+}/\text{Fe}^{3+}$ ) with biochar powder and pyrolyzed at 400°C, which resulted in iron oxide magnetite formation. The iodine numbers that are closely related to the surface area were determined as 521(±17) mg/g for biochar at 1 hr, 526 (±64) mg/g for biochar at 2 hr while 635 mg/g for the commercial activated carbon. Boehm titration was performed to investigate the acidic and basic sites of biochars for their activity with other substances. Concentrations of caboxylic group, lactonic group, phenolic group, and basic group were 0.27, 1.94, 3.57, 4.75, respectively. FT-IR of magnetic biochar was taken to



characterize the presence of Fe in the magnetic biochar. Sorption of Zn and Pb on biochar and magnetic biochar was performed and measured by ICP-AES. In future, the real food waste obtained from school cafeteria will be converted to biochar and magnetic biochar using HTC for comparing the adsorption of the biochar to that of Fe-biochar. keywords: biochar, magnetic biochar, Fe-coating, food waste, iron, biosorbent



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장소: 일산KINTEX

발표코드: ENVR.P-1339

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## The production of dissolved iron from iron oxides in ice

정다운 최원용<sup>1</sup>

포항공과대 환경공학과 <sup>1</sup>포항공과대 환경공학부

Iron is an important micronutrient controlling the growth and metabolism of living organisms. The environmental significance of iron biogeochemistry in the ocean has arrested much attention due to its sequestration of atmospheric CO<sub>2</sub> by stimulating the biological pump. Bioavailable iron is mainly provided via atmospheric deposition of dissolved iron. In this work, we investigated the formation of dissolved iron from iron oxide particles in the presence of various organic acids under dark condition. The dissolution of iron oxides in the aqueous phase is negligible even in low pH conditions whereas those in ice were significantly accelerated upon freezing. The enhanced dissolution of iron in ice is explained by the “freeze concentration effect”. When ice crystals begin to form, iron oxides, organic acids, and protons are concentrated in the ice grain boundary region and accelerate the dissolution of iron. The enhanced dissolution of iron oxide in ice might propose an important release path of bioavailable iron in environments deficient of light.

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장소: 일산KINTEX

발표코드: ENVR.P-1340

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## **Simultaneous conversion of heavy metals and organic compounds using the redox cycles of Iron**

이동우 최원용

포항공과대 환경공학부

It is a challenging process for degrading anthropogenic sources of heavy metals and toxic organic compounds in water at the same time. In this work, redox cycle of  $\text{Fe}^{3+}/\text{Fe}^{2+}$  was utilized as a photocatalyst for the simultaneous reduction of chromate and oxidation of aromatic compounds in aqueous suspension under UV irradiation. The photocatalytic efficiency of the oxidation was enhanced in the presence of chromate due to its efficient interaction with the degradation intermediates. Increase in concentration of iron which further produces  $\text{OH}^\bullet$  radicals and presence of oxygen which recycles iron through the system enhance both reactions. The removal of organic compounds with simultaneous reduction of chromate was achieved. This study provides an efficient photocatalytic system for the treatment of wastewater co-contaminated with heavy metals and organic compounds.

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장소: 일산KINTEX

발표코드: ENVR.P-1341

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Organic Dye Based 9-Ethyl Carbazole for Dye-Sensitized Solar Cells

변여진 김효정<sup>1</sup> 이창섭 강진규<sup>1</sup>

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염료감응태양전지(DSSCs)는 실리콘태양전지보다 생산기술비용이 저렴하여 널리 연구되고 있다. DSSCs의 핵심재료인 염료는 크게 유기염료와 유기금속염료가 있으며 유기염료는 금속을 사용하지 않으므로 금속유기염료에 비해 자원적인 제약이 없고 가시광선 영역에서 높은 흡광효율을 가지며 저가합성이 가능하고 다양한 구조의 염료를 디자인하기가 용이하다는 장점을 가지고 있어 유기염료의 연구가 많이 진행되고 있다. 본 연구에서는 electron donor 물질로 잘 알려진 carbazole을 사용하였으며, 용해도 증가 및 회합방지를 위해 carbazole의 amine 부분에 ethyl 기가 달려있는 9-ethyl carbazole을 사용하였다. 9-Ethyl carbazole을 Bis 형태로 합성하는 과정을 거친 후, 이 화합물이 금속산화물에 잘 흡착될 수 있도록 anchoring 그룹(-COOH)을 도입하여 donor-acceptor 구조로 합성하였으며 NMR과 Mass를 통해 구조를 확인하였고, 유기염료의 광전변환효율을 측정하였다.

일시: 2012년 4월 25~27일(수~금) 3일간

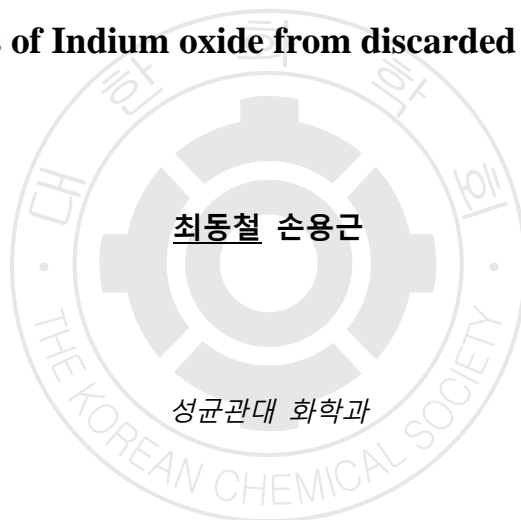
장소: 일산KINTEX

발표코드: ENVR.P-1342

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis of Indium oxide from discarded TFT-LCD



Indium tin oxide (ITO) has been widely used in Mobile Personal Information Apparatus (MPIA). As indium reserves has been decreased, the MPIAs display price increased. So we consider the recycle of indium from discarded MPIA. One of MPIAs, we selected laptop computer, monitor, and navigation display. Because nowadays many people used these MPIA and the a lot of MPIAs were abandoned. In this study, our interests were focused on the recovery indium materials from discarded TFT-LCD. We synthesized indium hydroxide nanoparticles from discarded TFT-LCD, hydrochloric acid, ammonia solution. Indium oxide nanoparticles were prepared via dehydration of indium hydroxide nanoparticles synthesized by hydrothermal process. Analysis of the indium material was done by using X-ray photoelectron spectroscopy (XPS), Energy dispersive x-ray spectroscopy (EDX), X-ray diffraction (XRD), Thermogravimetric Analysis (TGA) and Inductive coupled plasma (ICP). This work was supported the Energy & Resource Recycling of the Korea Institute of Energy Technology Evaluation and

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발표종류: 포스터, 발표일시: 수 18:00~21:00

## The Preparation Effect of Graphene/TiO<sub>2</sub> composite for Photo(electro)catalytic Activity

김형일

포항공과대 환경공학부

The core/shell structure of the semiconductor and carbon material hybrids can be carefully designed for higher solar conversion efficiency. In this work, nano-sized graphene-coated TiO<sub>2</sub> nanoparticles (r-NGOT) were successfully synthesized and compared with the typical graphene/TiO<sub>2</sub> composite (r-LGOT) that has the particles-on-a-sheet geometry for photocatalytic and photoelectrochemical (PEC) activities. r-NGOT showed significantly enhanced activities in both hydrogen production and PEC tests compared to r-LGOT. All experimental evidences obtained in this work indicate that the addition of r-NGOs onto TiO<sub>2</sub> NPs enhanced the photocatalytic and PEC activities, which can be attributed to the retarded charge recombination and the enhanced electron transfer on the surface of r-NGOT. The enhanced activities of r-NGOT in both photocatalytic and photoelectrocatalytic measurements are attributed to the unique core/shell structure of r-NGOT which has the larger contact area between r-NGO and TiO<sub>2</sub> NPs and the

closer contact between Pt and  $\text{TiO}_2$  compared with r-LGOT. The present core/shell geometry could serve as an effective design of graphene/ $\text{TiO}_2$  composite for solar conversion applications.





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발표코드: ENVR.P-1344

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Degradation of pyrene in cetylpyridinium chloride solution by pyrite Fenton reaction

최경훈 이우진

KAIST 건설 및 환경공학과

Degradation of pyrene with cetylpyridinium chloride (CPC) in pyrite Fenton system was investigated. Significant portion of pyrene (61%) on pyrite surface without CPC was adsorbed while relatively small sorption (15%) on pyrite surface was observed in the presence of CPC. Approximately, 96% of pyrene with CPC was removed by the pyrite Fenton system in 180 min, while 35% of pyrene with CPC was removed by classic Fenton system. The degradation pattern of pyrene with CPC showed pseudo-1st-order reaction kinetics ( $0.0194 \text{ min}^{-1}$ ) while pyrene without CPC in pyrite Fenton system followed 2nd-order reaction kinetics. Transformation study on pyrene with and without CPC in pyrite Fenton system showed that there was no significant toxic by-product. The degradation of pyrene with CPC by pyrite Fenton reaction resulted in the transformation to some acids such as isooctyl phthalate and n-octadecanoic acid. Meanwhile, CPC was degraded to  $\text{CO}_2$  and  $\text{H}_2\text{O}$  accompanied with ammonia production by pyrite Fenton reaction. These results suggest that pyrite Fenton system can be a novel remediation alternative to

treat groundwater and wastewater containing poly aromatic hydrocarbons solubilized in surfactants emitted from soil washing processes.



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장소: 일산KINTEX

발표코드: ENVR.P-1345

발표분야: 환경에너지

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## Driving factors of energy final use in urban area

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According to the bluemap scenario presented by IEA, energy end-use sector has the largest potential to reduce Greenhouse gas(GHG) emission, while energy supply sector has relatively small potential to reduce GHG. Moreover urbanism is accounted as the most significant factor to drive increase of energy consumption. It has been discovered that several factors of urbanism, such as income growth, drive increase energy consumption in lots of literature. However very few study has investigated relative importance of driving factors in urban final energy use. In order to implement energy policies which are suitable to individual city(especially developing cities), it is essential to know why a city has that kind of energy pattern, what drives it, and more importantly what factor is more significant than others. Even though income has been proved as the most significant factor, income as a single factor hardly explain the energy consumption. Therefore I will conduct a multi-variate analysis and define the significance of driving factors in each city. Talca, Chile and a similar city in Korea will be analyzed as a case study before main analysis with more amount of cities.

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발표코드: ENVR.P-1346

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Formic acid as a reducing agent and limiting reagent in the catalytic nitrate reduction

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Formic acid was employed for the nitrate reduction as a reductant in the presence of the alumina supported bimetallic Pd:Cu catalysts. Almost 100% nitrogen conversion of nitrate was due to the in situ buffering effect of CO<sub>2</sub>, which formed by the decomposition of formic acid on the surface of catalyst. To prevent formic acid from being left and to control the nitrate concentration below regulation at the same time, formic acid was used as a limiting reagent. The pH control by formic acid itself was not enough to ensure the maximum reduction efficacy of this system and additional pH control was necessary to achieve the goal. Our result shows that formic acid can convert the nitrate into nitrogen without producing the detectable amount of nitrite and ammonia and no formic acid remained after the treatment.

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발표코드: ENVR.P-1347

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Recovery of palladium from wastewater using a microbial fuel cell method

최찬수

대전대 응용화학과

The purpose of this study is to develop a cost-effective recovery system of palladium metal from wastewaters that contain Pd(II) ion. The A built-in electromotive force from a microbial fuel cell (MFC) was used while recovering the electric energy. After 40 hours reaction, Pd recovery rates as high as  $99.58 \pm 0.01$ ,  $99.74 \pm 0.00$ ,  $99.16 \pm 0.02\%$  were achieved when the initial concentrations of were 50 ppm, 100 ppm, and 200 ppm, respectively (the remaining concentrations were  $0.21 \pm 0.01$ ,  $0.26 \pm 0.00$ ,  $1.68 \pm 0.05$ ). The limiting current densities (LCJ) obtained from the voltage vs. current density (V-J) curves with different initial Pd(II) as  $[\text{PdCl}_4]^{2-}$  concentrations ( $C_{\text{bulk}}$ ) were found to greatly increased greatly with increase of the initial concentration of Pd(II). However, the slope of the LCJ vs.  $C_{\text{bulk}}$  curve in the low concentration range was 3.7 times higher than that in of the high concentration range. This indicates that the anode reaction rate affects cathode reaction rate in the higher concentration range due to the relatively low donor reaction ratio. The maximum power of  $7.03 \text{ W/m}^2$  with a fill factor of 0.638 was

achieved at 1000 ppm Pd(II) concentration. Using an initial concentration of 500 ppm, the fed-batch system yielded in discharge curves showing electric energy higher than about 39.2 Wh/Kg as a byproduct.



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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 수 18:00~21:00

## Synthesis and Characterization of Magnetic-cored dendrimer with photocatalytic terminals

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한양대 건설환경공학과 <sup>1</sup>한양대 토목공학과

We have shown that photoresponsible magnetic-cored dendrimer with photocatalytic functional groups can use nanoscale magnetite and  $\text{TiO}_2$  for magnetic recovery, photocatalytic activity. Nanomagnetite of magnetic core part was prepared by coprecipitating ferric and ferrous iron ion solution using ammonium hydroxide. The synthesized magnetic-cored dendrimers were modified with photocatalytic functionals for environmental application. Magnetic-cored dendrimer with photocatalytic terminal (MDP) took functional group of  $\text{TiO}_2$  nanoparticles by functional group bonded surface of  $\text{TiO}_2$  chemically. The morphology of MDP depended on the  $\text{TiO}_2$  nanoparticles. The prepared MDP has the optimal structure as a catalyst for advanced oxidation processes (AOPs) because of available surface of  $\text{TiO}_2$  and magnetite. In terms of catalytic activity the synthesized MDP were almost comparable to the commercial P25  $\text{TiO}_2$  photocatalyst. In addition, the easily recoverable magnetic photocatalysts showed good reusability.